PRINCIPLES FOR QUANTUM ALGORITHMS

Johannes Bausch

Quantum Information for Developers 2018

OVERVIEW

Goal: Get an intuitive understanding of quantum algorithm design.

Real goal: There is a *lot* of algorithms out there. Make use of them.

SESSION 1

- Warmup: Grover Search
- Brief Recap:
 - Complexity Classes
 - Basic Arithmetic
 - Qudits
- Szegedy Walks: better than flipping a coin
- Quantum Backtracking

SESSION 2

- Warmup: Let's predict (in retrospect) who wins the World Cup
- Gate Teleportation and Clifford Circuits: Magic!
- Repeat until Success
- How to load data into a quantum memory

BONUS

- Quantum Machine Learning
- Hamiltonian Simulation

SESSION 1

COMPLEXITY CLASSES

- 1. P
- 2. BPP
- 3. NP, MA

P

- PTIME, "poly-time"; $\mathcal{L} = \mathcal{L}_{YES} \dot{\cup} \mathcal{L}_{NO}$
- For a given input of size n, a classical Turing Machine can decide the problem in polynomial runtime.
- ullet For circuits: family of Boolean circuits $C_n:n\in\mathbb{N},$ such that there exists a TM M which, on input 1^n outputs C_n , in poly-time.
- ullet Example: unstructured search, computing digits of π

BPP

- Bounded-error poly-time; $\mathcal{L} = \mathcal{L}_{YES}\dot{\cup}\mathcal{L}_{NO}$
- Same as P, but you have coins

$$egin{cases} \mathbb{P}(M(x)=1) \geq rac{2}{3} & x \in \mathcal{L}_{YES} \ \mathbb{P}(M(x)=1) \leq rac{1}{3} & x \in \mathcal{L}_{YES} \end{cases}$$

BPP

- Bounded-error poly-time; $\mathcal{L} = \mathcal{L}_{YES}\dot{\cup}\mathcal{L}_{NO}$
- Same as P, but you have coins

$$egin{cases} \mathbb{P}(M(x) = 1) \geq rac{1}{2} + \left|x
ight|^{-c} & x \in \mathcal{L}_{YES} \ \mathbb{P}(M(x) = 1) \leq rac{1}{2} - \left|x
ight|^{-c} & x \in \mathcal{L}_{YES} \end{cases}$$

BPP

- Bounded-error poly-time; $\mathcal{L} = \mathcal{L}_{YES}\dot{\cup}\mathcal{L}_{NO}$
- Same as P, but you have coins

$$egin{cases} \mathbb{P}(M(x)=1) \geq 1-2^{-p(|x|)} & x \in \mathcal{L}_{YES} \ \mathbb{P}(M(x)=1) \leq 2^{-p(|x|)} & x \in \mathcal{L}_{YES} \end{cases}$$

PROBABILITY AMPLIFICATION

 X_t outcome of run t, coin flip w/ prob 1/2+q.

$$S_t := \sum_t X_t$$
.

Let
$$\mathbb{E}(S_t) := tq$$
, then $Var(S_t) = tq(1-q)$.

Chebyshev's inequality: Majority voting. Denote with A_t .

$$\mathbb{P}(A_t(x)=1)=\mathbb{P}(S_t\geq t/2)$$

$$=rac{1}{t}igg(rac{q^{-c}}{4}-1igg)$$

PROBABILITY AMPLIFICATION

Chernoff bound:

$$\mathbb{P}(S_t \leq \lfloor t/2
floor) \leq \exp \left| -rac{t}{2q} \left(q - rac{1}{2}
ight)^2
ight|$$

PROBABILITY AMPLIFICATION

Takehome Message:

The output probability of your randomized algorithm matters less than you think.

But:

It does matter.

NP

- "Non-deterministic poly-time"
- Any set of problems for which YES/NO can be decided with a P machine.
- Example: 3SAT, Knapsack, Subset Sum, Travelling Salesman, Hamiltonian Cycle

MA

- "Merlin-Arthur"
- Any set of problems for which YES/NO can be decided with a BPP machine
- Probabilities inherited from BPP
- Example: stoquastic k-SAT

BQP

- "Bounded-error quantum poly-time"
- For a given input of size n, a quantum Turing Machine can decide the problem in polynomial runtime.

BUT: QTM's ARE DIFFICULT.

- For circuits: family of quantum circuits $C_n:n\in\mathbb{N}$, such that there exists a **classical** TM M which, on input 1^n outputs C_n , in poly-time.
- Same acceptance/rejection bounds as BPP
- Example: Prime Factoring

QMA

- "Quantum Merlin-Arthur"
- Any set of problems for which YES/NO can be decided with a BQP machine
- Probabilities inherited from BQP
- Example: the local Hamiltonian problem

A FEW KNOWN RELATIONS

 $P \subset BPP \subset BQP$

 $P \subset NP \subset MA \subset QMA$

 $BPP \subset MA$

 $BQP \subset QMA$

BASIC ARITHMETIC OPERATIONS

IMPORTANT GATES

H, X, Y, Z, T, S

CNOT, CCNOT (Toffoli)

Controlled-U

+

$$\ket{a} \stackrel{+b}{\longmapsto} \ket{a+b \mod 2^n}$$

We use QFT.

$$|a
angle \stackrel{\mathcal{F}}{\longrightarrow} rac{1}{\sqrt{2^n}} \sum_{t=0}^{2^n-1} \exp\left(rac{at}{2^n}
ight) |t
angle$$

$$|a
angle \stackrel{\mathcal{F}}{\longrightarrow} rac{1}{\sqrt{2^n}} |\phi_n(a)
angle \otimes \ldots \otimes |\phi_2(a)
angle \otimes |\phi_1(a)
angle$$
 where $|\phi_k(a)
angle = (|0
angle + \exp(a/2^k))|1
angle)/\sqrt{2}$

Remember: $\exp(a/2^k) = 0.a_k \cdots a_2 a_1$

$$egin{align} |\phi_k(a)
angle &= (|0
angle + \exp(0.a_k\cdots a_2a_1))|1
angle)/\sqrt{2} \ |b_1
angle |b_2
angle \cdots |b_n
angle \end{aligned}$$

Then

$$egin{aligned} |\phi_k(a)
angle &= (|0
angle + \exp(0.a_k\cdots a_2a_1))|1
angle)/\sqrt{2} \ &
ightarrow (|0
angle + \exp(0.a_k\cdots a_2a_1+0.b_k))|1
angle)/\sqrt{2} \ &
ightarrow (|0
angle + \exp(0.a_k\cdots a_2a_1+0.b_kb_{k-1}))|1 \ &dots \ &
ightarrow (|0
angle + \exp(0.a_k\cdots a_2a_1+0.b_kb_{k-1}))|1 \ &dots \end{aligned}$$

Gates work on qubits. But if you program in python, you don't think in bits.

THINK OF QUDITS

QUDIT LAND

- ullet Take some number $a\in\mathbb{N}$
- ullet Encode it in $n=\lceil \log_2 a
 ceil$ many qubits $\in (\mathbb{C}^2)^{\otimes n}$.
- ullet Treat it as one qudit in \mathbb{C}^{2^n}

$$\begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ \vdots & & \ddots & \ddots & \\ 0 & & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

COMPLEXITY OF BASIC ARITHMETIC OPERATIONS

Don't expect a speedup.

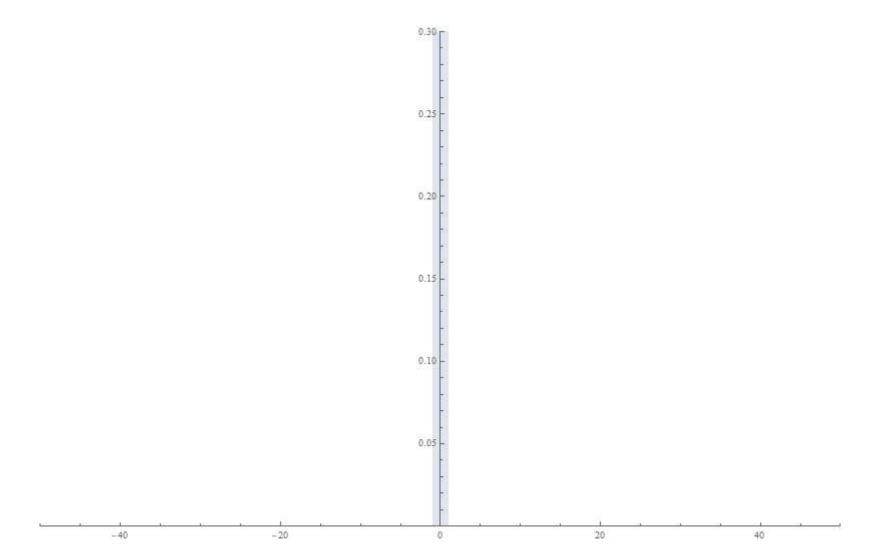
HIGH-LEVEL ALGORITHMS

https://math.nist.gov/quantum/zoo/

CLASSICAL RANDOM WALKS

- 1. Markov chain: Graph G=(V,E) with transition probabilities $p_e,e\in E$
- 2. We will usually assume ergodicity (non-patologic) and symmetry (undirected)
- 3. Classically: described by stochastic matrix M such that $Mx_t=x_{t+1}$

What would be a good quantum analogue of this?

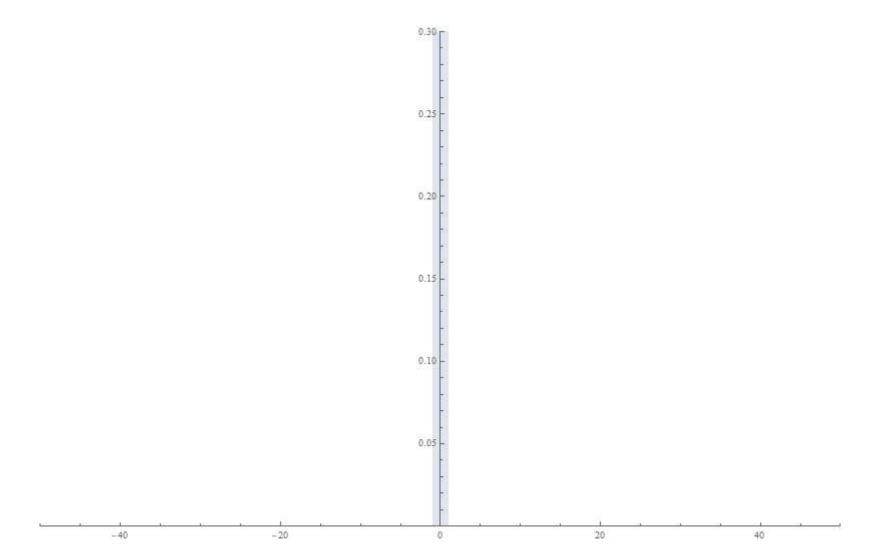


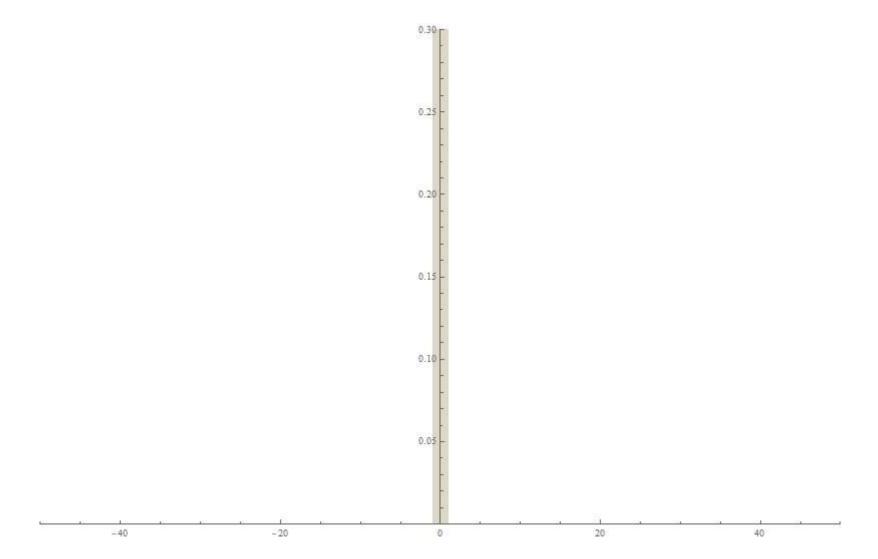
QUANTUM WALKS

- 1. Start with a bipartite Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^L$, which is and location space, respectively
- 2. Quantum walk on a line (Aharonov): perform a coin fli shift:

$$|0
angle|l
angle \stackrel{H}{\longmapsto} rac{1}{\sqrt{2}}(|0
angle + |1
angle)|l
angle \stackrel{S}{\longmapsto} rac{1}{\sqrt{2}}|0
angle|l-1
angle +$$

- 3. Continuous time (Farhi)
- 4. Finding marked vertices in graph (Szegedy)
 - How do we make the walk detect marked elements?
 - What's the speedup?





SZEGEDY WALKS

Walk on a graph G=(V,E) with transition probabilities p_{xy} to find some target.

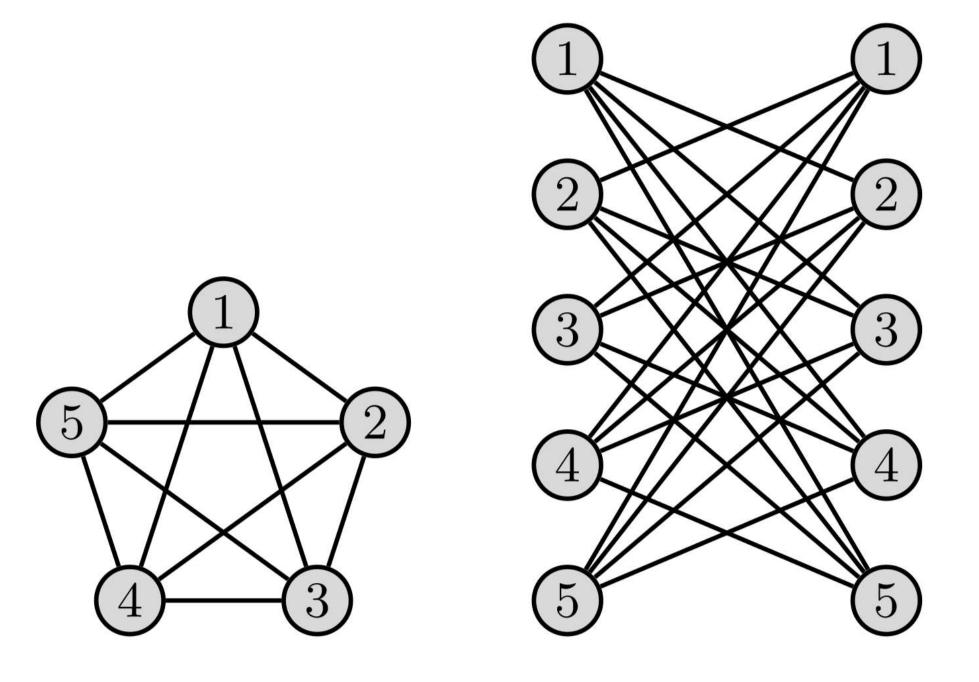
- Let $\mathcal{H} = \mathbb{C}^n \otimes \mathbb{C}^n$ represent *two* copies of the graph.
- ullet computational basis $|x,y
 angle:x,y\in V$
- Define

$$egin{aligned} \ket{\Psi_x} &:= \ket{x} \otimes \sum_y \sqrt{\overline{p_{x,y}}} \ket{y} \ \ket{\Phi_y} &:= \sum \sqrt{\overline{p_{xy}}} \ket{x} \otimes \ket{y} \end{aligned}$$

Iterate the reflections

$$egin{aligned} R_A := 2 \sum_{x \in E} |\Psi_x
angle\!\langle\Psi_x| - 1_n \ R_B := 2 \sum_{y \in E} |\Phi_y
angle\!\langle\Phi_y| - 1_n \end{aligned}$$

- 1. Walk on the *edges* of the graph: each map maps an edge $|x,y\rangle$ to a superposition of edges (Santos).
- 2. How can we make it stop at a marked vertex $x \in M$? We have to redefine the transition probabilities



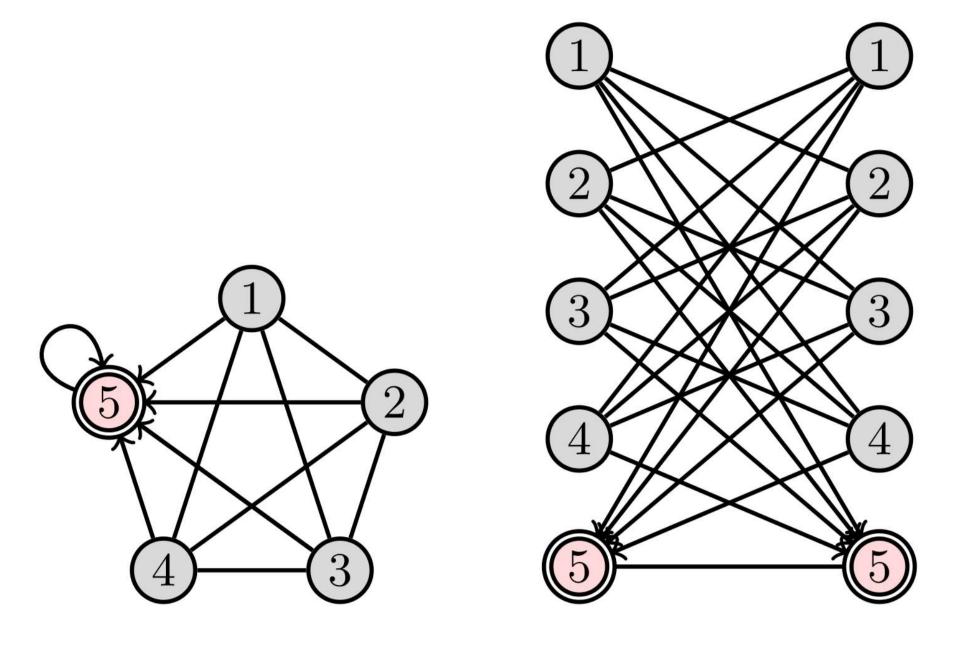
ABSORBING RANDOM WALK

If p_{xy} is original transition probability, and M a set of marked vertices, then define

$$p'_{xy} := egin{cases} p_{xy} & x
otin M \ \delta_{xy} & x \in M \end{cases}$$

Initial state is stationary distribution of graph

$$|\psi(0)
angle = rac{1}{\sqrt{n}} \sum_{xy} \sqrt{p_{xy}} |x,y
angle$$



ABSORBING RANDOM WALK

One can show that

- 1. The weight does not stay at the marked vertex—since the evolution is unitary
- 2. If there are m=|M| out of n=|V| marked vertices, then a marked element will be measured
 - ullet within $t=O(\sqrt{n/m})$ steps, and
 - ullet with probability $\geq 1/2 + O(\sqrt{m/n})$

Great—but if we already know the solution in order to modify the original transition probabilities p_{xy} for all elements in $x \in M$, why do we need to look for them at all?

ORACLES

ORACLES AND SZEGEDY WALKS

- 1. Standard phase kickback: the oracle maps $|x
 angle\mapsto -|x
 angle$ iff $x\in M$
- 2. Equivalent operation: reflection around marked elements $R_M := 2 \sum_{x \in M} |x \rangle\!\langle x| 1_n$
- 3. Promote to operator on \mathcal{H} (= $\mathbb{C}^n \otimes \mathbb{C}^n$): $R := R \otimes 1_n$
- 4. Change walk to $R_A R_B R R_A R_B R \dots$

ORACLES AND SZEGEDY WALKS

One can show that the following states span invariant subspaces under $U=R_AR_BR$:

$$egin{aligned} |a,a
angle &= rac{1}{\sqrt{(n-1)(n-2)}} \sum_{x,y
otin M} |x,y
angle \ |a,b
angle &:= rac{1}{\sqrt{n-1}} \sum_{x
otin M,y\in M} |x,y
angle \ |b,a
angle &:= rac{1}{\sqrt{n-1}} \sum_{x\in M,y
otin M} |x,y
angle \end{aligned}$$

1. This means that the operator U is a rotation in three dimensions:

$$U = egin{pmatrix} \cos^2\phi & \cos\phi\sin\phi & -\sin\phi \ \sin\phi & -\cos\phi & 0 \ \cos\phi\sin\phi & \sin^2\phi & \cos\phi \end{pmatrix}$$

- 2. The initial state is roughly $|a,a\rangle$
- 3. Repeated applications of U map it to |b,a
 angle
- 4. Measurement returns a marked element with probability 1
- 5. Number of timesteps $O(\sqrt{n/m})$.

So we can use Szegedy walks to find marked elements in a graph, even if the vertex is determined by a subroutine.

But what if we don't know the graph beforehand?

BACKTRACKING

BACKTRACKING

- Algorithm to solve constraint satisfaction problems
- Tree exploration, where vertices are partial solutions
- Early dropout: often better than brute force
- Examples: Sudoku solver, SAT solver

BACKTRACKING

$$f: \{1, \ldots, d\}^n \longrightarrow \{\text{true}, \text{false}\}$$

Algorithm:

```
# f can return True, False, or Indetermined
def backtrack(f, x : list = []):
    # early stopping
    if f(*x) == True:
        print("solution found:", x)
        return True
    if f(*x) == False:
        return False

# next solution; use heuristic
for i in range(d):
        if backtrack(f, [*x, i]):
            return True
    return False
```

BACKTRACKING

Query complexity:

brute force	d^n
Grover	$d^{n/2}$
backtracking	\overline{T}
quantum backtracking	$O(\sqrt{Tn}\log(1/\delta))$

- 1. $0 < \delta < 1$ failure probability
- 2. to also *find* a solution, extra $n \log n$.
- 3. uses poly(n) space

QUANTUM BACKTRACKING

Ingredients:

1. Quantum Phase Estimation, to differentiate when a unitary U has eigenvalue 1: e.g. for

$$U = \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}lpha} \end{pmatrix}$$

2. If for two states, $||\psi_1\rangle - |\psi_2\rangle|| = \epsilon$, then if measured in the computational basis, the total variation distance is $\leq \epsilon$

QUANTUM BACKTRACKING

We will look at the special case of **trees** where one starts at the **root** of the tree.

- ullet T vertices labeled $r,1,\ldots,T-1,r$ being the root
- Distance from root $\leq n$; denote with $\ell(i)$
- ullet A is the vertices with even ℓ, B with odd ℓ
- ullet Write x o y if y is a child of x
- d_x is the degree of vertex x:

$$d_x = \left\{ egin{array}{ll} |\{y:x
ightarrow y\}| + 1 & x
eq r \ |\{y:x
ightarrow y\}| & ext{otherwise} \end{array}
ight.$$

QUANTUM BACKTRACKING

- ullet Label states $|r
 angle, |1
 angle, \ldots, |T-1
 angle$
- Define a diffusion operator D_x that only requires *local* knowledge of the tree:
 - 1. If x is marked, $D_x=\mathbb{1}_T$
 - 2. Otherwise, and if x
 eq r, then $D_x = 1_T 2 |\psi_x
 angle \! \langle \psi_x |$ with

$$\ket{\psi_x} = rac{1}{\sqrt{d_x}} \Biggl(\ket{x} + \sum_{y:x o y} \ket{y} \Biggr)$$

3. $D_r=1_T-2|\psi_r
angle\!\langle\psi_r|$ with

$$\ket{\psi_x} = rac{1}{\sqrt{1+nd_x}} \Biggl(\ket{x} + \sqrt{n} \sum_{y:x
ightarrow y} \ket{y} \Biggr)$$

ullet Let $R_A = igoplus_{x \in A} D_x$, $R_B = |r
angle\!\langle r| + igoplus_{x \in B} D_x$

Why diffusion operator?

Think of a vertex x in the tree that $D_x=1_T-2|\psi_x\rangle\!\langle\psi_x|$ acts on. Then e.g.

$$|\psi_x
angle\!\langle\psi_x| = egin{pmatrix} 1 & 1 & 1 & 1 \ 1 & 1 & 0 & 0 \ 1 & 0 & 1 & 0 \ 1 & 0 & 0 & 1 \end{pmatrix}$$

is like the adjacency matrix of that graph segment; D_x is thus like a Laplace operator.

Algorithm:

- 1. Repeat K times:
 - ullet apply QPE to R_AR_B
 - if eigenvalue is 1, accept, else reject
- 2. If the number of acceptance is $\geq 3K/8$, a marked vertex exists.

Why does this work?

- 1. If x is marked, $D_x=\mathbf{1}_T$
- 2. Otherwise, D_x diffuses the weight.
- 3. D_r , where r is the root element, *also* concentrates weight around r.

This means that if there is *no* marked element in the tree, there will be a single eigenvector with eigenvalue 1. This eigenvector is roughly $|r\rangle$.

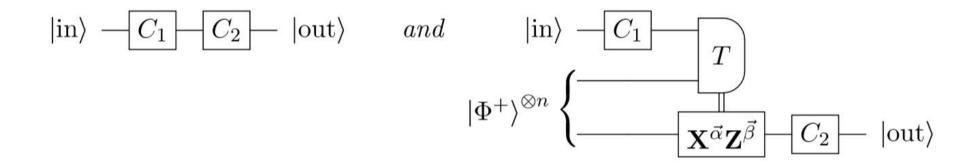
SESSION 2

WHO WON THE WORLD CUP?

https://bitbucket.org/rumschuettel/quantum-ranking

GATE TELEPORTATION

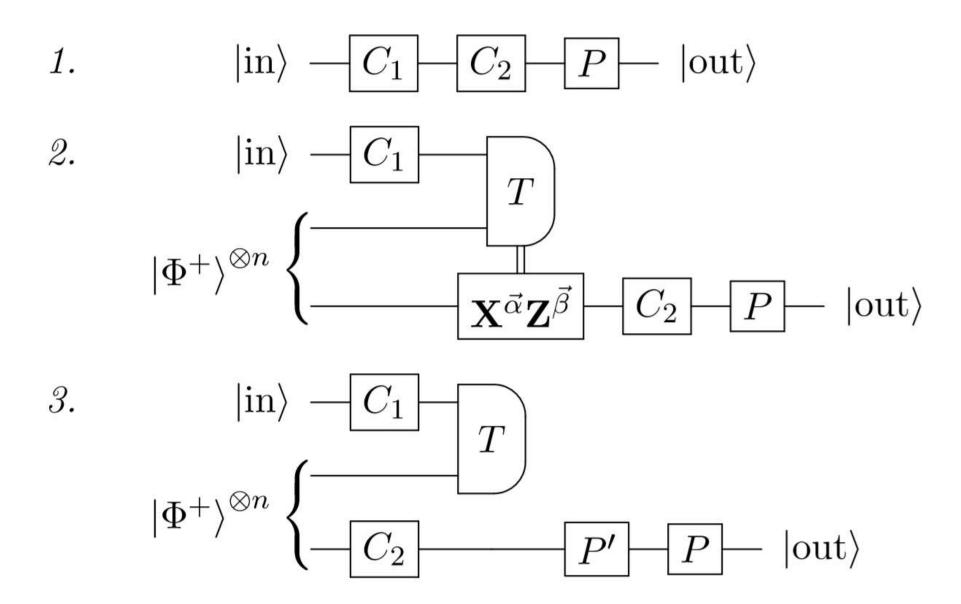
Quantum state teleportation can also be used to teleport operations around.



CLIFFORD CIRCUITS

- 1. Preparation of computational basis states, e.g. |0
 angle
- 2. gates: CNOT, H, S, Paulis (normalizers of the Pauli group)
- 3. Measurement in the computational basis.
- Those are not yet universal
- In fact, they are classically simulable ([Gottesman-Knill])

SO WHY ARE THEY INTERESTING?



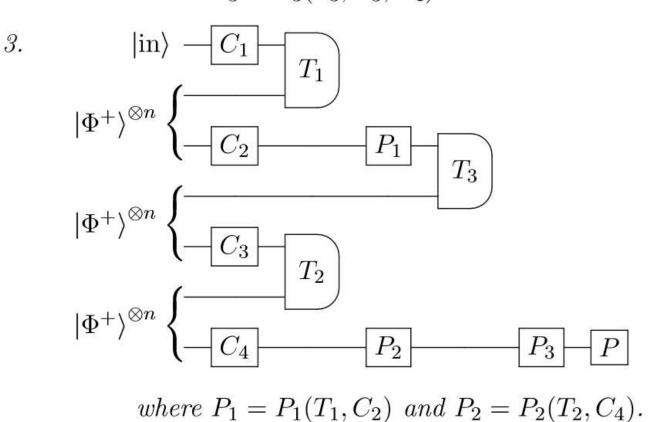
P, P' are depth-1 Pauli circuits.

1.
$$|\text{in}\rangle - C_1 - C_2 - C_3 - C_4 - P - |\text{out}\rangle$$

2.
$$|\operatorname{in}\rangle - C_1 - C_2 - T_3$$

$$|\Phi^{+}\rangle^{\otimes n} \left\{ - C_3 - C_4 - P_3 - P - |\operatorname{out}\rangle \right\}$$

where $P_3 = P_3(T_3, C_3, C_4)$.



Clifford circuits are a kind of sub-circuit that can be teleported in; a type of quantum speculative execution.

T

$$\left(egin{array}{cc} 1 & 0 \ 0 & \mathrm{e}^{\mathrm{i}\pi/4} \end{array}
ight)$$

CLIFFORD + T IS UNIVERSAL.

MAGIC STATE INJECTION

Prepare the following state:

$$|A
angle=(|0
angle+\mathrm{e}^{\mathrm{i}\pi/4}|1
angle)/\sqrt{2}$$

$$|\phi\rangle$$
 — T — T $|\phi\rangle$ — T $|\phi\rangle$ — T $|\phi\rangle$ — T $|\phi\rangle$

Like this, *any* quantum circuit can be decomposed into Clifford + Magic State injection.

MAGIC STATE INJECTION

REPEAT UNTIL SUCCESS (RUS)

REPEAT UNTIL SUCCESS

- 1. Prepare some states in some magic gate factory.
- 2. Your device can only perform a limited set of operations (e.g. measurements, and Pauli gates).
- 3. You attempt a gate; if it fails, apply recovery operation, and repeat.

HOW TO LOAD DATA INTO A QUANTUM MEMORY

Imagine you have a list of numbers that you want to load into your quantum device, e.g. to perform Grover search on it.

If that list is long, in time I have loaded the list I've already found the element, no?

YES, BUT...

QUANTUM DATA LOADING

REPRESENTING DATA

```
1 : list = [m00, m01, m10, m11]

1[2]
# == m10

[ f(item) for item in 1 ]
# == [ f(m00), f(m01), f(m10), f(m11) ]
```

IN QUANTUM LAND

- $|1.|m
 angle = |00
 angle \otimes |m_{00}
 angle + |01
 angle \otimes |m_{01}
 angle + |10
 angle \otimes |m_{10}
 angle + |11
 angle \otimes |m_{00}
 angle \otimes |m_{00}
 angle + |11
 angle \otimes |m_{00}
 angle + |11
 angle \otimes |m_{00}
 angle \otimes |m$
- 2. read data: project onto corresponding address register, i.e. $(\langle 10|\otimes 1_{
 m mem})|m
 angle=|m_{10}
 angle$
- 3. **BUT**: Let's exploit coherence for the function application! $(1_4 \otimes U_f)$

How do we get this type of quantum memory of data?

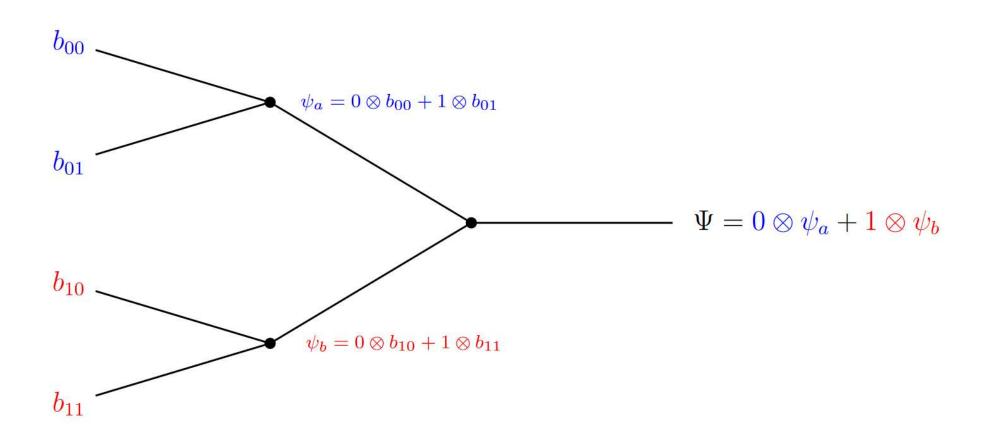
APPROACH A

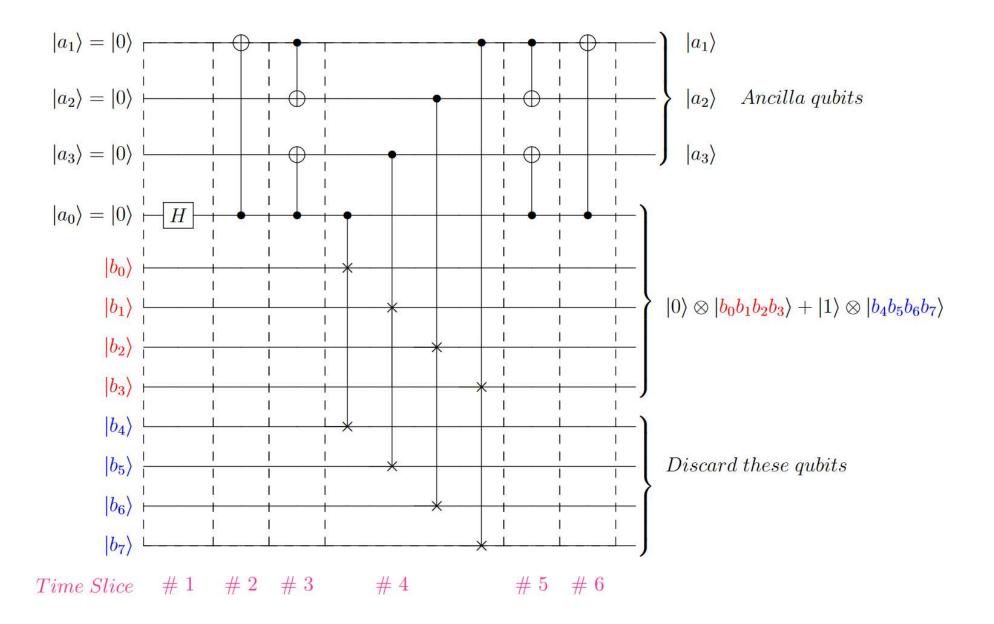
Load data serially.

APPROACH B

Load data in parallel.

PARALLEL DATA LOADING





The gate depth of loading classical data into a quantum memory can be reduced exponentially.

But we still need to read the information once in first place.

QRAM is somewhat unrealistic.

QUANTUM MACHINE LEARNING

- 1. Use ML to learn something about quantum systems.
- 2. Use quantum algorithms to speed up classical neural nets.
- 3. Quantum neural nets.

NEURAL NETWORK STATES

If $|\psi\rangle=\sum_{i=1}^{2^n}\alpha_i|i\rangle$, we need exponentially many weights to represent the state. So do a *variational* ansatz:

- 1. Find a function $i \longmapsto f(i) \approx \alpha_i$.
- 2. Find a function which maintains some property of the state, e.g. entanglement entropy, fidelity wrt. some observable, ...

We know this from physics: a family of wavefunctions is used to minimize the energy wrt. some Hamiltonian.

NEURAL NETWORK STATES

f(i) is a neural network, e.g. RBM, feed forward, recurrent, autoencoder, name your favourite.

I sense... competition.

- 1. Matrix Product States (MPS)
- 2. Projected Entangled Pair States (PEPS)
- 3. Tensor network states

NEURAL NETWORK STATES

Surprisingly good for a range of tasks.

- 1. Representing ground states of Hamiltonians.
- 2. Communication and error correction

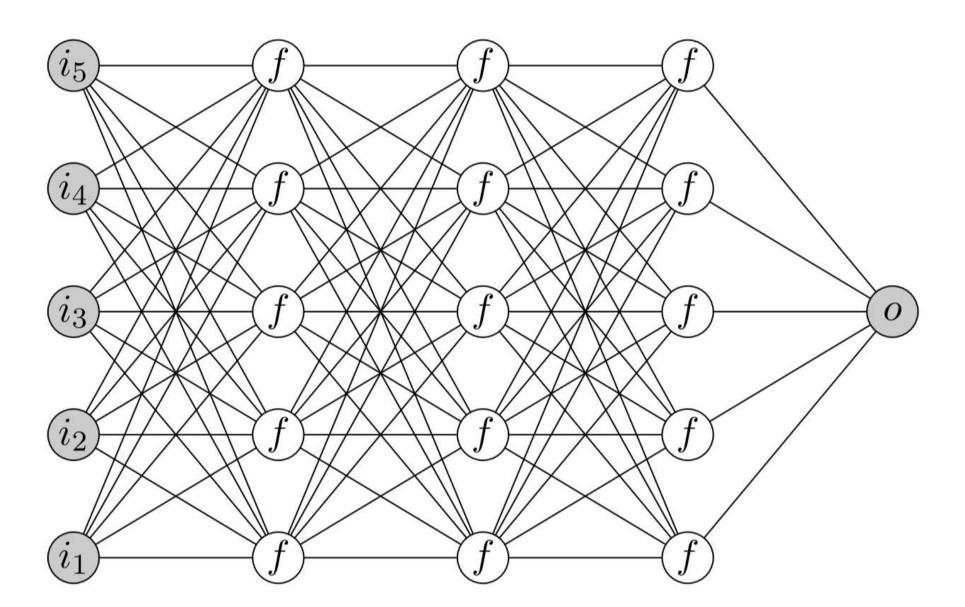
https://bitbucket.org/rumschuettel/coherent-information-optimizer

SPEEDING UP LEARNING

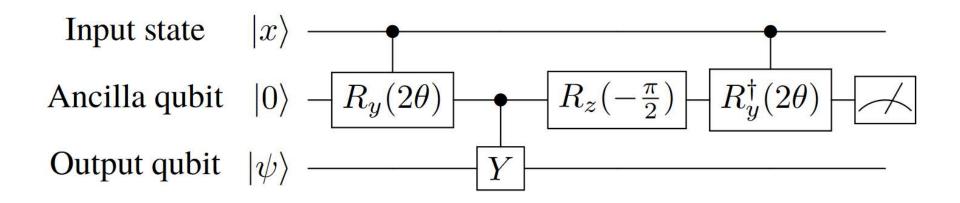
- 1. SVMs, principal component analysis: HHL
- 2. Use any quantum optimization algorithm:
 - Grover-type algorithms
 - Adiabatic evolution, annealing
 - Quantum gradient decent
- 3. Quantum approximate optimization algorithm (QAOA)

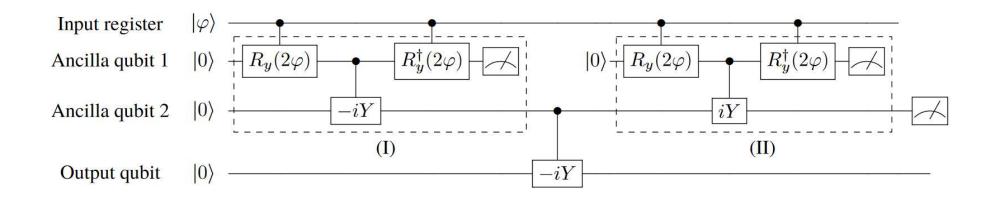
QUANTUM NEURAL NETWORK

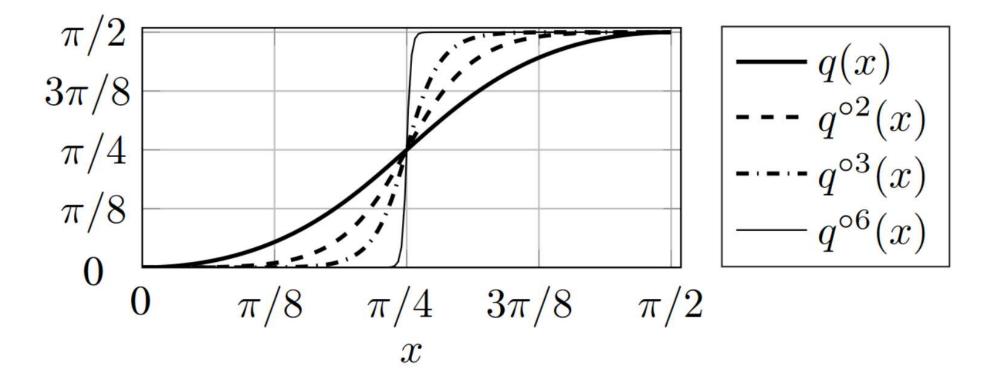
If quantum mechanics is linear, how do we encode a non-linear activation function, like Sigmoid, or ELU?

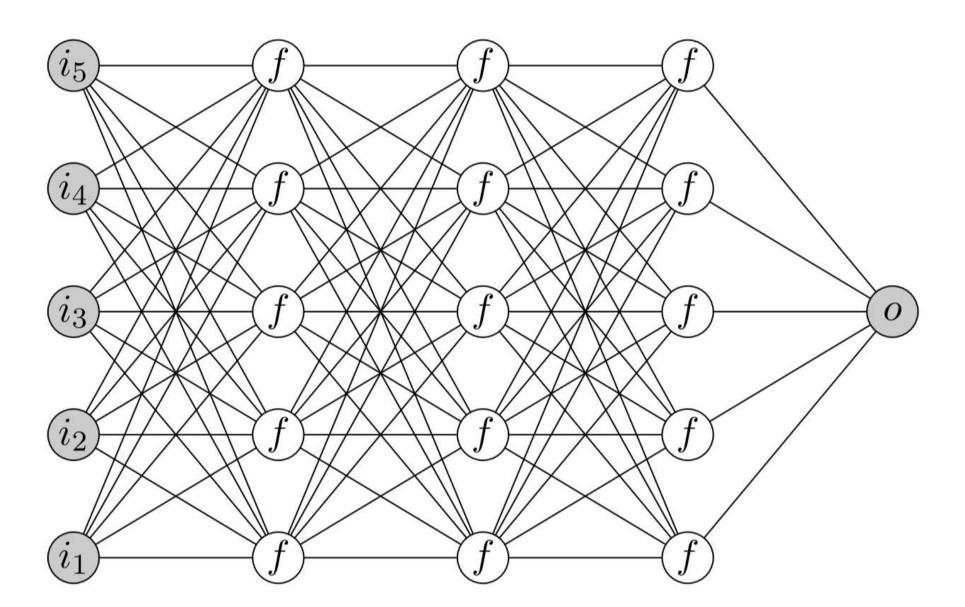


There is a quantum neuron:



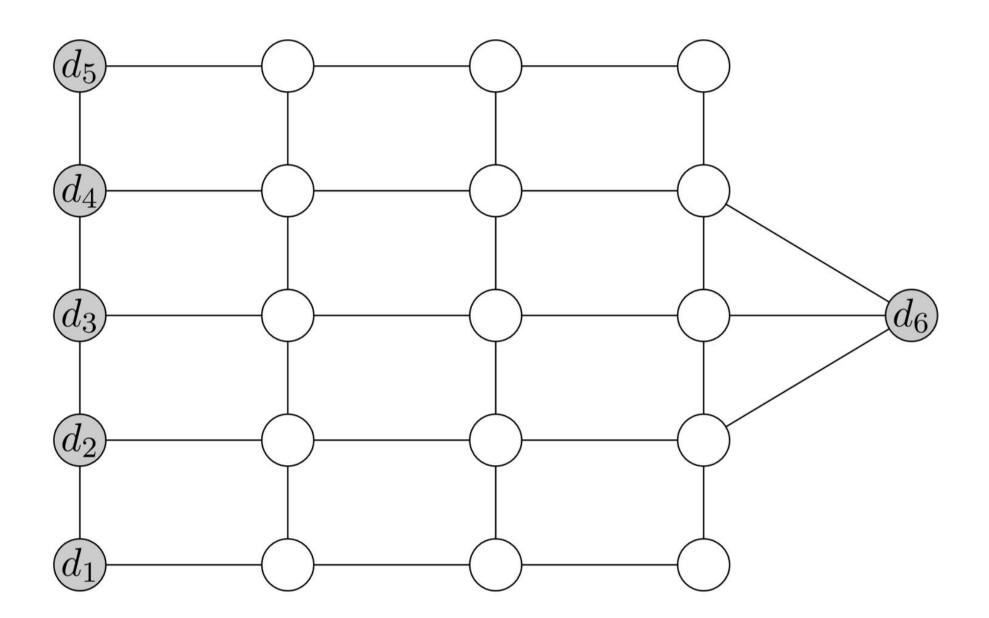


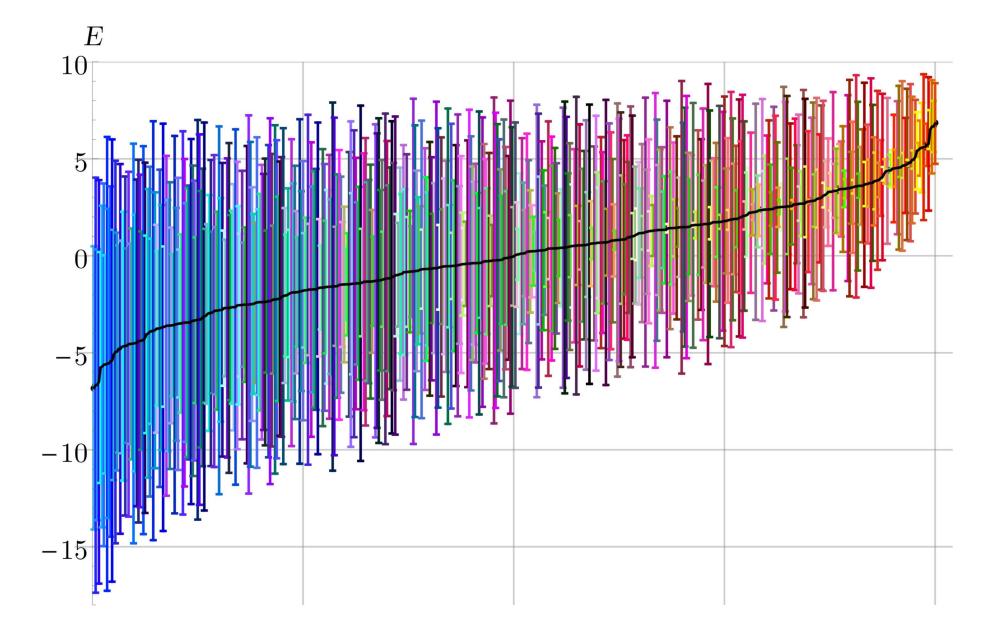


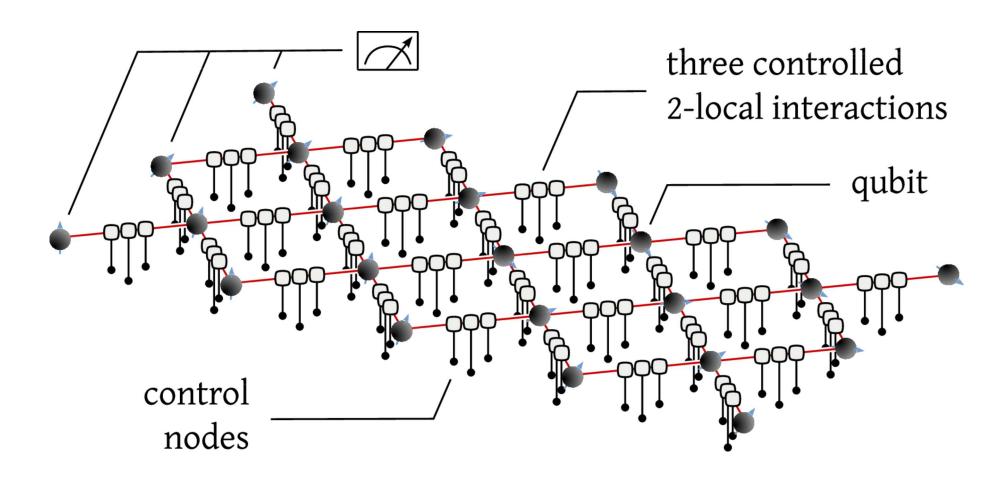


QUANTUM ANNEALING

Hamiltonian Ground States







https://bitbucket.org/rumschuettel/liquidlearn

HAMILTONIAN SIMULATION

A Hamiltonian is a big matrix that describes the energy of a quantum system.

For instance: transverse Ising model:

$$H = \sum_{i \sim j} J_{ij} \sigma_z^{(i)} \otimes \sigma_z^{(j)} + \sum_i h_i \sigma_x^{(i)}$$

HAMILTONIAN SIMULATION

- 1. Simulating static properties: ground state energy
- 2. Simulating dynamics: approximate $\exp(itH)$.

These tasks are *hard*—at least on a classical computer.

(1) is known to be QMA-complete (depending on the precision), and (2) is known to be BQP-complete: we can, in fact, run a quantum computation with a Hamiltonian.

The problems we can exactly solve are very few. QC promise an exponential speedup over classical algorithms.

SUZUKI-TROTTER

$$\mathrm{e}^{t(A+B)} = (\mathrm{e}^{tA/r}\mathrm{e}^{tB/r})^r + O\left(rac{t^2}{r}
ight)$$

- There exist much more sophisticated techniques
- The basic building blocks always show up: RUS, QPE, (oblivious) Grover, Quantum Walks...

THANK YOU! QUESTIONS?