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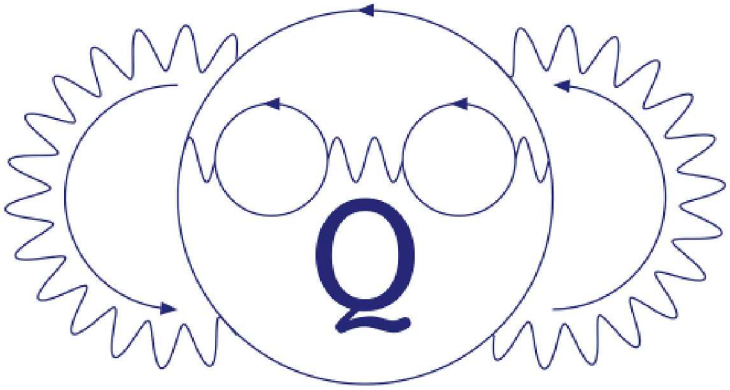

QOALAS

Quantum Optimization and Learning and Simulation

Lead PI: Ojas Parekh, Sandia National Laboratories

(Mohan Sarovar, Sandia National Laboratories)

ASCR PI meeting, Oak Ridge, September 2018

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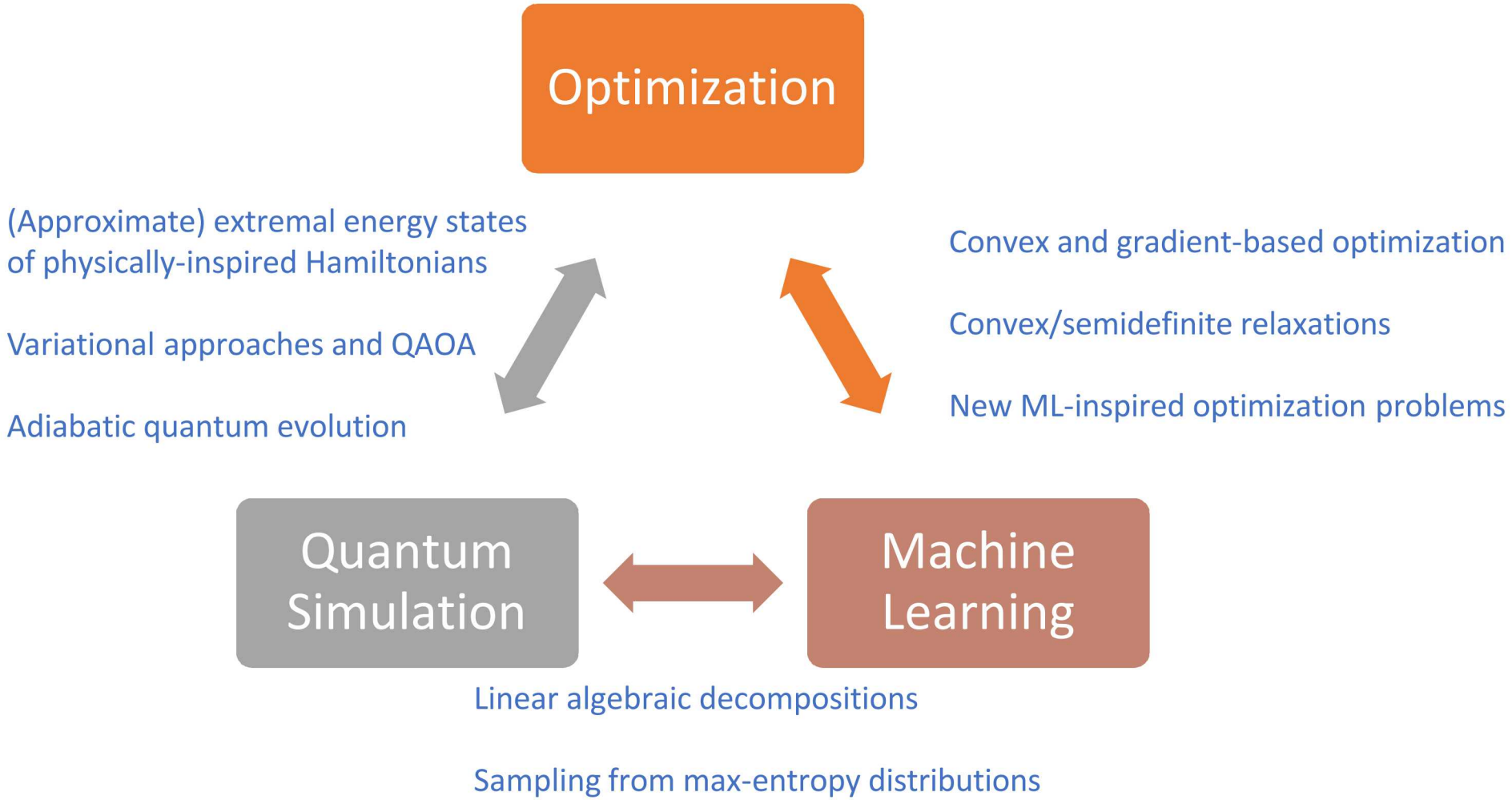
Outline

- Project introduction
  - Project goals
  - Team and expertise
  - Impact and challenges
- Preview of posters
  - “Quantum-Adiabatic like algorithms for solving linear systems of equations”
  - “Engineered thermalization of many-body quantum systems”
  - “Faster quantum simulation by randomization”
- Highlights of recent work or work in progress
  - “Approximate Solutions for Quantum Heisenberg Models via Discrete Optimization”
  - “Optimally Controlled Quantum Optimization”

Project summary

Goal: New quantum techniques and algorithms from the interplay of quantum simulation, optimization, and machine learning



Team and expertise

Sandia National Laboratories

- Ojas Parekh
- Andrew Baczewski
- Matthew Grace
- Kenneth Rudinger
- Mohan Sarovar

Quantum approaches to discrete optimization, Theoretical computer science, Quantum and classical simulation of many-body quantum systems, QCVV, Quantum dynamics and Control

University of Maryland, College Park

- Andrew Childs
- Stephen Jordan (also Microsoft Research)
- Yi-Kai Liu (also NIST)
- Brian Swingle
- Jacob Taylor (also NIST)
- Xiaodi Wu

Quantum computing, Quantum algorithms, Quantum complexity theory, Machine learning, Quantum many-body physics, Quantum gravity, Quantum machine learning, Optimization

Los Alamos National Laboratory

- Rolando Somma
- Yigit Subasi

Quantum computing, Condensed matter theory

California Institute of Technology

- John Preskill

Quantum computing, High-energy physics, Quantum error correction and fault tolerance

Virginia Commonwealth University

- Sevag Gharibian (also Universität Paderborn, Germany)

Quantum algorithms and complexity theory

Sandia National Laboratories

University of Maryland 18 56

Joint Center for Quantum Information and Computer Science

Los Alamos National Laboratory EST. 1943

California Institute of Technology 1891

VCU Virginia Commonwealth University

Project challenges

Challenge: collaboration among large interdisciplinary team with complementary backgrounds

Mitigation strategies:
Bi-weekly global team meetings in addition to more frequent local meetings,
Informal technical seminars presenting and discussing ongoing work,
Plan to organize a group retreat this year

Challenge: deep mathematical or theoretical results may require significant time to incubate

Mitigation strategies:
New areas of exploration leverage existing expertise and work,
Interdisciplinary interactions may lead to cross-semination,
Modularization of broad goals and aspirations into series of more focused results/papers

Challenge: balancing fundamental scientific research with DOE mission impact

Mitigation strategies:
Consultation with applied machine learning experts and analysts at Sandia,
Focus on fundamental problems and techniques with wide applicability:
(e.g. solving linear systems, convex optimization, approx. ground states of local Hamiltonians)

Project outputs

Publications

Quantum algorithms and lower bounds for convex optimization

Shouvanik Chakrabarti, Andrew M. Childs, Tongyang Li, Xiaodi Wu
https://arxiv.org/abs/1809.01731

Quantum algorithms for linear systems of equations inspired by adiabatic quantum computing

Yigit Subasi, Rolando D. Somma, Davide Orsucci
https://arxiv.org/abs/1805.10549

Faster quantum simulation by randomization

Andrew M. Childs, Aaron Ostrander, Yuan Su
https://arxiv.org/abs/1805.08385

Approximate Constraint Satisfaction in the Quantum Setting

Sevag Gharibian, Ojas Parekh, and Ryan Ciaran-Anderson
Submitted to the ACM/SIAM Symposium on Discrete Algorithms, 2019

Synergistic activities

Quantum Computing for Scientific Applications

with LBNL and ORNL QATs, Google, IBM, NASA, Rigetti Computing
Accepted tutorial at ACM/IEEE Supercomputing, 2018.

Workshop on Quantum Machine Learning

Organized by and hosted at QuICS, University of Maryland, September 24-28, 2018
http://qml2018.umiacs.io/

Poster previews

Poster 1 [Yigit Subasi, Rolando Somma]

Quantum-Adiabatic like Algorithms for Solving Linear Systems of Equations

Scientific Achievement

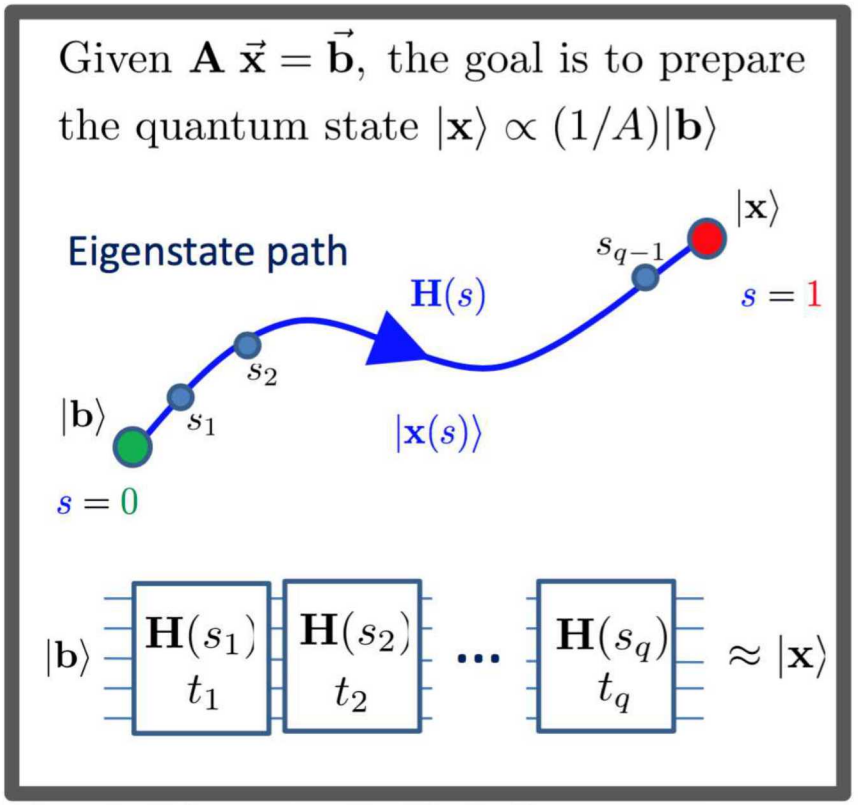
A quantum algorithm to *solve* linear systems of equations much more efficiently than classical computers

Significance and Impact

Evolutions induced by simple Hamiltonians prepare a quantum state that encodes the solution to a linear system of equations. This new idea will find applications in Machine Learning and Optimization, where linear systems play an important role

Research Details

- A Hamiltonian path is built such that the ground states (or other eigenstates) encode the solution to an increasingly difficult linear system of equations
- A variant of adiabatic quantum computing allows one to prepare the ground states or eigenstates
- The complexity of our method is given by the total evolution time and is shown to be optimal



Schematic of the quantum algorithm for linear systems: To prepare a quantum state that is proportional to the solution of a linear system of equations, evolutions under certain Hamiltonians are required. These evolutions can be implemented efficiently on a quantum computer in many cases, achieving an exponential speedup.

Y. Subasi, R.D. Somma, and D. Orsucci, *arXiv:1805.10549* (2018).

Poster 1 [Yigit Subasi, Rolando Somma]

Quantum-Adiabatic like Algorithms for Solving Linear Systems of Equations

The randomization method (RM)

A variant of adiabatic quantum computing in which the parameters of the Hamiltonian are changed discretely and the evolution is for a random time. The time complexity is

$$T_{\mathbf{RM}} \propto \frac{L^2}{\epsilon.\Delta}$$

- L is the length of the path of the state
- Δ is the smallest spectral gap of the Hamiltonians
- ϵ is the accuracy of the state preparation

Hamiltonians and linear systems

We observe the property

$$\mathbf{P}_{\mathbf{b}}^{\perp}.\mathbf{A}\ \vec{\mathbf{x}} = \mathbf{P}_{\mathbf{b}}^{\perp}\ \vec{\mathbf{b}} = 0$$

$$\mathbf{B} \Rightarrow \left(\mathbf{B}^{\dagger}\mathbf{B}\right)\ \vec{\mathbf{x}} = 0$$

The family of Hamiltonians is

$$\mathbf{H}(s) = \mathbf{B}^{\dagger}(s)\mathbf{B}(s)\ ,\mathbf{B}(0) = \mathbf{P}_{\mathbf{b}}^{\perp}\ ,\mathbf{B}(1) = \mathbf{B}$$

Important variables for this problem

The path length satisfies $L = O(\log \kappa)$

The spectral gap satisfies $\Delta = O(1/\kappa^2)$

κ is the condition number

$$T_{\mathbf{RM}} \propto \frac{\kappa^2 \log^2(\kappa)}{\epsilon}$$

Polynomial dependence in condition number and no dependence in dimension imply quantum speedup

Y. Subasi, R.D. Somma, and D. Orsucci, *arXiv:1805.10549* (2018).

Poster 1 [Yigit Subasi, Rolando Somma]

Quantum-Adiabatic like Algorithms for Solving Linear Systems of Equations

The randomization method (RM)

A variant of adiabatic quantum computing in which the parameters of the Hamiltonian are changed discretely and the evolution is for a random time. The time complexity is

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- ϵ is the accuracy of the state preparation

Hamiltonians and linear systems: spectral gap amplification

We observe the property

$$\mathbf{P}_{\mathbf{b}}^{\perp}.\mathbf{A}\ \vec{\mathbf{x}} = \mathbf{P}_{\mathbf{b}}^{\perp}\ \vec{\mathbf{b}} = 0$$

The gap-amplified family of Hamiltonians is:

$$\mathbf{H}(s) = \mathbf{B}(s) \otimes \sigma^{+} + \mathbf{B}^{\dagger}(s) \otimes \sigma^{-}$$

Important variables for this problem

The path length satisfies $L = O(\log \kappa)$

The spectral gap satisfies $\Delta = O(1/\kappa)$

κ is the condition number

$$T_{\mathbf{RM}} \propto \frac{\kappa \log^2(\kappa)}{\epsilon}$$

Linear dependence in condition number results in an optimal quantum algorithm for linear systems

Y. Subasi, R.D. Somma, and D. Orsucci, *arXiv:1805.10549* (2018).

Poster 2 [Mekena Metcalf, Jonathan Moussa, Mohan Sarovar]

Engineered thermalization of many-body quantum systems

Scientific Achievement

Designed and demonstrated protocol for generating thermal states of many-body quantum systems using coupled, driven ancilla spins.

Significance and Impact

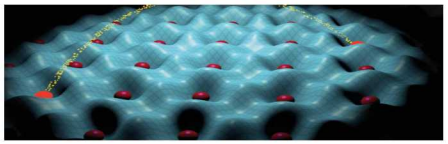
Quantum simulation of thermal states is useful for extracting finite temperature properties of many-body quantum systems, and we have developed a practical protocol for doing this.

Research Details

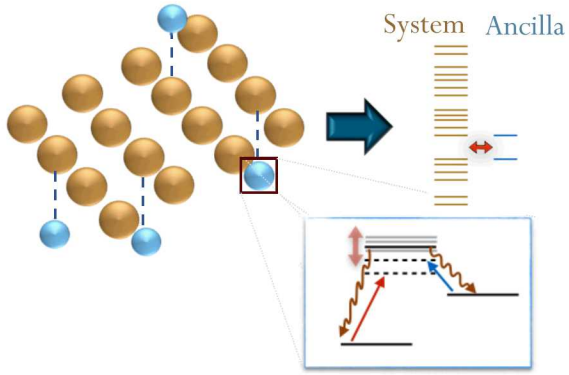
Thermalizing a many-body quantum system requires coupling it to an engineered reservoir. The conditions required for thermalization are known if one has access to a macroscopic reservoir, but this is not typical.

We have developed a protocol that results in thermalization using driven, dissipated ancilla spins that are coupled to the system in a way that results in engineered energy exchange.

Numerical and analytical results demonstrate that the steady-state of the engineered dynamics is the desired thermal state of the many-body system.



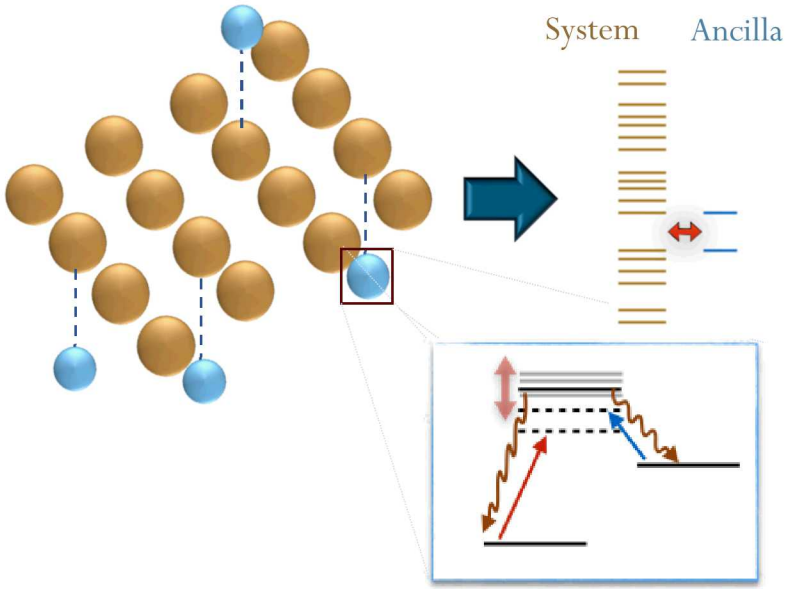
Example target system: cold atom lattice, Esslinger Lab, ETH Zurich



Schematic of protocol: Ancilla systems that are optically pumped to local thermal states are coupled to the system to thermalize. The resonant energy of the ancilla systems are swept across the spectrum of the primary system, and over a few sweeps this dynamics generates a thermal distribution in the principal system.

Poster 2 [Mekena Metcalf, Jonathan Moussa, Mohan Sarovar]

Engineered thermalization of many-body quantum systems



A time-dependent term is added to the ancilla energy to *sweep the system's full energy spectrum.*

$$\Omega_m(t) = \Delta_0 f(t)$$

$$H_T(t) = H_{sys} - \sum_{m=1}^{M} \frac{\Omega_m(t)}{2} \tau_z^m + \sum_{m=1}^{M} g_m \left(\sigma_x^{k_m} \tau_x^m\right)$$

Ancilla optically pumped to thermal state

Timescale Hierarchy

$$\left|\frac{df(t)}{dt}\right| << g_m \sim \Gamma^m << \|H_{sys}\|, \forall m, t$$

$$\Gamma^m = \gamma_+^m + \gamma_-^m$$

A reduced master equation describes system evolution

when the ancilla dynamics is averaged over

$$\dot{\rho} = g^2 \sum_{\omega} \gamma(t,\omega) \left(X(\omega)\rho X^\dagger(\omega) - \frac{1}{2}\{X^\dagger(\omega)X(\omega), \rho\} \right)$$

Operator on System

$$X(\omega) = \sum_{\epsilon' - \epsilon = \omega} |\epsilon\rangle \langle\epsilon| \sigma_x^k |\epsilon'\rangle \langle\epsilon'|$$

Ancilla Correlation Functions

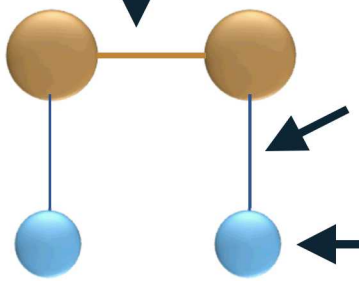
$$\gamma(t,\omega) = \frac{P_0(t)\Gamma}{\left(\frac{\Gamma}{2}\right)^2 - (\omega - \Omega(t))^2} + \frac{P_1(t)\Gamma}{\left(\frac{\Gamma}{2}\right)^2 - (\omega + \Omega(t))^2}$$

Poster 2 [Mekena Metcalf, Jonathan Moussa, Mohan Sarovar]

Engineered thermalization of many-body quantum systems

Two Site System

$$H_{sys} = -\frac{\omega_1}{2}\sigma_z^1 - \frac{\omega_2}{2}\sigma_z^2 + J_x\sigma_x^1\sigma_x^2 + J_y\sigma_y^1\sigma_y^2 + J_z\sigma_z^1\sigma_z^2$$

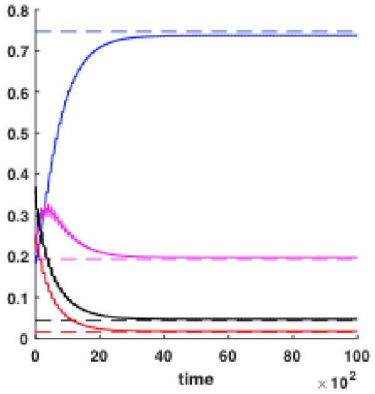


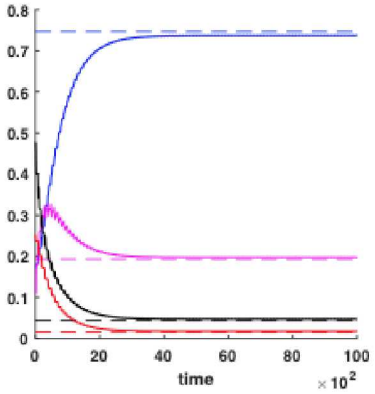
$$H_{s-a} = \sum_{i=1}^{2} g\left(\sigma_x^i\tau_x^i\right)$$

$$\Omega_i(t) = \Delta_{max}\sin^2(\omega t)$$

$$\Delta_{max} = E_{sys}^{max} - E_{sys}^{min}$$

Markovian Evolution of Random Initial State



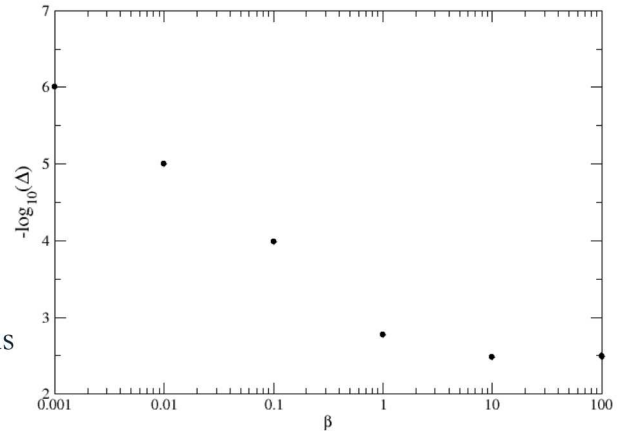


How close is the time averaged state to thermal state?

$$\Delta = \|\rho_{th} - \bar{\rho}\|$$

$$\rho_{th}(\beta) = \frac{e^{-\beta H}}{\mathrm{Tr}(e^{-\beta H})}$$

$$\mathcal{T}\left[e^{\int_0^T dt\mathcal{L}(t)}\right]\rho_{th} = \bar{\rho}$$



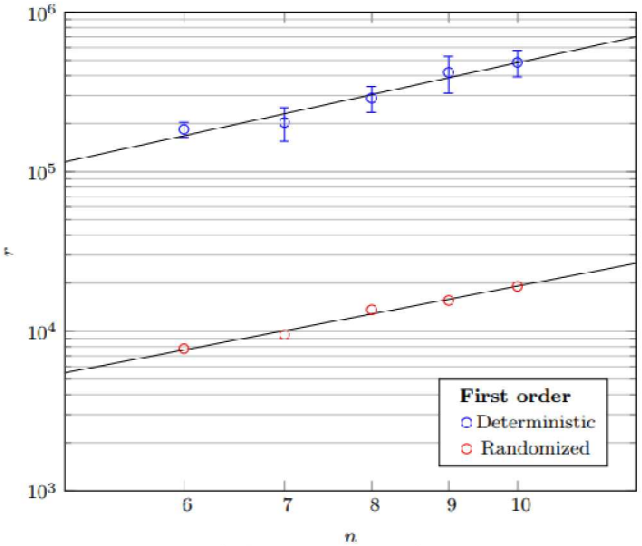
Ongoing Research:

- Analytical calculations to approximate the time-averaged, effective generator of evolution

- Prove fixed point of the dynamics and provide a bound on the thermalization time, respectively.
- Demonstrate this scheme is generalizable to generic system Hamiltonians.

Poster 3 [Yuan Su, Andrew Childs]

Faster quantum simulation by randomization



Comparison of the number of trotter steps between deterministic and randomized first-order product formulas. Error bars are omitted when they are negligibly small on the plot. Straight lines show powerlaw fits to the data.

Scientific Achievement

Stronger product-formula bounds were proved by randomization, and their advantage for near-term quantum simulation was evidenced by numerics.

Significance and Impact

Product formula algorithm is a straightforward yet surprisingly efficient approach to simulating quantum dynamics on a quantum computer. Recent results show that this approach can outperform more sophisticated algorithms, and it is important to understand why it has such outstanding performance.

Research Details

– Proved stronger error bounds for product formulas by randomizing how the terms in the Hamiltonian are ordered.

– Showed that randomized bounds can be asymptotically better than previous bounds that exploit commutation between the terms in the Hamiltonian.

– Numerically compared the deterministic and randomized product formulas, showing improvement even with respect to the empirical performance.

Andrew Childs, et al., arXiv:1805.08385 (2018)

Poster 3 [Yuan Su, Andrew Childs]

Faster quantum simulation by randomization

Quantum simulation

Given a description of a Hamiltonian *H* and an evolution time *t*, perform $U(t) = e^{-itH}$ up to some error ε.

Product formula algorithm

- Target system $H = \sum_{\ell=1}^{L} \alpha_\ell H_\ell$
  - $0 \le \alpha_\ell \le 1$;
  - H_ℓ is a tensor product of Paulis (up to a sign).
- Can use the first-order product formula

$$\left\| e^{-it\sum_{j=1}^{L}\alpha_j H_j} - \left[\prod_{j=1}^{L} e^{-i\frac{t}{r}\alpha_j H_j}\right]^r \right\| \le O\left(\frac{(Lt)^2}{r}\right)$$

- Generalizations to *(2k)*th-order are known [Suzuki 92].
- Advantage: straightforward; can empirically outperform more sophisticated simulation algorithms.
- Problem: error bounds are loose in practice.

Andrew Childs, et al., arXiv:1805.08385 (2018)

Poster 3 [Yuan Su, Andrew Childs]

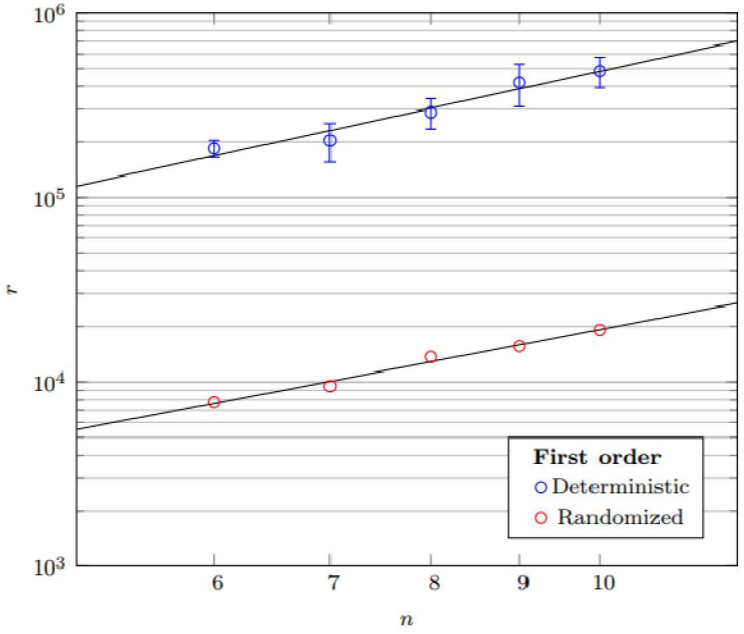
Faster quantum simulation by randomization

New bounds by randomization

- We prove stronger bounds by randomizing how terms in the Hamiltonian are ordered.
- New error bound: $O\left(\frac{(Lt)^3}{r^2}\right)$ improving over the old bound

$$O\left(\frac{(Lt)^2}{r}\right)$$

- We also derive new bounds for higher-order formulas.
- Numerical simulations show improvement even with respect to the empirical performance.



Comparison of the number of trotter steps between deterministic and randomized first-order product formulas.

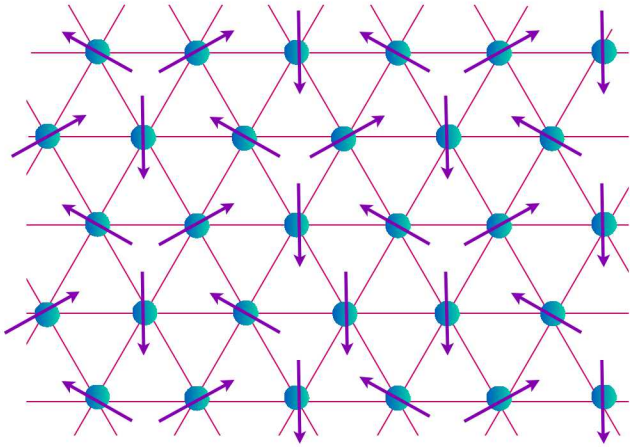
Andrew Childs, et al., arXiv:1805.08385 (2018)

Highlights of recent and ongoing work

Highlight 1 [Sevag Gharibian, Ojas Parekh, Ciaran Ryan-Anderson]

Approximate Solutions for Quantum Heisenberg Models via Hyperplane Rounding

Discrete optimization techniques enable new rigorous approximations of low-energy states of quantum Heisenberg Hamiltonians, a central topic in condensed matter physics.



Anti-ferromagnetic Heisenberg model: roughly neighboring quantum particles aim to align in opposite directions. This kind of Hamiltonian appears, for example, as an effective Hamiltonian for so-called Mott insulators.
(Image: Sachdev, http://arxiv.org/abs/1203.4565)

Significance and Impact

The Heisenberg model is fundamental for describing quantum magnetism, superconductivity, and charge density waves. Beyond 1 dimension, the properties of the anti-ferromagnetic Heisenberg model are notoriously difficult to analyze. Exploiting analytical tools from discrete optimization, a team led by Sandia National Labs has developed new algorithms to rigorously approximate hard-to-compute properties of this model beyond 1-D.

Research Details

- The researchers introduce a new quantum Hamiltonian model that simultaneously generalizes the quantum Heisenberg anti-ferromagnet and hard classical graph partitioning problems.
- A new classical algorithm produces approximate solutions for the above model that are mathematically guaranteed to be relatively close in quality to optimal quantum solutions.

Highlight 1 [Sevag Gharibian, Ojas Parekh, Ciaran Ryan-Anderson]

Approximate Solutions for Quantum Heisenberg Models via Discrete Optimization

New maximum-energy version of the antiferromagnetic Heisenberg model, generalizing the fundamental Maximum Cut discrete optimization problem:

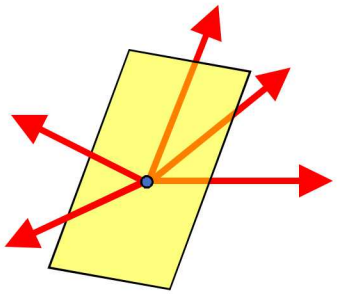
Max Cut Hamiltonian:

$$\sum(I - Z_i Z_j)$$

⇨

Quantum Heisenberg generalization:

$$\sum(I - X_i X_j - Y_i Y_j - Z_i Z_j)$$



- The hard-to-solve Heisenberg maximum energy optimization problem is relaxed to an easier-to-solve semidefinite program
- A generalization of the celebrated Goemans-Williamson hyperplane rounding method produces an approximate max-energy product state

We obtain the first nontrivial rigorous approximations for these problems:
0.498-approx via a product state, where 1/2 is best possible for product states
(also 0.649-approx for XY model, where 2/3 is best possible for product states)

Our results extend to approximating max-energy of any "symmetric" 2-local Hamiltonian:

$$I - \sum_{\{k=1\}}^{3} (\alpha_{k,i} X_i + \beta_{k,i} Y_i + \gamma_{k,i} Z_i)(\alpha_{k,j} X_j + \beta_{k,j} Y_j + \gamma_{k,j} Z_j)$$

Highlight 2 [Aniruddha Bapat, Stephan Jordan]

Optimally Controlled Quantum Optimization

General Framework

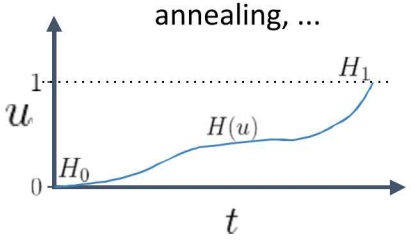
$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = -iH(u)|\psi\rangle$$

$$H(u) = (1-u)H_0 + uH_1$$

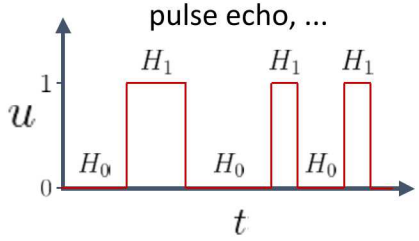
H_0 : "Easy" Hamiltonian (e.g. TFIM)
Ground state = Initial state

H_1 : Cost Hamiltonian
Ground state = Global cost minimum

Adiabatic: QAO, Quantum annealing, ...

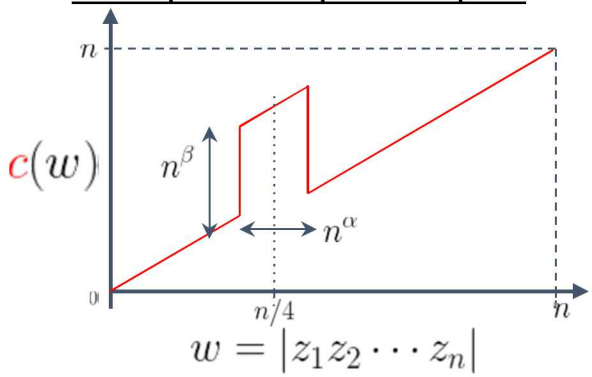


Bang-bang: QAOA, VQE, Spin pulse echo, ...



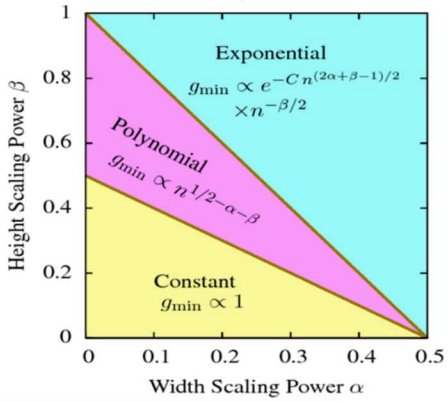
Pontryagin's Minimum Principle
⇓
Optimal controls are bang-bang [1]

Example: Ramp with Spike

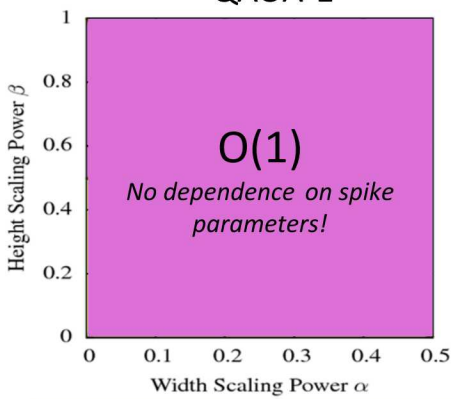


$$w = |z_1 z_2 \cdots z_n|$$

QAO [2]



QAOA-1



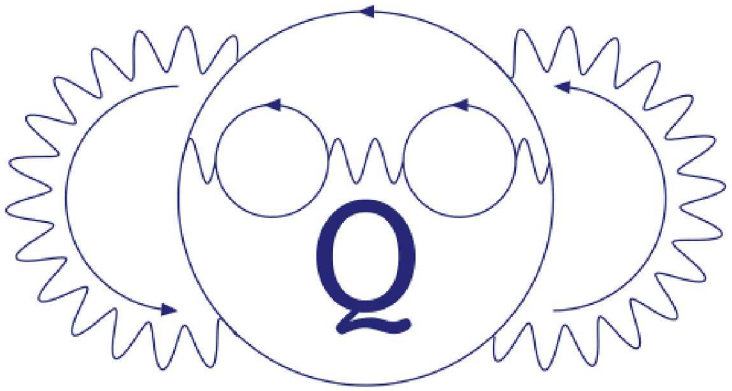
Key intuition: QAOA-1 samples local gradient on hypercube, and imparts a momentum kick to wavepacket, allowing barrier jumps.

?

Quantum-inspired Classical Heuristic

[1] Z.C. Yang *et al.*, Optimizing Variational Quantum Algorithms using Pontryagin's Minimum Principle, Phys. Rev. X 7, 021027 (2017).

[2] L.T. Brady, W. van Dam, Spectral Gap Analysis for Efficient Tunneling in Quantum Adiabatic Optimization, *arXiv:1601.01720v2* (2016).



Thanks!

Sandia National Laboratories

University of Maryland

Joint Center for Quantum Information and Computer Science

Los Alamos National Laboratory EST. 1943

California Institute of Technology

Virginia Commonwealth University VCU