Optimal Hamiltonian Simulation by Quantum Signal Processing

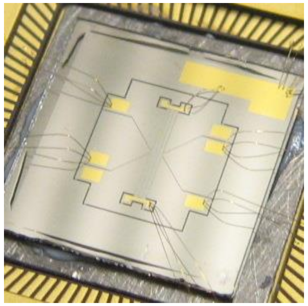
Guang-Hao Low, Isaac L. Chuang

Massachusetts Institute of Technology

QIP 2017

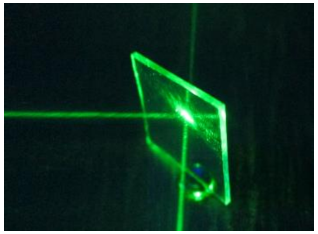
January 19

Physics ↔ Computation



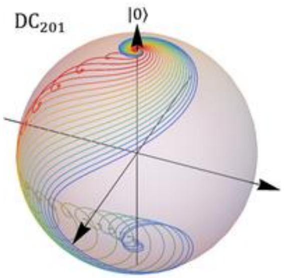
Physical concepts inspire problem-solving techniques

- Adiabatic evolution, Quantum walks
- Universal quantum computation
- Compiling to specific architecture has large overheads



Physical systems solve problems

- Boson sampler, Analog quantum simulator
- Very elegant, simple, fast; Near future prospects
- Generally not fault-tolerant



Quantum Signal Processing: Abstraction of physical dynamics into a computing module `**Quantum Signal Processor'** that

- Preserve intuition of how original physical system computes
- Preserve simplicity, optimality of original physical system
- In a FTQC compatible manner

Outline

1. Hamiltonian Simulation
    - A Brief History of Simulation
2. Overview of Algorithm
    - Quantum Signal Processing
    - Optimal Hamiltonian Simulation
3. Conclusion

1. Hamiltonian Simulation

$$i\frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle \Rightarrow e^{-i\hat{H}t}$$

Simulate nature:

Chemistry, materials, etc.

Run quantum algorithms:

Quantum walks, span programs etc.

"… nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

Richard Feynman (1982)

Difficult for classical computers in general

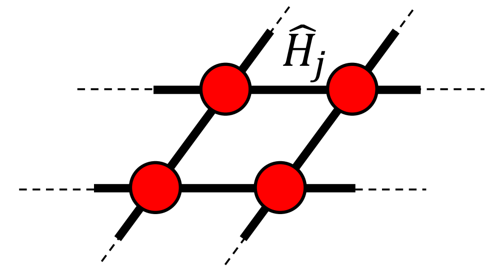
Curse of dimensionality: n qubits $\Rightarrow N = 2^n$ states

PromiseBQP-complete

Assumptions

$\boldsymbol{k}$-local interactions [Lloyd 1996]

- $\hat{H} = \sum_{j=1}^{m} \hat{H}_j, \quad \hat{H}_j$ on $k = O(1)$ qubits
- Naturally describes physical systems
- $e^{-i\hat{H}_j t}$ are easy; $e^{-i(\hat{A}+\hat{B})} = (e^{-i\hat{A}/r} e^{-i\hat{B}/r})^r + O(1/r)$



$\boldsymbol{d}$-sparse matrices [Aharanov & Ta-Shma 2002]

- d non-zero entries per row, e.g. $d = 2^k m$
- Oracles for positions & values of non-zero elements
- Exponential speedups claimed when $d = \mathrm{polylog}(N)$
- Popular in quantum algorithm design by quantum walk

$$\underbrace{\begin{pmatrix} 0 & -2 & 0 & 0 & 0 & \cdots \\ -2 & 0.333 & 0 & 1 & -i & \cdots \\ 0 & 0 & -1 & 1 & 1 & \cdots \\ 0 & 1 & 1 & 2 & 0 & \cdots \\ 0 & i & 1 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}}_{N}$$

Unitary access model [Childs & Wiebe 2012]

- $\hat{H} = \sum_{j=1}^{m} \alpha_j \hat{U}_j, \quad \hat{U}_j$ are Unitary, Oracles for α_j & $\hat{U}_j$
- New promising approach to quantum physics simulations

A Brief History of Simulation

Parameters:
t time
ε error
N dimension
m terms
d sparsity
$\delta > 0$

Richard Feynman 1982

k-local era
[L96] $O\left(m\frac{(mt\|H\|)^2}{\varepsilon}\right)$

[BACS07] $O\left(m\frac{(mt\|H\|)^{1+\delta}}{\varepsilon^\delta}\right)$

[PZ10] $O\left(m\frac{(mt\|H_1\|)(mt\|H_2\|)^\delta}{\varepsilon^\delta}\right)$

Unitary access era [CW12]
$\mathbf{O}\left(m^2\|H_j\|t\exp\left(1.6\sqrt{\log\left(\frac{m\|H_j\|t}{\varepsilon}\right)}\right)\right)$
Better than product formulas

***d*-sparse Graph coloring era**
[AT02] $\text{poly}(d,\log N)(\|H\|t)^{3/2}/\sqrt{\varepsilon}$

[C04] $O(d^4\log^4 N\|H\|t)^{1+\delta}/\varepsilon^\delta$

[BACS07] $O(d^4\log^* N\|H\|t)^{1+\delta}/\varepsilon^\delta$

[CK11] $O(d^3\log^* N\|H\|t)^{1+\delta}/\varepsilon^\delta$

***d*-sparse Quantum walk era**
[C10][BC12] $O(d\|H\|_{\max}t\,/\varepsilon)$
Optimal time & sparsity

Aharanov Ahokas Berry Childs Cleve Kothari Lloyd Novo Papageorgiou Sanders Somma Ta-Shma Wiebe Zhang

Modern History

Parameters:
t time
ε error
N dimension
m terms
d sparsity

Qubitization[2] Era?
$\hat{H} \propto \langle G|\hat{U}|G\rangle$

[BCCKS14B] $O\left(\tau \frac{\log(\tau/\varepsilon)}{\log\log(\tau/\varepsilon)}\right)$

[LC16B][2] $O\left(\tau + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right)$

[NB16] $O\left(\tau \frac{\log \tau}{\log\log \tau} + \log\left(\frac{1}{\varepsilon}\right)\right)$

[BCK15] $O\left(\tau \frac{\log(\tau/\varepsilon)}{\log\log(\tau/\varepsilon)}\right)$

Lower bound $\Omega\left(\tau + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right)$

[LC16A][1] $O\left(\tau + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right)$
Optimal

[BN16] $O\left(\tau \frac{\log\log \tau}{\log\log\log \tau} + \log\left(\frac{1}{\varepsilon}\right)\right)$

Our results!

[BCCKS14A] $O\left(\tau\, d \frac{\log(\tau/\varepsilon)}{\log\log(\tau/\varepsilon)}\right)$
Optimal error

Legend

- **Unitary access** $\tau = t\sum_{j=1}^{m} \alpha_j \geq \|H\|t$
- ***d*-sparse Quantum walk** $\tau = d\|H\|_{\max}t$
- ***d*-sparse Graph coloring** $\tau = d\|H\|_{\max}t$

[1]Low, Chuang, arXiv:1606.02685 | Phys. Rev. Lett. 118, 010501
[2]Low, Chuang, arXiv:1610.06546

2. Overview of Algorithm

Input: d-sparse oracles **Output: $\approx e^{-i\hat{H}t}$**

$\mathrm{COLUMN}|i\rangle|l\rangle = |i\rangle|f(l,j)\rangle$ $\mathrm{ELEMENT}|i\rangle|j\rangle|z\rangle = |i\rangle|j\rangle|z \oplus \hat{H}_{ij}\rangle$

row l^{th} non-zero column row column

Discrete-time quantum walk for any Hamiltonian [Childs 2010]

Implement $e^{i\,\arcsin(\hat{H}/d\|H\|_{\max})}$ with 2 COLUMN & 4 $\mathrm{ELEMENT}$ queries

Linearize with `quantum signal processing'

Linearize spectrum with eigenphase transformation $e^{i\,\lambda} \mapsto e^{-id\|H\|_{\max}\sin(\lambda)}$

$O\left(td\|H\|_{\max} + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right)$ single qubit gates & queries to controlled-walk

1 ancilla qubit

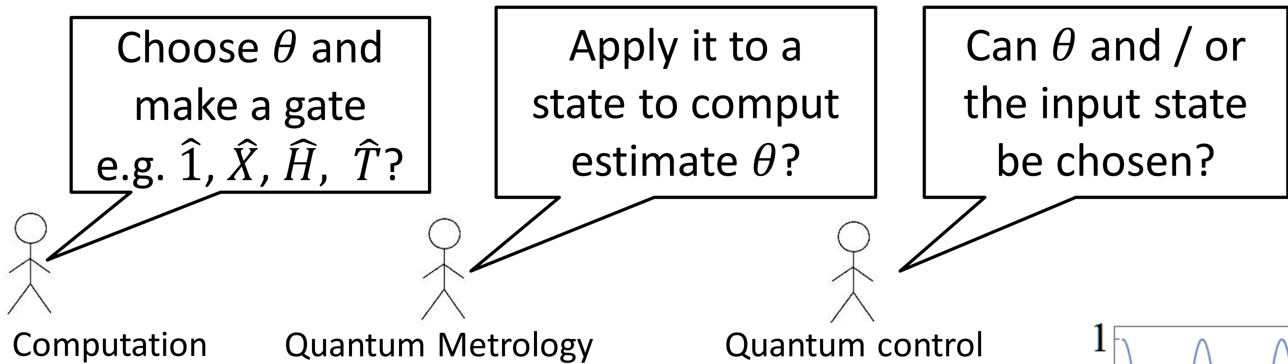
Extremely small overhead:
Candidate for small quantum computer!

Quantum Physics 8.01

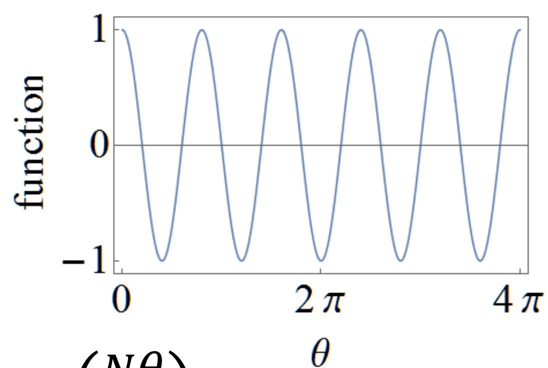
Single-qubit unitary

$$\hat{R}[\theta] \equiv e^{-i\frac{\theta}{2}\hat{X}} \equiv \cos\left(\frac{\theta}{2}\right)\hat{1} - i\sin\left(\frac{\theta}{2}\right)\hat{X} \equiv -\boxed{\hat{R}}-$$

Q: How does this compute?



Combination of Ideas: $\hat{R}[\theta]$ is a computational module that computes some function depending on input parameter θ, input state and measurement basis.



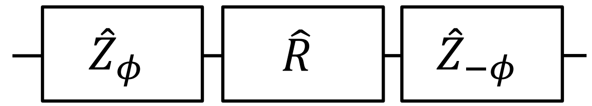
Composite gate: $\langle 0|\hat{R}[\theta]\hat{R}[\theta]\cdots\hat{R}[\theta]|0\rangle = \cos\left(\frac{N\theta}{2}\right)$

The Single-Qubit Processor

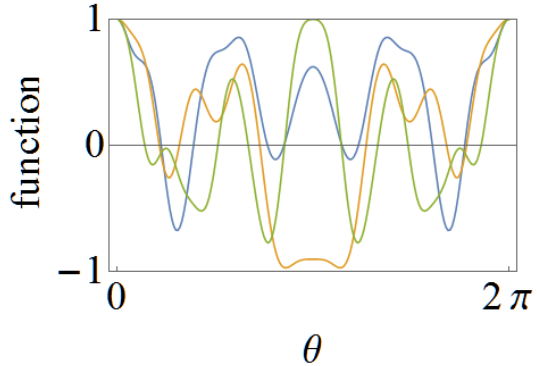
Q: Can this compute anything interesting?

Idea: Less trivial primitive unitary by with discrete quantum control

$\hat{R}_\phi[\theta] \equiv e^{-i\frac{\phi}{2}\hat{Z}}\hat{R}[\theta]e^{i\frac{\phi}{2}\hat{Z}}$ $\equiv$



Composite gate $\langle 0|\hat{R}_{\phi_N}[\theta]\cdots\hat{R}_{\phi_2}[\theta]\hat{R}_{\phi_1}[\theta]|0\rangle$ **for some choice** $\overrightarrow{\boldsymbol{\phi}}$



Very non-trivial functions for random choice of $\boldsymbol{\phi}$

Idea: $\overrightarrow{\boldsymbol{\phi}}$ **assembly code for single-qubit processor**

Compute unitary function $A[\theta]\,\hat{1} + iB[\theta]\hat{Z} + iC[\theta]\hat{X} + iD[\theta]\hat{Y}$

Select desired components with choice of input state and measurement

Qubit Unitary Function Synthesis

Q: Why is this hard? Analogy:

- Single-qubit gate synthesis from $\{\mathrm{H}, \mathrm{T}\}$
- Single-qubit function synthesis from $\{\hat{R}_\phi[\theta],\ \overrightarrow{\boldsymbol{\phi}} \in \mathbb{R}\}$

Exponential time for finding best-fit $\overrightarrow{\boldsymbol{\phi}}$ via gradient descent

- $\hat{R}_{\phi_N}[\theta] \cdots \hat{R}_{\phi_2}[\theta]\hat{R}_{\phi_1}[\theta] = A[\theta]\hat{1} + iB[\theta]\hat{Z} + iC[\theta]\hat{X} + iD[\theta]\hat{Y}$

Necessary & sufficient constraints on achievable $\boldsymbol{A[\theta]}, \boldsymbol{C[\theta]}$[1]

1. $A[0] = 1$
2. $A[\theta]^2 + C[\theta]^2 \leq 1$
3. $A[\theta] = \sum_{k=0}^{N/2} a_k \cos(k\theta)$
4. $C[\theta] = \sum_{k=1}^{N/2} c_k \sin(k\theta)$

(3–4: Fourier series)

- Given $A[\theta], C[\theta]$, can compute $\overrightarrow{\boldsymbol{\phi}}$ in classical poly*(N)* time

[1]Low, Yoder, Chuang, Phys. Rev. X 6, 041067 (2016)

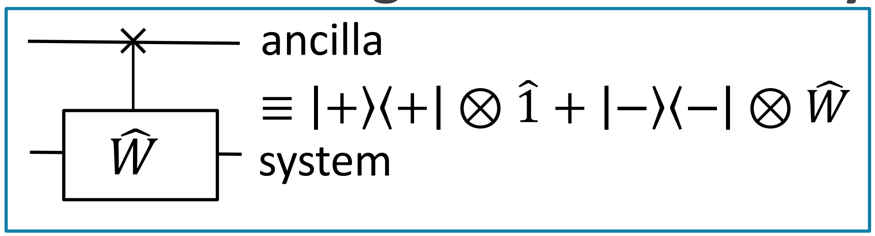
1-qubit Quantum Signal Processing

Q: How relevant is this to multi-qubit problems?

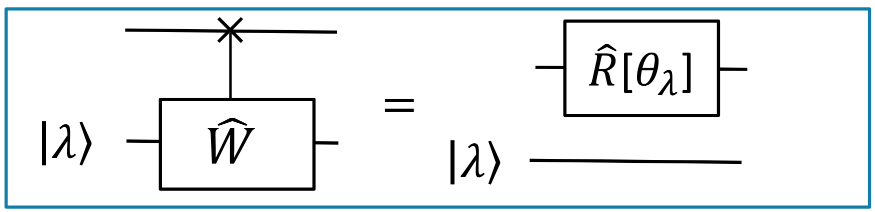
Idea: Single-qubit rotation angle θ controlled by system

- Controlled-$\widehat{W}$

$\widehat{W}|\lambda\rangle = e^{i\theta_\lambda}|\lambda\rangle$



- On input $|\lambda\rangle$



Up to global phase uncomputed with $\widehat{W}^\dagger$

- Replace all $\hat{R}$ in $\hat{R}_{\phi_N}[\theta]\cdots\hat{R}_{\phi_2}[\theta]\hat{R}_{\phi_1}[\theta]$ with controlled-$\widehat{W}$

Idea: Project ancilla to apply coefficient on eigenstate

$$\langle+|\hat{R}_{\phi_N}[\theta]\cdots\hat{R}_{\phi_2}[\theta]\hat{R}_{\phi_1}|+\rangle = A[\theta] + iC[\theta]$$

$$\langle+|\widehat{U}|+\rangle|\lambda\rangle = A[\theta_\lambda] + iC[\theta_\lambda]|\lambda\rangle$$

Quantum Signal Processing (cont.)

Q: What can this do?

Approximate $e^{i\,\theta} \rightarrow e^{i\,h(\theta)}$ with degree *N/2* Fourier series

- **Input**: Objective function h: $[0,2\pi) \rightarrow [0,2\pi)$
- $\left\| A[\theta] + iC[\theta] - e^{i\,h(\theta)} \right\|_\infty \leq \epsilon \Rightarrow$ can find achievable $A_1[\theta] + iC_1[\theta]$ s.t. $\left\| A_1[\theta] + iC_1[\theta] - e^{i\,h(\theta)} \right\|_\infty \leq 8\epsilon$

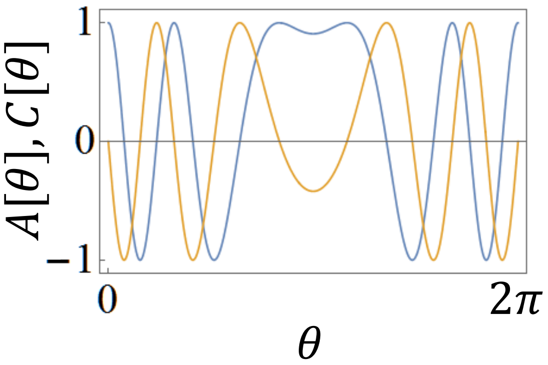
Eigenphase transformation

- **Output**: $\langle + | \hat{U} | + \rangle | \lambda \rangle = A_1[\theta_\lambda] + iC_1[\theta_\lambda] | \lambda \rangle \approx e^{i\,h(\theta_\lambda)} | \lambda \rangle$
- Query Complexity *N* vs. ϵ depends on smoothness / analyticity of $e^{i\,h(\theta)}$
- Trace distance $\leq 8\epsilon$
- Success probability $\geq 1 - 16\epsilon$

k-smooth: $\epsilon^{-1/k}$
Analytic: log(*1/* ϵ)
Entire: super-logarithmic

[1]Methodology of … Composite Quantum Gates, Low, Yoder, Chuang, Phys. Rev. X 6, 041067 (2016)

Optimal Hamiltonian Simulation



Eigenphase transformation with QSP

- Objective function $e^{i\,h(\theta)} = e^{-i\,\tau\,\sin(\theta)}$
- Linearize quantum walk spectrum to $e^{-i\,\lambda\,t}$

Degree *N* Fourier approximation error

- Truncate Jacobi-Anger expansion $e^{-i\,\tau\,\sin(\theta)} = \sum_{k=-\infty}^{\infty} J_k(\tau)\, e^{-ik\theta}$
- Super-exponential scaling $\varepsilon \leq \sum_{k>N}^{\infty} 2|J_k(\tau)| \leq O\left((e\tau/2N)^N\right)$

Query complexity by solving for $N = O\left(\tau + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right)$

***d*-sparse PARITY lower bound** [Berry Childs Cleve Kothari Somma 2015]

- $\Omega(N)$ for any N s.t. $\varepsilon = O\left((\tau/N)^N\right)$

~~Big Crunch~~ Big Rip

Many open problems in Quantum simulation

Gate optimal simulation

Time-dependent simulation

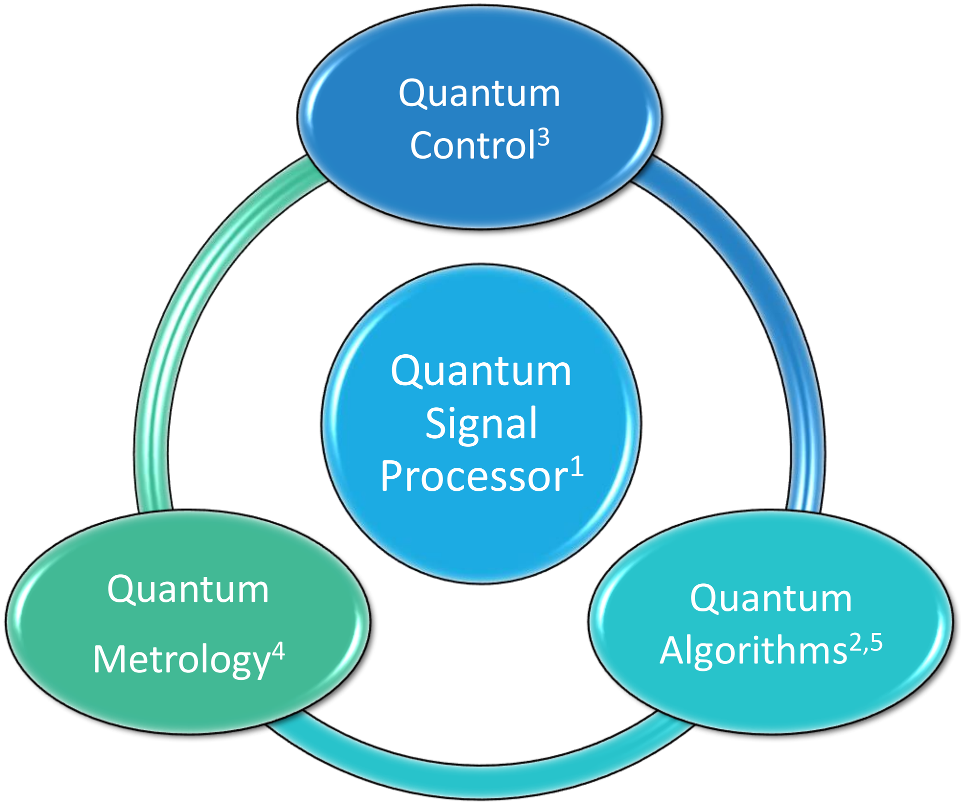
Open quantum system simulation

Hamiltonians with structured information

Analog simulation [Stephen Piddock 2:00-2:40 !]

Other query models

3. Conclusion



Thank you!

Work related to the single-qubit quantum signal processor

1) Hamiltonian simulation by qubitization, Low, Chuang, arXiv preprint arXiv:1610.06546
2) Optimal Hamiltonian simulation by quantum signal processing, Low, Chuang, Physical Review Letters 118 (1), 010501
3) Methodology of resonant equiangular composite quantum gates, Low, Yoder, Chuang, Physical Review X 6 (4), 041067
4) Quantum imaging by coherent enhancement, Low, Yoder Chuang, Physical Review Letters 114 (10), 100801
5) Fixed-point quantum search with an optimal number of queries , Yoder, Low, Chuang, Physical Review Letters 113 (21), 210501