

SHORTCUTS TO QUANTUM ADVANTAGE

With superconducting circuits Work with D. Bagrets, G. Bishop, T. Bode, A. Misra-Spieldenner, P. Schuhmacher, T. Stollenwerk, D. Shapiro, R. Roma

18.6.24 I FRANK WILHELM-MAUCH, INSTITUTE FOR QUANTUM COMPUTER ANALYTICS



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Institute for Quantum Computing Analytics - Groups





Mitglie Tobias Stollenwerk | January 16, 2024, Besuch BMW, Prof. Unruh | Institute for Quantum Computing Analytics (PGI-12) | Slide 6 of 25

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- Mixed qubit-resonator architectures



WHAT IS NISQ AND WHY DO WE CARE?



BASIS OF QUANTUM SUPREMACY

- saving a 50 qubit quantum states requires 2⁵⁰=1.126E15 complex numbers
- need to accomplish a sufficiently general task (otherwise it is not a computer)
- need to be coherent enough / low enough errors (otherwise it is classical)
- needs to be certified without simulation
- Shown in 2019 with a synthetic benchmarks

$$|\psi\rangle = \frac{1}{2^{n/2}} \sum_{s=0}^{2^n - 1} c_s |s\rangle$$



STATUS OF HARDWARE

Error rate, not qubits

- Quantum computers are intrinsically highly **sensitive to errors** (more mature hardware will reduce but not eliminate that!)
- Current error rate: 0.1% per hard operation 1000 steps
- Applied benchmarks use 10ish qubits within large chips
- Next goal: Use more than 50 qubits for real-world applications
- Roadmaps for 1000 qubits need an error roadmap
- (Making 1000 Josephson junctions is routine)
- Key ingredient: Improvement of materials







THE ERA OF EARLY QUANTUM SUPREMACY

Meaning of the Google 2019 and later results

Up to 50 qubits	Beyond 50 qubits	NISQ-Era	Beyond 1MQubits
Basic research in physics	Quantum advantage In synthetic benchmarks	Applied quantum advantage possible?	Provable quantum advantager

- Quantum advantage based on exponential need for memory: Most likely irreversible
- N qubits correspond to 2^N floating point numbers - beyond large HPC at N>50
- Current goal: Better machines and more efficient algorithms: NISQ Era (NISQ: Noisy intermediatescale quantum technologies)
- NISQ-Macines are R&D infrastructure



WIR RECHNEN MIT QUANTENCOMPUTERN für Bildung und Forschung

gefördert durch



NISQ: QUANTUM COPROCESSOR

Classical algorithm calls a shallow and fat routine

- Inside: Parameterized quantum circuit = Algorithm that depends on classical numbers
- Outside: Classical optimizer improving that numbers
- Uses fast quantum sampling of space
- Example: Quantum Approximate Optimization Algorithm (QAOA)
- Speedup conjectured
- Shallow circuit + reset during classical optimization: NISQ friendly

Needs: Reasonable qubits, fast I-O and low-latency Reprogramming



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OPTIMIZING ON QUANTUM COMPUTERS AND QAOA



(Random) Optimization problems

• Many NP-hard or/and complete probelms afford *classical* Ising formulation:

$$H_{P} = -\sum_{i < j}^{N} J_{ij} \sigma_{z}^{(i)} \sigma_{z}^{(j)} - \sum_{j=1}^{N} h_{j} \sigma_{z}^{(j)}$$

- Optimal string corresponds to the ground state !
- For random couplings/graphs Ising Hamiltonian defines the spin glass
- Examples:
 - Number partitioning problem
 - Graph coloring
 - Hopfield neural network

See A. Lucas "Ising formulations of many NP problems", 2014



Quantum annealing

• Use of adiabatic theorem to find the ground state

$$H(s) = s H_P + (1 - s)H_D, \quad H_D = -\sum_{j=1}^N \sigma_x^{(j)}$$

- D-wave system:
 - 5000+ flux qubits with tunable couplings

Imbedding of a problem graph into Chimera one of D-wave





SOLVING BY PHYSICS

Adiabatic algorithms

- Transform a simple into a hard optimization problem
- Stay in the ground state
- Speed protected by energy gap, based on the superconducting tunnel effect
- Predicting the gap is NP-hard
- Has reached more than 2000 qubits already
- Discussion about inefficiencies
- Speedup debated

Needs: Many qubits, a pre-settable interaction, Global adiabatic control Mitglied der Helmholtz-Gemeinschaft



Quantum Approximate Optimization Algorithm (QAOA) E.Farhi, J.Goldstone, S. Gutmann⁴ 2014

• Evolution: variational ansatz for the ground state ~ Trotterization of adiabatic protocol

$$|\beta,\gamma\rangle = \prod_{j=1}^{p} e^{-iH_{D}\beta_{j}} e^{-iH_{P}\gamma_{j}} \left(|+\rangle_{X}\right)^{\otimes N}$$

• Optimum: to be minimized over a set of (β_j, γ_j)

$$E_*(\beta,\gamma) = \langle \beta,\gamma | H_P | \beta,\gamma \rangle$$



NISQ: QAOA ALGORITHM

Classical algorithm calls a shallow and fat routine

- Speedup conjectured
- Shallow circuit + reset during classical optimization: NISQ friendly
- Allows to implement higher-order / long range interactions by compilation (rather than hard-wire)
- Feedback loop allows to adjust to variable gap
- Speedup claimed for MAXCUT (Farhi) then quantum-inspired algorithm with same complexity appeared (Hastings)



Needs: Reasonable qubits, fast I-O and low-latency Reprogramming



WHERE CAN SPEEDUP (NOT) COME FROM?

A physical argument

Exponential speedup on general NP-hard combinatorical optimization problems extremely unlikely (viz: Optimality of Grover)

A lot of heuristics and empiricism

Our goal: Get a good solution for cost fuctional with high probability - why should that work?

Note: Other quantum algorithms (Shor, Grover) contain uncomputing of superpositions for that purpose

So - under which conditions does the state converge onto a narrow distribution, centered at low values?

Our statement is: Often this has to do with classical simulability



QAOA AS A DISCRETE PATH INTEGRAL

Start: Hadamard State - all at once Give all of them a phase factor





Mix-Phase etc.

Continuous path integral: Compute time evolution in space

$$\mathcal{U}(x_i, x_f) = \sum_{x_1} \lim_{\delta t \to 0} \left\langle x_i \left| e^{-i\delta t E_{kin}} \left| x_1 \right\rangle \left\langle x_1 \right| e^{-i\delta t E_{pot}} \cdots \left| x_f \right\rangle \right. = \int_{x_i}^{x_f} \mathcal{D}x(t) e^{iS[x(t), \dot{x}(t)]}$$

Path integral = sum over all paths, each with their phase factor

Aha: Kinetic energy similar to driver / mixer - potential energy similar to problem Hamiltonian - can we access path integral methods?

Analogy even closer for AQC with arbitrary annealing schedule



SEMICLASSICS

Emergence of a particle-like theory from a wave-like theory

We can do a lot of optics without waves - a lot of mechanics without quanta - classical / particle limit

Those are driven by variational principles for wavepackets

Optics: Fermat principle - Light ray maximizes the total time $t = \int \frac{ds}{c}$

Mechanics: Newtons equation follow from the stationary action $\delta S = 0$



 $\int_{x_i}^{x_f} \mathscr{D}x(t) e^{iS[x(t),\dot{x}(t)]}$

Dominated by $\delta S = 0$ - else oscillatory integrand

Semiclassics: Take $\delta^2 S$ into account



WHAT CAN WE DO FOR QAOA / AQC

Main ingredient: Qubits / spins instead of scalar waves

Mean field theory (in real time):
$$H_p = \sum_i h_i Z_i + \sum_{i < j} J_{ij} Z_i Z_j$$
 replaced by $H_{MF} = \sum_i h_{i,mf} Z_i$ with self-consistent field $h_{i,mf} = h_i + \frac{1}{2} \sum_{j \neq i} J_{ij} \langle Z_j \rangle$

Know in equilibrium thermodynamics: Works well in high (graph) dimension Keeps two real coordinates for qubit state, keeps some correlation, throws away entanglement



Mean-field AOA

Hamiltonian with the SU(2) Poisson bracket for classical spins •

$$H(n) = -\gamma(t) \sum_{i < j}^{N} J_{ij} n_z^{(i)} n_z^{(j)} - \beta(t) \sum_{j=1}^{N} n_x^{(j)}, \quad \left\{ n_a^{(i)}, n_b^{(j)} \right\} = \delta^{ij} \varepsilon_{abc} n_c^{(i)}$$



Initial state:

$$\overrightarrow{n}^{(i)} = (1, 0, 0)$$
 for all

spins Classical (~mean-field) evolution, ٠

$$\frac{d}{dt} n_a^{(k)}(t) = \left\{ n_a^{(k)}(t), H \right\}$$

can be solved *exactly* using **Trotterization scheme**



Mean-field AOA

• The Bloch vectors evolve according to $\overrightarrow{n}^{(i)}(j) = \prod_{k=1}^{n} \stackrel{\wedge}{V}_{D}(k) \stackrel{\wedge}{V}_{P}(k) \stackrel{\wedge}{n}^{(i)}(0)$

where

$$\hat{V}_{D} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(2\beta(k)) & \sin(2\beta(k)) \\ 0 & -\sin(2\beta(k)) & \cos(2\beta(k)) \end{pmatrix} - \text{driver matrix}$$

$$\hat{V}_{P} = \begin{pmatrix} \cos(2\gamma(k)m_{i}(k)) & \sin(2\gamma(k)m_{i}(k)) & 0 \\ -\sin(2\gamma(k)m_{i}(k)) & \cos(2\gamma(k)m_{i}(k)) & 0 \\ 0 & 0 & 1 \end{pmatrix} - \text{problem matrix}$$

$$m(k) = \sum_{i=1}^{n} L_{i} r_{i}^{(j)}(k) + k$$

 $m_i(k) = \sum_j J_{ij} n_3^{(s)}(k) + h_i$ - mean-field at discrete time k

Note: only the problem matrix depends on the mean-field m(k)

• Total time scales as $\sim pN^2$, $p \gg 1$

Sherrington-Kirkpatrick model

$$H_P = -\sum_{i < j}^N J_{ij} \sigma_z^{(i)} \sigma_z^{(j)}, \quad \left\langle J_{ij}^2 \right\rangle = 1/N$$

i.i.d. random Gaussian

Parisi'79:

$$\lim_{N \to \infty} \left\langle E_0 / N \right\rangle_J = -0.763166...$$

• results from spin-glass replica symmetry breaking theory



Bencmarking of QAOA for SK-model



• QAOA is not able to achieve Parisi's result at finite p

Large-N scaling



M. Palassini' 2003, $\omega \approx 2/3 = 0.666...$

Fluctuations of E_0 (MF-AOA vs. exact)

- Hybrid of genetic algorithm (GA) & local optimization
- Mean-field AOA outperforms QAOA on average at large N



- Exponentially small gaps are due to MBL physics (~ NP hardness)
- The 1st gap at Γ_c is polynomial in N

ANALYZING FLUCTUATIONS

Judging the quality of MF-AOA

- MF-AOA=stationary action path
- Leading correction is of second order $\delta^2 S$ Gaussian path integral $\int_{x_i}^{x_f} \mathscr{D}x(t) e^{iS[x(t),\dot{x}(t)]} \simeq e^{iS_{cl}} \int \mathscr{D}\delta x(t) e^{-\delta xK\delta x} \quad \delta x = x - x_{cl}$
- Here coded via spins quadratic correction to the action

$$\mathcal{S}[\eta,\bar{\eta}] = \frac{i}{2} \int_0^t (\bar{\eta},\eta) \begin{bmatrix} -i\partial_t + \hat{A} & \hat{B} \\ \hat{B}^{\dagger} & i\partial_t + \hat{A}^* \end{bmatrix} \begin{pmatrix} \eta \\ \bar{\eta} \end{pmatrix}$$

- Eigenmode analysis of this Dirac-type equation steep or flat landscape / encoded as Lyapunov exponents
- Fluctuations = paramagnons







Spectrum of Lyapunov exponents

easy instance hard instance Fluctuations: N = 11Exact $\langle |\eta_i(t)|^2 \rangle \sim \frac{1}{N} e^{2\lambda_0(t)}$ E_0 Mean-field maximal exponent Ξ • 2nd peak: ergodic-to-MBL transition 1.0 $\stackrel{\sim}{\prec} 0.5$ 0.00.50.51.0 0.0 1.00.0ss

SIMULATING STRONGLY CORRELATED ELECTRONS



1. Motivation (i) Electronic correlation is captured in the Fermi-Hubbard model

Fermi-Hubbard model



Orbitals	Byte	
2	64B	
4	256B	
8	4MB	
36	1TB	
49	9PB	



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1. Motivation (iii)

Green's function gives access to phase space

Δ



Selection of observables

- Average particle density $\langle n_{i,\sigma} \rangle$
- Superconducting gap
- Density of states $N(\omega)$
- Cooper pair coherence length ξ

Requires exact Green's function, e. g. via Variational Cluster Approach (VCA)

Variational Cluster Approach





1. Motivation (ii) Introducing the single-particle (retarded) Green's function

Retarded single-particle Green's function

$$\begin{aligned} G_{ij}^{R} &= \theta(\tau) [G_{ij}^{<}(\tau) - G_{ij}^{>}(\tau)] \\ G_{ij}^{<}(\tau) &= -i \langle \Psi | e^{iH\tau} c_{i} e^{-iH\tau} c_{j}^{\dagger} | \Psi \rangle \\ G_{ij}^{>}(\tau) &= i \langle \Psi | c_{j}^{\dagger} e^{iH\tau} c_{i} e^{-iH\tau} | \Psi \rangle \end{aligned}$$



Linear response Green's function





3. Toy model: Two-site dimer (i) Course of action



Forschungszentrum

3. Two-site dimer (ii)

Ground state preparation via Variational Hamiltonian Ansatz





4. Results





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USING ALL DEGREES OF FREEDOM

Resonators are easy to add to superconducting procesors

Add extra resonators ... coherent, easy to make, high-dimensional: What can they do?



Martinis Group 2012 (!)



Current plan at FZJ















Electronic correlation captured in Fermi-Hubbard model Solve FH by means of many-body Green's function, build from singleparticle Green's function

Directly measure the correlators within the Green's function

Apply error mitigation to results Extrapolate to larger system sizes via VCA



PHONONIC MODELS

Hubbard Holstein and friends



Qubit encodings

	Unary	Binary
Complexity for N levels	N qubits	Log N qubits
Number of qubits required	High	Low
CNOT overhead	Low	High



A GATE ON THE MODE



Jaynes-Cummings Hamiltonian:



Coupling Terms: Hubbard Holstein





Coupling Terms (2): generalised hopping

$$\hat{H}_{\rm XY} = g \sum_{i \neq j,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}^{}_{j,\sigma} \right) \left(\hat{a}^{\dagger} + \hat{a} \right)$$



The Variational Hamiltonian Ansatz

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$$\begin{split} \mathsf{A}(\boldsymbol{\theta}) &= \hat{D}\left(\boldsymbol{\phi}\right) \prod_{i,\sigma}^{N-1} \mathsf{Y} \mathsf{Y}_{i,\sigma}(v_{i,\sigma}) \mathsf{X} \mathsf{X}_{i,\sigma}(v_{i,\sigma}) \hat{U}_{\Theta}^{i,\sigma;i+1,\sigma}(\gamma_{i,\sigma}) \\ &\times \prod_{i=1}^{N} \mathsf{Z} \mathsf{Z}_{i}(u_{i}) \prod_{\sigma} \hat{U}_{\Theta}^{i,\sigma}(\zeta_{i,\sigma}) R_{z}(2\epsilon_{i,\sigma}) \end{split}$$

Displacement operator

$$\hat{D}(\alpha) = e^{\alpha \hat{a}^{\dagger} - \alpha^* \hat{a}}$$



SUPERRADIANCE WITH INTERACTIONS

Ising Dicke model





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Approximation of the superradiant state via quench





Density matrix and Wigner functions after the quench



Quantum circuit

Qubit-boson architecture



 flux-tunable transmons (Q) and couplers (C), capacitively coupled to resonators (R)

Simulation protocol for quench dynamics

• evolution operator for Ising-Dicke Hamiltonian

$$\tilde{S}_{\rm ID}(t_p) = \prod_{k=0}^{p-1} e^{-i\tau H_Z} e^{-i\tau H_{ZZ}} \tilde{S}_D(t_k + \tau, t_k), \qquad t_k = k\tau$$

- Dicke Hamiltonian gate $\tilde{S}_D(t+\tau,t) = \text{SWAP}^{(12)}\tilde{S}_R^{(1)}(t+\tau,t+\tau/2)\text{SWAP}^{(12)}\tilde{S}_R^{(1)}(t+\tau/2,t)$
- Rabi Hamiltonian gate $\tilde{S}_R(t+\tau,t) = \tilde{S}_{
 m JC}(\theta/2,t+\tau)\sigma_x\tilde{S}_{
 m JC}(\theta,t+\tau/2)\sigma_x\tilde{S}_{
 m JC}(\theta/2,t)$
- · Janes-Cummings gate $S_{\rm JC}(\theta, t) = e^{-ih_z t} e^{-i\theta(\sigma a + \sigma a)} e^{ih_z t}, \theta = \tau g$

Quantum circuit

Quantum gates





CONCLUSIONS

- Mean Field AOA often a good proxy for QAOA
- Green's function measurement physics inspired method to simulate manybody systems
- If your experimental colleague gives you resonators ... simulate Bosons

Misra-Spieldenner et al., PRX Quantum 4, 030335 G. Bishop, D. Bagrets, FKW, arXiv:2310.10412

