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Department of Physics and Astronomy

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Creating Materials & Energy Solutions

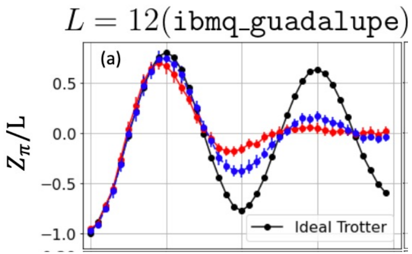
U.S. DEPARTMENT OF ENERGY

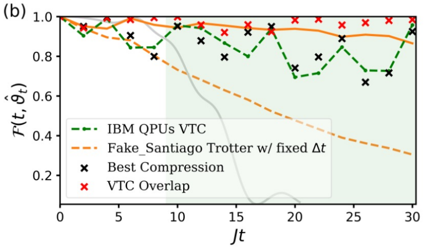
The Future of Computation: Unleashing the Power of Quantum Computers

Peter P. Orth (Iowa State University & Ames Laboratory)

Collaboration with Josh Aftergood, Noah Berthusen, I-Chi Chen, Joao Getelina, Niladri Gomes, Kai-Ming Ho, Thomas Iadecola, Anirban Mukherjee, Cai-Zhuang Wang, Yongxin Yao, Feng Zhang (Iowa State University & Ames Laboratory)

Physics Colloquium, MSU Mankato, April 11, 2022





References:

- I.-C. Chen et al., arXiv:2203.08291 (2022)
- N. Berthusen et al. arXiv:2112.12654 (2021)
- N. Gomes *et al.*, Adv. Qu. Tech. 2100114 (2021)
- Y. Yao *et al.*, PRX Quantum **2**, 030307 (2021)

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SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

What is a quantum computer?

A quantum computer is a programmable computing device that works according to the fundamental physical laws of quantum mechanics.

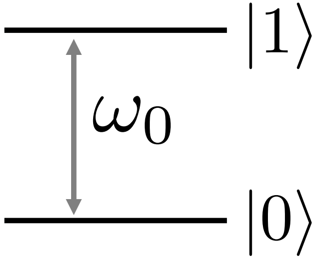
Properties of a digital quantum computer

- Contains **qubits** = quantum mechanical 2-level systems = Spin-1/2
  - Sounds similar to a classical bit {0, 1}, but is a totally different beast
  - Can be in a **superposition** of two basis states |0> and |1>

Hamiltonian of a qubit

$$H = -\omega_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

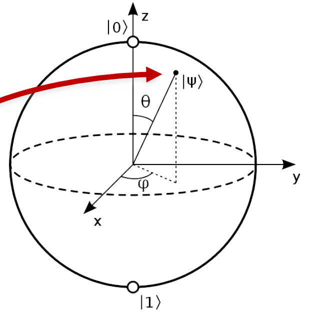
Pauli-Z operator



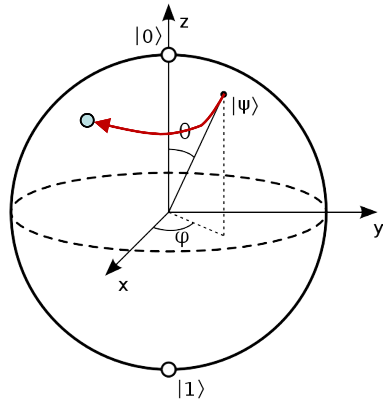
General state of a qubit

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

Bloch sphere



Quantum gate operations



Properties of a digital quantum computer

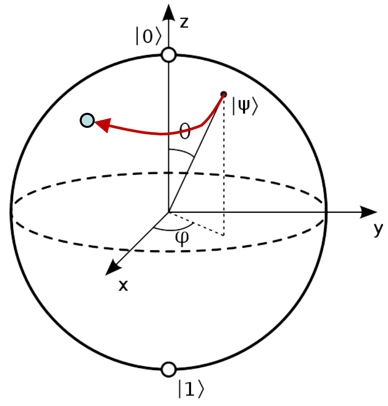
- Contains qubits = quantum mechanical 2-level systems
- **Quantum gate operations** act on qubits and change their states
  - Sounds similar to classical gates {NOT, OR, …}, but must be reversible
  - Single-qubit gates is unitary 2x2 matrix [SU(2)] = Rotations on Bloch sphere

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Longrightarrow X|0\rangle = |1\rangle, X|1\rangle = |0\rangle$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \Longrightarrow \begin{aligned} H|0\rangle &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ H|1\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{aligned}$$

- X gate flips qubit. Acts like a NOT gate.
- H: generates superposition (Hadamard gate).

Multi-qubit gates and entanglement



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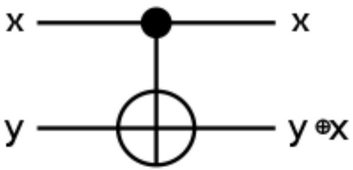
  - Sounds similar to classical gates {NOT, OR, …}, but must be reversible
  - Single-qubit gates is unitary 2x2 matrix [SU(2)] = Rotations on Bloch sphere
  - Multi-qubit gates are unitary rotations in $SU(2^N)$

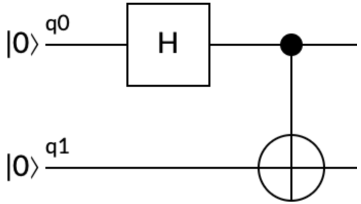
Controlled-NOT (CNOT)



$$\mathrm{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

CNOT creates entanglement

Quantum circuit (Bell pair)

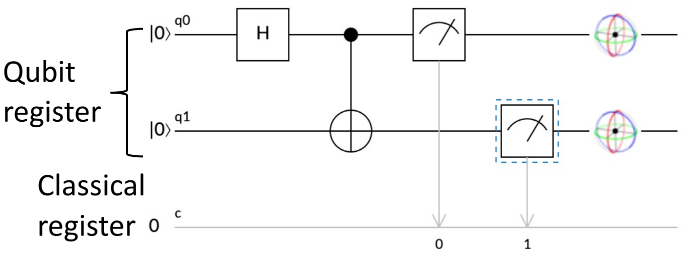


- Non-local quantum correlations
- Cannot be written as $|\psi_1\rangle \otimes |\psi_2\rangle$

$$|00\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Measurement of qubits

Quantum circuit (Bell pair)



Properties of a digital quantum computer

- Contains qubits = quantum mechanical 2-level systems
- Quantum gate operations act on qubits and change their states
- **Quantum state is transformed to classical information by measurements**
  - Choose a basis in which to measure (usually Pauli-Z)
  - Measurement outcomes are operator eigenvalues: +1,-1 for Pauli-Z
  - Measurement outcome is probabilistic (Born rule)

2^10 = 1024:	{'11': 501, '00': 523}
2^12 = 4096:	{'11': 2035, '00': 2061}
2^14:	{'11': 8154, '00': 8230}
2^16:	{'11': 32773, '00': 32763}

Outcomes for different number of measurements

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Measurement probabilities

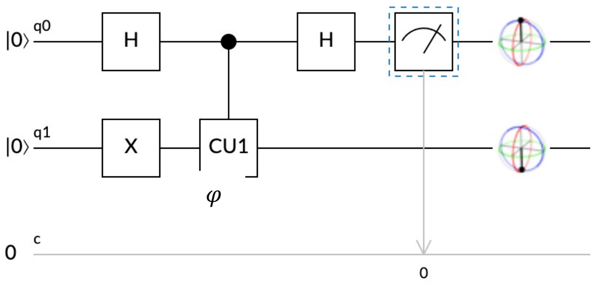
$$|\langle 00|\psi\rangle|^2 = |\langle 11|\psi\rangle|^2 = 1/2$$

$$|\langle 10|\psi\rangle|^2 = |\langle 01|\psi\rangle|^2 = 0$$

- One of four bitstrings is measured each time
- Probability given by quantum wavefunction
- Infer that by repeated measurements (build histogram of #(observed bitstrings)

Interference in quantum circuits

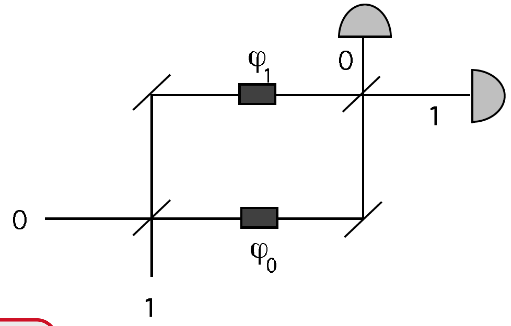
Quantum circuit (interference):



Controlled-Z phase gate

$$\mathrm{CU1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\varphi} \end{pmatrix}$$

Corresponding light interferometer (Mach-Zehnder)



$$|00\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + e^{i\varphi}|1\rangle)|1\rangle$$

$$\rightarrow \frac{1}{\sqrt{2}}(\cos\frac{\varphi}{2}|0\rangle - i\sin\frac{\varphi}{2}|1\rangle)|1\rangle$$

Interference of different circuit paths

- Outcome depends on phase difference φ along two paths
  - Qubit q0 in state |0> for φ=0,
  - Qubit q0 in state |1> for $\varphi=\pi$

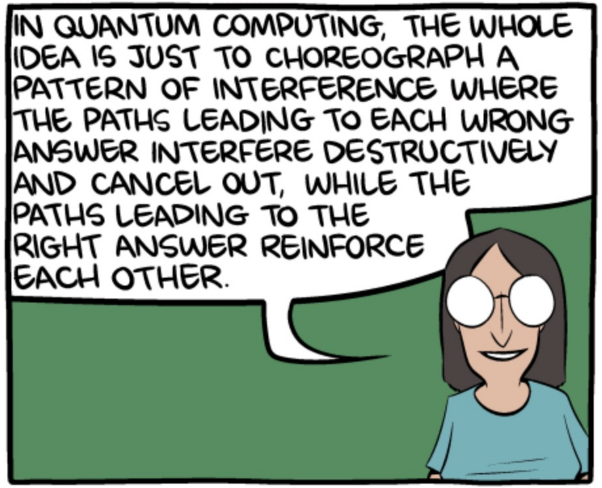
- Hadamard gate H acts as semi-transparent mirror
- Qubit q0 stores information about phase evolution of qubit q1
- Qubit q1 acts as state dependent phase delay

Quantum versus classical computer

Most important differences between classical and quantum computer

- QC can be in a superposition of bit states
- QC exhibits interference of different circuit paths, analogous to waves or light
- QC exhibits entanglement and thus non-local effects
- QC intrinsically probabilistic
- QC more powerful for certain tasks: factoring, searching, quantum simulation,…

Figure by C. Addams (NYT)



www.scottaaronson.com/blog, smbc-comics.com

How does a quantum computer look like?

Various implementation platforms are being built. Too early to tell which ones succeed.

DiVincenzo criteria for scalable quantum computer

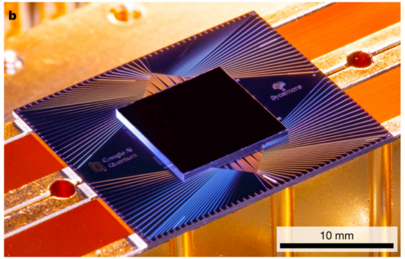
> Well-characterized qubits, scalability to large systems

> Ability to initialize state & perform “universal” set of gate operations

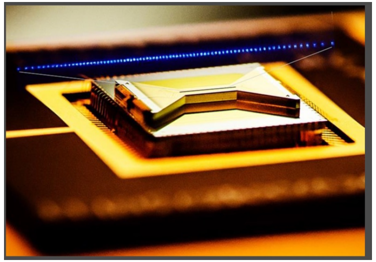
> Long lifetime of quantum state >> gate operation

> Measurement capability with high fidelity

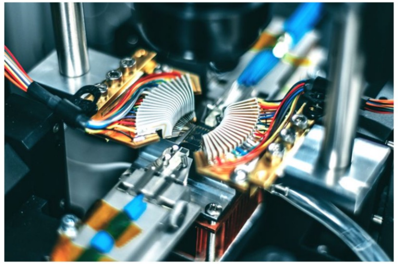
& others (neutral atoms, bosonic processors, …)



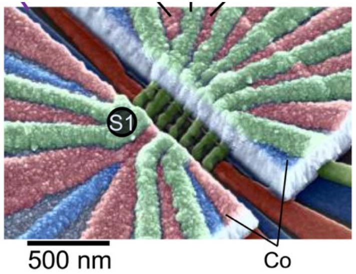
Superconducting qubits (Yale, UCSB, ETH, IBM, Google, Rigetti, Intel…)



Trapped ions (NIST, Innsbruck, IonQ, Honeywell, …)



Photonic QC (Xanadu, PsiQ, QuiX, …)

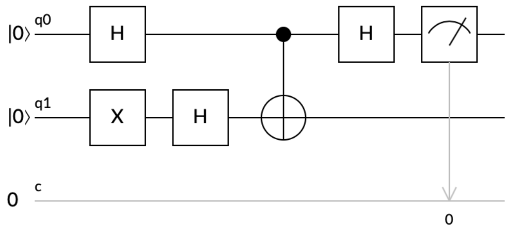


Silicon spin qubits (Princeton, New South Wales, SQC, …)

Implement quantum circuits and run using quantum cloud services

Different quantum programming frameworks are available

- IBM Qiskit, Circ (Google), PyQuil (Rigetti), Q# (Microsoft): syntax similar to Python
- Quantum Programming Studio (QPS): easy drag&drop circuits
- Many open quantum software projects: Unitary Fund, Qiskit, OpenFermion, Circ, Quest, Yao, …
- Run quantum circuits using quantum simulators (incl. noise models) and/or on IBM hardware

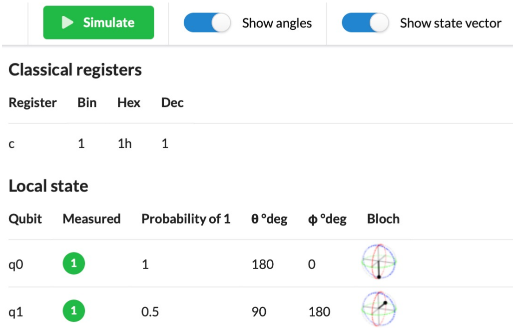


State vector

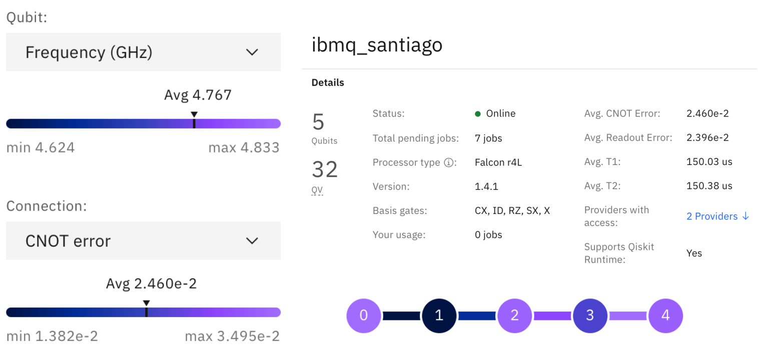
```
0.70710678+0.00000000i|10>     50.00000%
-0.70710678+0.00000000i|11>    50.00000%
```

Export circuits to Circ, Qiskit, PyQuil, …

From Quantum Programming Studio



From IBM Quantum Experience



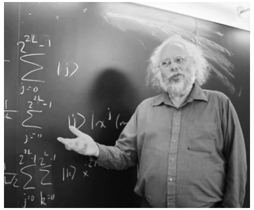
What can you do with a quantum computer?

Quantum computers promise dramatic speedups over classical computers for certain tasks. New computing paradigm!

Longer term applications

- Factoring integers using Shor's algorithm: break public-key RSA encryption
- Speed-up searches of unstructured databases using Grover's algorithm
- Simulate quantum dynamics: protein folding, molecular dynamics, chemical reactions, …

Codebreaking is a lot faster with this one…



Peter Shor (from dotquantum.io)

Deutsch-Josza algorithm (example of exponential speedup):

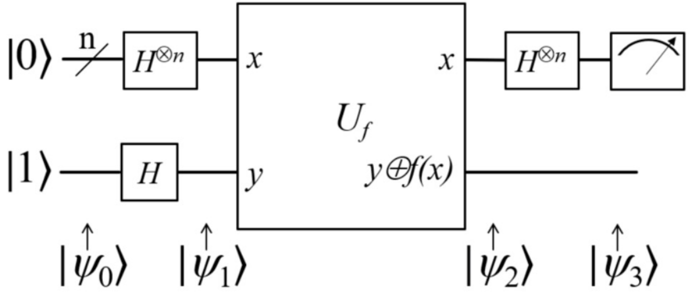
Task: A black box U_f performs transformation $|x\rangle|y\rangle \rightarrow |x\rangle|y \oplus f(x)\rangle$ with $x \in \{0,1\}^n$ and $f(x) \in \{0,1\}$. It is promised that $f(x)$ is either constant or balanced (= 1 for half of all x and zero otherwise). Is $f(x)$ constant or balanced?

Deutsch-Josza algorithm

Task: A black box U_f performs transformation $|x\rangle|y\rangle \to |x\rangle|y \oplus f(x)\rangle$ with $x \in \{0,1\}^n$ and $f(x) \in \{0,1\}$.

It is promised that $f(x)$ is either constant or balanced (= 1 for half of all x and zero otherwise).

Determine whether $f(x)$ is constant or balanced?



Example for $n = 1$:

$$|\psi_0\rangle = |01\rangle \longrightarrow |\psi_1\rangle = \frac{1}{2}\Big[|0\rangle + |1\rangle\Big]\Big[|0\rangle - |1\rangle\Big]$$

$$|\psi_2\rangle = \frac{1}{2}\Big((-1)^{f(0)}|0\rangle + (-1)^{f(1)}|1\rangle\Big)\Big(|0\rangle - |1\rangle\Big) =$$

$$= \begin{cases} \pm\frac{1}{2}\Big(|0\rangle + |1\rangle\Big)\Big(|0\rangle - |1\rangle\Big) & \text{if } f(0) = f(1) \\ \pm\frac{1}{2}\Big(|0\rangle - |1\rangle\Big)\Big(|0\rangle - |1\rangle\Big) & \text{if } f(0) \neq f(1) \end{cases}$$

$$|\psi_3\rangle = \begin{cases} \pm|0\rangle\Big(|0\rangle - |1\rangle\Big) & \text{if } f(0) = f(1) \\ \pm|1\rangle\Big(|0\rangle - |1\rangle\Big) & \text{if } f(0) \neq f(1) \end{cases}$$

We used that:

$$U_f|x\rangle(|0\rangle - |1\rangle) = (-1)^{f(x)}|x\rangle(|0\rangle - |1\rangle)$$

One function call instead of two.

For n qubits:

- Classically need $2^{n-1} + 1$ calls
- Quantum: only one function call
- Exponential speedup

Simulating nature using quantum computers

- R. Feynman: “Nature isn't classical, dammit, and if you want to make a simulation of Nature, you'd better make it quantum mechanical.”
- Hilbert space dimension grows exponentially with the number of particles: $N = 2^n$
- Example: $n = 1000 \;\rightarrow N = \; 2^n = 10^{300} \;\gg$ number of baryons in the universe 10^{80}
- Cannot even store wavefunction, but QC can create it!

Idea: Prepare wavefunction on QC using gates and measure its properties

- Find ground state energy of an interacting Hamiltonian H
- Algorithm: Prepare non-interacting initial state and slowly turn on interactions

$$H(t) = H_0 + tH_{\text{int}}, 0 \leq t \leq 1$$

Richard Feynman

Noisy intermediate-scale quantum computing (NISQ) era

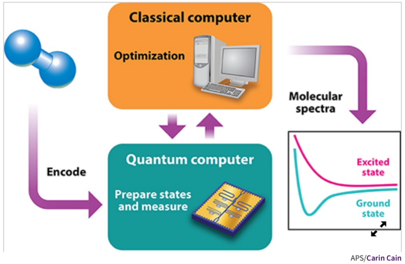
Google's Sycamore QPU

Important caveat: Current quantum computers are too noisy to allow for quantum error correction. Intermediate = 10 – 100s of qubits.

- Without error correction, errors accumulate over time and the maximal gate depth is limited

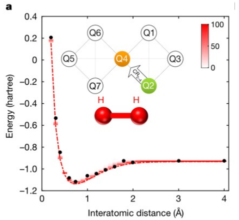
Near-term applications:

- Generate truly random numbers by sampling from a random wavefunction
- Hybrid quantum-classical algorithms using parametrized quantum circuits
  - Optimization problems
  - Optimize cost function in variational state
  - Very general!



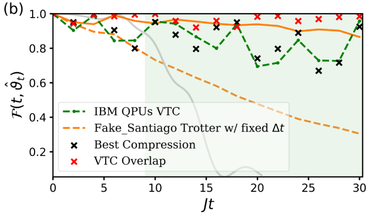
Sim, Alán Aspuru-Guzik et al., Physics Viewpoint (2018).

Ground state preparation



Kandala et al (IBM) (2017)

Quantum dynamics (this talk!)



Berthusen, PPO et al. (2022)

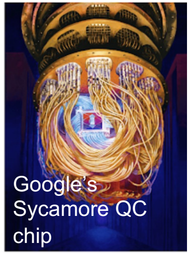
Quantum advantage

Quantum Advantage: perform tasks (of practical relevance) with controlled quantum systems going beyond what can be currently achieved with classical digital computers.

- Google announced quantum advantage (or supremacy) in 2019: Performed calculation on "Sycamore" chip in 200 sec that Googles estimated would take 10'000 years on classical hardware
- Led to classical algorithmic development that showed it can be done (potentially) much faster
- Take-away: Google's calculation was important proof-of-principle (similar to Wright flyer)

Wright Flyer

Seconds into the first airplane flight, near Kitty Hawk, North Carolina; December 17, 1903, Photo first published in 1908

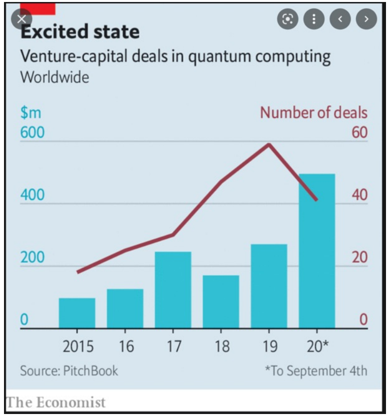


Most likely need quantum error correction for full quantum advantage!!!

But let's do the research!

Quantum gold rush (before quantum winter?)

Progress in quantum technology has spurred large investments & a lot of industry activity.



https://www.indeed.com › q-Quantum-Computing-jobs

Quantum Computing jobs - Indeed

4342 **Quantum Computing** jobs available on **Indeed**.com. Apply to Software Engineer, Researcher, Scientist and more!

- Many job opportunities
- Both hardware & software development
- Both large companies and startups

Quantum dynamics simulations

- I-Chi Chen, Benjamin Burdick, Yongxin Yao, PPO, Thomas Iadecola
  Error-Mitigated Simulation of Quantum Many-Body Scars on Quantum Computers with Pulse-Level Control
  arXiv:2203.08291 (2022).
- Noah F. Berthusen, Thaís V. Trevisan, Thomas Iadecola, PPO
  Quantum dynamics simulations beyond the coherence time on NISQ hardware by variational Trotter compression
  arXiv:2112.12654 (2021).
- Yong-Xin Yao, Niladri Gomes, Feng Zhang, Thomas Iadecola, Cai-Zhuang Wang, Kai-Ming Ho, PPO
  Adaptive Variational Quantum Dynamics Simulations
  Phys. Rev. X Quantum **2**, 030307 (2021).

Quantum dynamics simulations

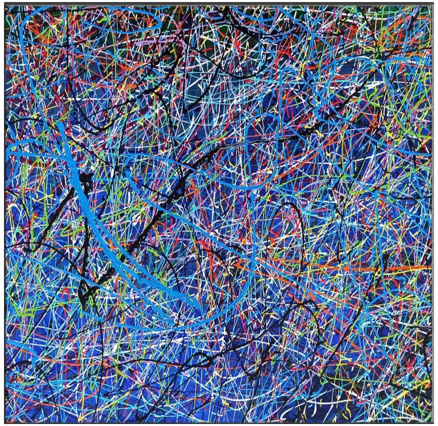
Initial state

$$|\Psi(0)\rangle = \sum_n c_n |n\rangle$$

Energy eigenstate of many-body H

Dynamics

$$|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t} |n\rangle$$



Dynamics of an observable O

$$\langle \mathcal{O}(t) \rangle = \sum_{n,m} c_n c_m^* e^{i(E_m - E_n)t} \langle m|\mathcal{O}|n\rangle$$

- Classically hard due to rapid growth of entanglement in nonequilibrium for generic H
- Reason: contains highly excited states ➢ Volume-law entanglement entropy

Entanglement = complexity of classical calculation

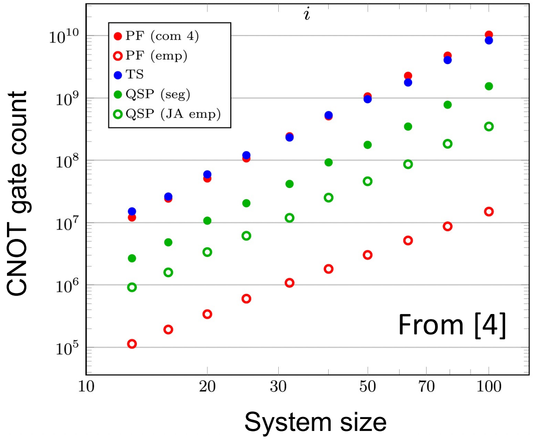
Exponential growth of classical resources like the bond dimension in tensor networks

Opportunity for quantum computing

Overview of quantum algorithms for dynamics simulations

- > Lie-Suzuki-Trotter Product formulas (PF)
  - > Simple yet limited to early times for current hardware noise
  - > Trotter circuit depth scales as $\mathcal{O}(t^{1+1/k})$ ☞ fixed t_{max}
- > Algorithms with best asymptotic scaling have significant overhead
  - > Linear combination of unitaries (TS) [1], quantum walk methods [2], quantum signal processing (QSP) [3]
- > Hybrid quantum-classical variational methods [5, 6]
  - > Work with fixed gate depth ☞ ideally tailored for NISQ hardware
  - > Trading gate depth for doing many QPU measurements

$$H = J\sum_i (Z_i Z_{i+1} + h_i Z_i)$$



Variational Dynamics Simulations

$$|\Psi[\boldsymbol{\theta}]\rangle = \prod_{\mu=0}^{N_{\boldsymbol{\theta}}-1} e^{-i\theta_\mu \hat{A}_\mu} |\Psi_0\rangle$$

E.g. MacLachlan principle [5, 6]

$$\sum_\nu M_{\mu\nu}\dot{\theta}_\nu = V_\mu .$$

[1] Berry et al. (2015); [2] Childs (2004); [3] Low, Chuang (2017); [4] Childs et al., PNAS (2018);
[5] Li, Benjamin, Endo, Yuan (2019); Y. Yao, PPO, T. Iadecola *et al.* (2021).

Overview of quantum algorithms for dynamics simulations

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In this talk:
- **Trotter dynamics**
- **Variational MacLachlan approach**
- **Combine simplicity of Trotter product with a variational approach to simulate for long times.**

Demonstrate full algorithm on IBM hardware [6].

[1] Berry et al. (2015); [2] Childs (2004); [3] Low, Chuang (2017); [4] Childs et al., PNAS (2018); [5] Li, Benjamin, Endo, Yuan (2019); Y. Yao, PPO, T. Iadecola *et al.* (2021); [6] Berthusen, Trevisan, Iadecola, PPO (2021).

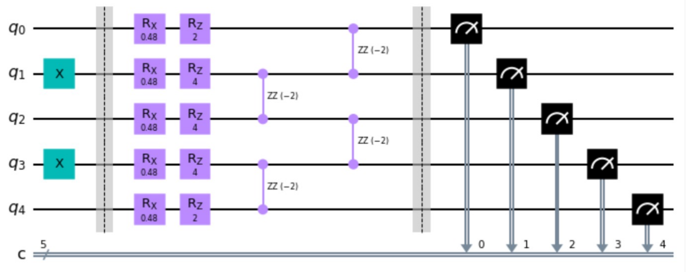
Trotter product formula simulations of quantum dynamics

- Decompose Hamiltonian into sum of terms that include commuting operators $H = H_{\text{even}} + H_{\text{odd}}$

$$H_{\text{even}} = \frac{J}{4}\sum_{i\,\text{even}}(X_iX_{i+1} + Y_iY_{i+1} + Z_iZ_{i+1}) \quad \text{and} \quad H_{\text{odd}} = \frac{J}{4}\sum_{i\,\text{odd}}(X_iX_{i+1} + Y_iY_{i+1} + Z_iZ_{i+1})$$

- 1st order Trotter product formula

$$\left[e^{-i(H_{\text{even}}+H_{\text{odd}})\frac{t}{N}}\right]^N = \prod_{\alpha=1}^{N}\left[e^{-iH_{\text{even}}\frac{t}{N}}e^{-iH_{\text{odd}}\frac{t}{N}} + \mathcal{O}(t^2/N^2)\right]$$



Trotter step size

$\tau = t/N$

Must be chosen small ➢ deep circuits

Can be easily implemented as product of two-qubit unitaries

➡ While product formulas are straightforward to implement, they result in **deep circuits for long and precise simulations**

Lloyd (1996)

NISQ Trotter simulations of mixed field Ising model

- Benchmark Trotter simulations on current NISQ hardware

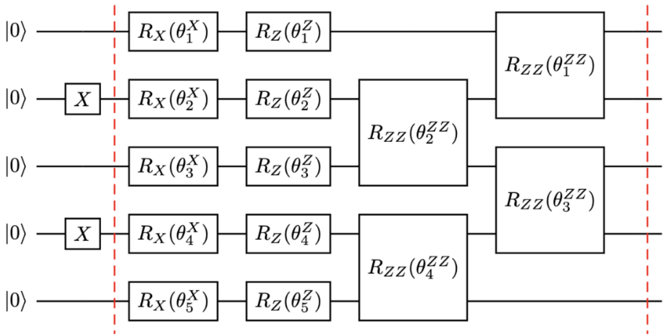
Mixed-field Ising model: $$H = \frac{V}{4}\sum_{i=1}^{L-1} Z_i Z_{i+1} + \frac{V}{2}\sum_{i=2}^{L-1} Z_i + \frac{V}{4}(Z_1 + Z_L) + \Omega \sum_{i=1}^{L} X_i$$

Displays many-body coherent dynamics for $V \gg \Omega$

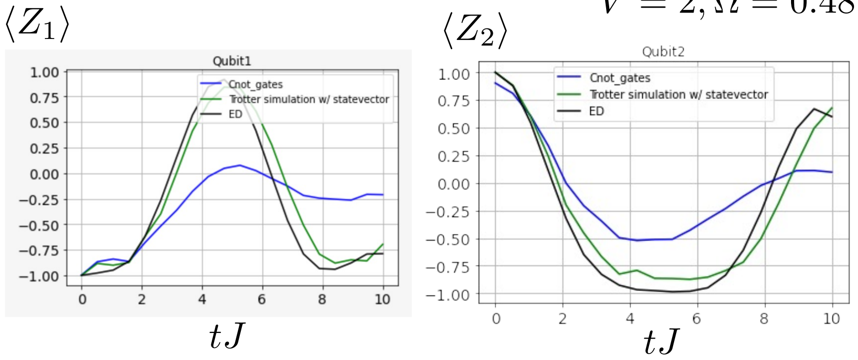
Bernien, Lukin (2017)

- Naïve Trotter simulation limited to $t \approx 1/J$ due to finite coherence time on device

$V = 2, \Omega = 0.48$



One step of Trotter circuit in L=5 system, starting from Neel state.



Trotter simulation on IBM Nairobi QPU

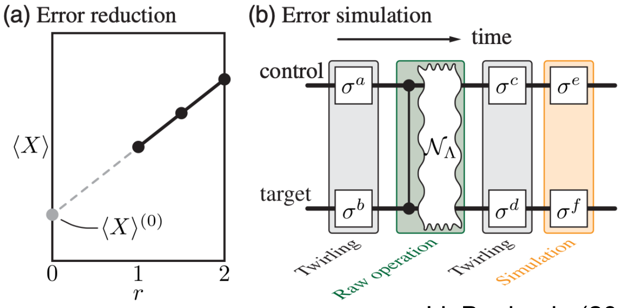
Use pulse level control and error mitigation strategies to extend simulation time

Pulse level control and error mitigation

- Pulse level control allows to make optimal use of finite coherence time on device
  - Direct implementation of R_{zz} gate via cross-resonance pulse ➢ shortens program by about half
- Error mitigation is key to extend final time of simulation
  - Zero-noise extrapolation (Mitiq) + Pauli twirling: $G \mapsto GG^\dagger G.$
  - Readout error mitigation (tensor product assumption):

$$C_{\text{ideal}} = M^{-1} C_{\text{noisy}}. \qquad M = \begin{bmatrix} 1-\epsilon_1 & \eta_1 \\ \epsilon_1 & 1-\eta_1 \end{bmatrix} \otimes \cdots$$

  - Symmetry-based postselection (tailored to specific model)
  - Dynamical decoupling: apply $X(\pi)$ and $X(-\pi)$ during qubit idle time



Li, Benjamin (2017)

Pauli twirling converts noise to stochastic form
➢ justification for ZNE

$$\mathcal{N}_\Lambda \rho = \sum_h E_h \rho E_h^\dagger$$

Kraus form

$$E_h = \sum_{a=0}^{3} \sum_{b=0}^{3} \alpha_{h;a,b} \sigma_c^a \sigma_t^b$$

$$\bar{\mathcal{N}}_\Lambda = F_\Lambda[\mathbb{1}] + \sum_{(a,b)\neq(0,0)} \epsilon_{a,b} [\sigma_c^a \sigma_t^b],$$

Qiskit Pulse

Qiskit

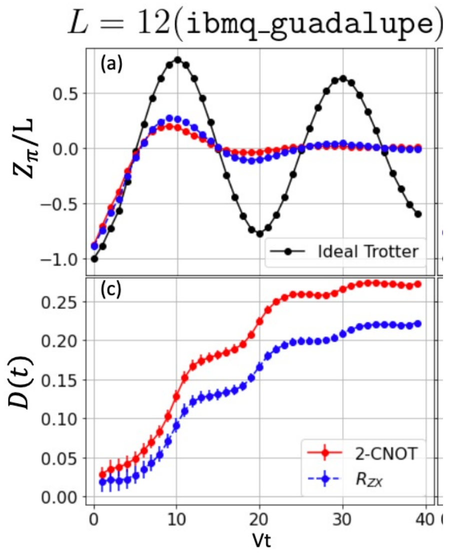
Error mitigation tools

mitiq

Pulse level control and error mitigation

Pulse and zero-noise extrapolation (ZNE) are effective strategies to reduce errors.

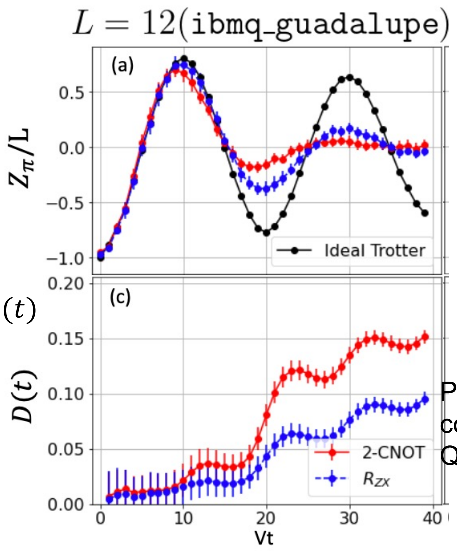
- Simulation of 12 qubits on IBM Guadelupe
- Comparison of pulse gate versus standard CNOT realization of Rzz
- Full error mitigation techniques for both

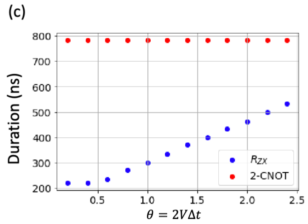


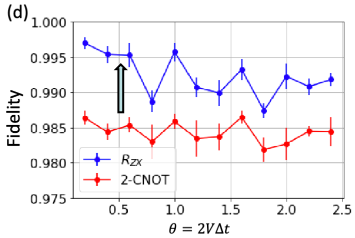
Pulse gate + error mitigation

Moving average error $D(t)$

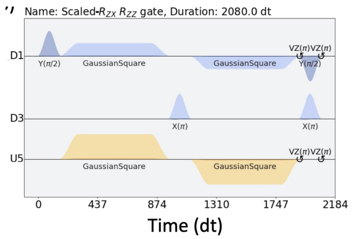
$$\frac{1}{Nt}\sum_{i=1}^{N}\int_0^t ds\left|\langle Z_{\mathrm{QPU}}\rangle - Z_{\mathrm{SV}}\right|$$







Pulse schedule control using Qiskit Pulse



$V = 0.9, \Omega = 0.6$

ZNE used linear extrapolation and scale factors {1, 1.5, 2}.

Results for 12 qubits on IBM Guadelupe

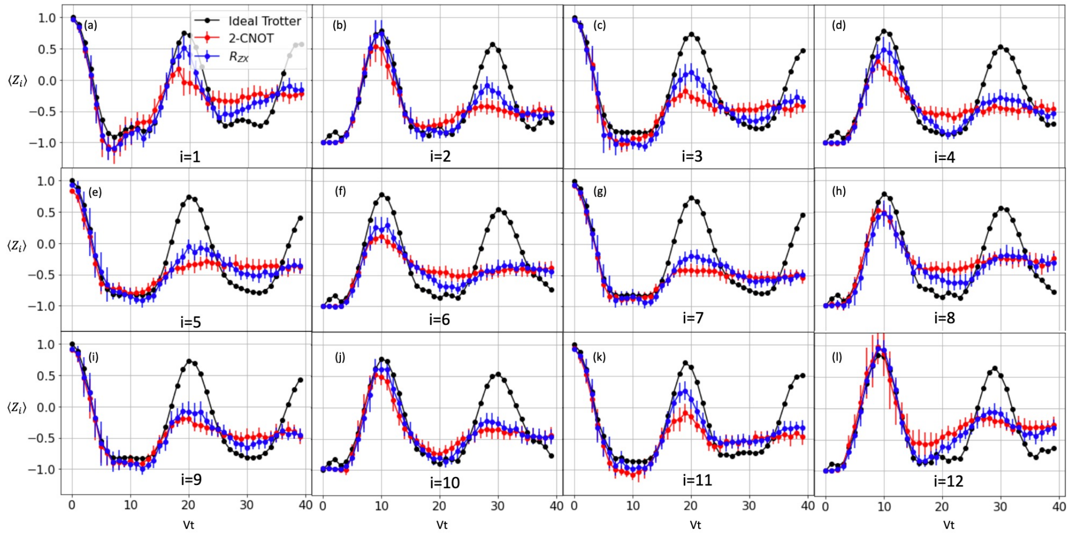


FIG. 11. Complete list of error-mitigated local magnetization results $\langle Z_i \rangle$ versus time Vt for a 12-site chain measured on **ibmq_guadalupe** using the scaled-R_{ZX} and two-CNOT implementations (blue and red, respectively). The ideal Trotter simulation data (black) are also shown for reference.

- Simulation of 12 qubits on IBM Guadelupe
- Comparison of pulse gate versus standard CNOT realization of Rzz
- Full error mitigation techniques for both
- Qubits have different quality
  - Compare i=1,2 with i=6 for example
  - Gate noise
  - Decoherence times

Custom pulse gate for R_{zz} shows advantage proportional to shortening of pulse sequence
☞ **Trotter simulations limited to early times**

$$V = 2, \Omega = 0.48$$

Quantum dynamics simulations

- I-Chi Chen, Benjamin Burdick, Yongxin Yao, PPO, Thomas Iadecola
  Error-Mitigated Simulation of Quantum Many-Body Scars on Quantum Computers with Pulse-Level Control
  arXiv:2203.08291 (2022).
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  Phys. Rev. X Quantum **2**, 030307 (2021).

Time-dependent variational quantum algorithms

Variational form of quantum state

$$|\Psi[\boldsymbol{\theta}]\rangle = \prod_{\mu=0}^{N_{\boldsymbol{\theta}}-1} e^{-i\theta_\mu \hat{A}_\mu} |\Psi_0\rangle$$

Variational parameters evolve in time

Von Neumann equation

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = -i[\mathcal{H}, \rho]$$

$$L^2 \equiv \left\| \sum_\mu \frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_\mu} \dot{\theta}_\mu - \mathcal{L}[\rho] \right\|^2$$

$$= \sum_{\mu\nu} M_{\mu\nu} \dot{\theta}_\mu \dot{\theta}_\nu - 2 \sum_\mu V_\mu \dot{\theta}_\mu + \mathrm{Tr}[\mathcal{L}[\rho]^2].$$

MacLachlan distance b/w exact and variational time evolution

Minimize L^2

M measures state change under parameter change

$$M_{\mu\nu} \equiv \mathrm{Tr}\left[\frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_\mu} \frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_\nu}\right]$$

$$V_\mu \equiv \mathrm{Tr}\left[\frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_\mu} \mathcal{L}[\rho]\right]$$

V depends on Hamiltonian

$$\sum_\nu M_{\mu\nu} \dot{\theta}_\nu = V_\mu.$$

EOM for variational parameters

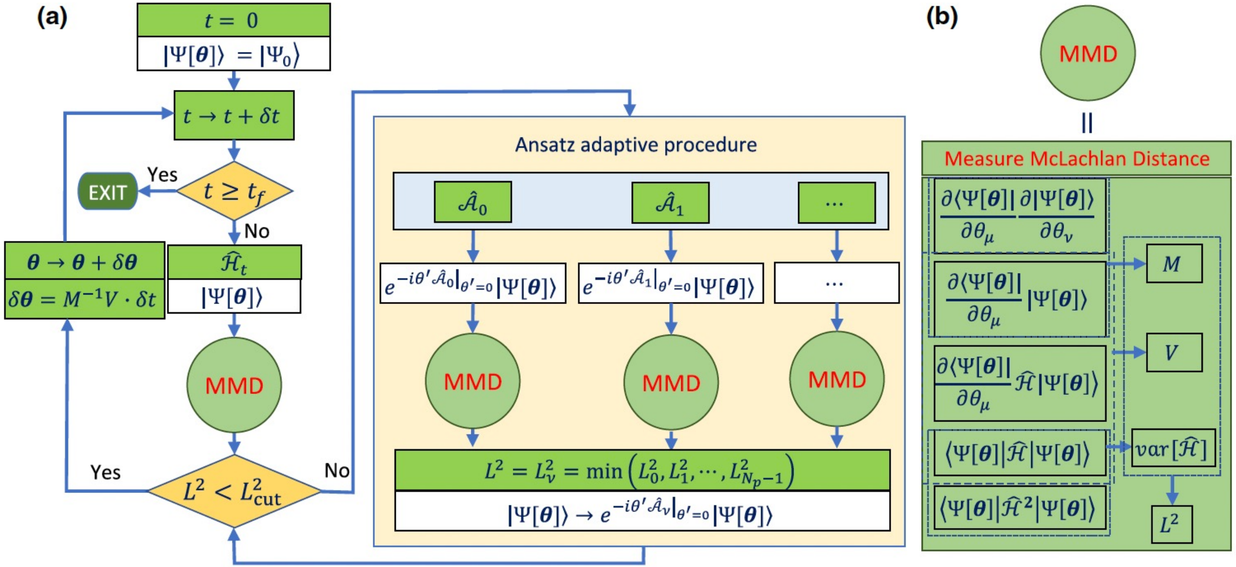
Matrix $M_{\mu\nu}$ and vector V_μ measured on QPU

Only so good as the ansatz can follow the dynamics

☞ **How to select an efficient yet flexible variational ansatz?**

[1] Li, Benjamin, Endo, Yuan (2019).

Adaptive Variational Quantum Dynamics simulation algorithm



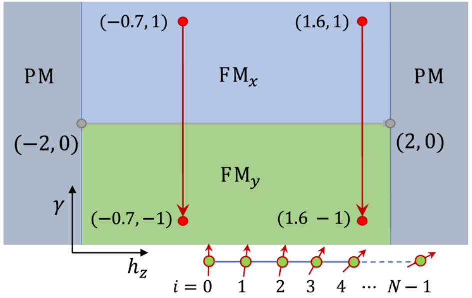
- Adaptive ansatz construction in pseudo-Trotter form: flexible and avoids pitfalls of fixed ansatz
- Add operator from predefined pool to ansatz if MacLachlan distance increases above set threshold
- Operator pool we use contains all Pauli strings that appear in Hamiltonian

[1] Y. Yao *et al.*, PRX Quantum **2**, 030307 (2021)

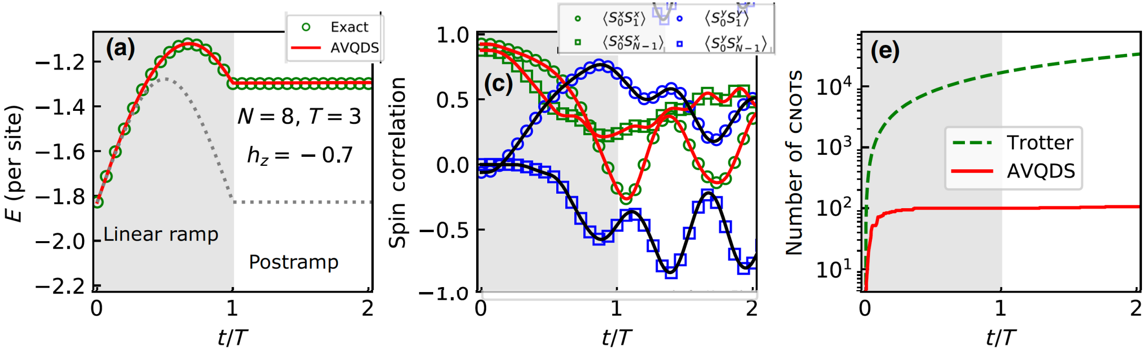
Application I: continuous quench in integrable spin chain

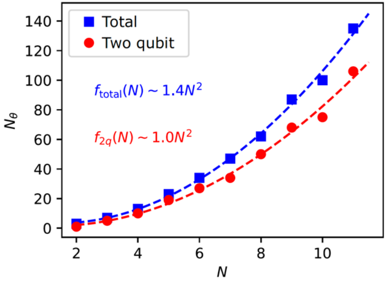
- Linear quench of anisotropic XY chain in transverse magnetic field

$$\hat{\mathcal{H}} = -J\sum_{i=0}^{N-2}\left[(1+\gamma)\hat{X}_i\hat{X}_{i+1} + (1-\gamma)\hat{Y}_i\hat{Y}_{i+1}\right] + h_z\sum_{i=0}^{N-1}\hat{Z}_i \quad \text{with} \quad \gamma(t) = 1 - \frac{2t}{T}$$



- AVQDS follows exact solution during and after quench, shown for $N = 8$
- Circuit depth saturates at 100 CNOTs << Trotter circuit depth 10^4 CNOTs
- Can simulate system with gate depth independent of time t ☞ can simulate to arbitrary times!





Saturated # of parameters

Application II: sudden quench in nonintegrable spin chain

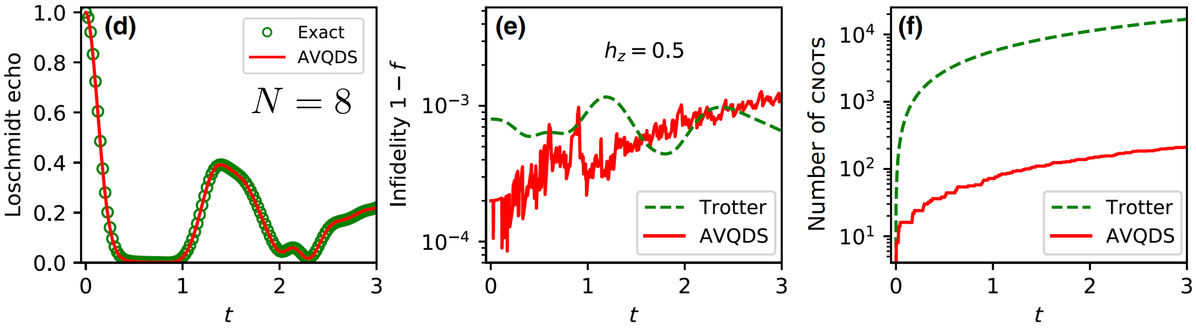
- Sudden quench in mixed-field Ising model

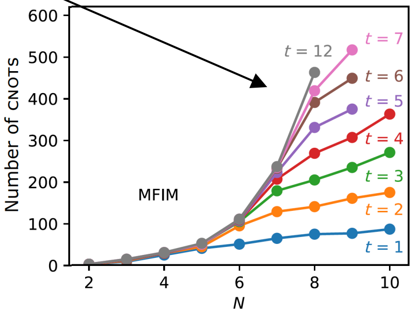
$$\hat{\mathcal{H}} = -J\sum_{i=0}^{N-1}\hat{Z}_i\hat{Z}_{i+1} + \sum_{i=0}^{N-1}\left(h_x\hat{X}_i + h_z\hat{Z}_i\right)$$

Loschmidt echo: $\mathcal{L}(t) = \left|\langle\Psi_0|e^{-i\hat{\mathcal{H}}_f t}|\Psi_0\rangle\right|^2$

Initial state: $|\Psi_0\rangle = |\uparrow\cdots\uparrow\rangle$

- Circuit depth two orders of magnitude smaller than Trotter circuit depth
- Saturated AVQDS circuit depth scales exponentially with system size N
- # measurements is main bottleneck of algorithm $\propto N_\theta^2$





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Variational Trotter Compression (VTC) algorithm

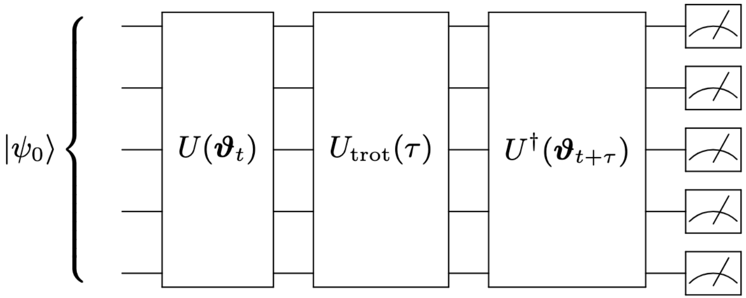
Key idea of VTC algorithm [1, 2]:

- First, propagate state using Trotter: $|\psi(\boldsymbol{\vartheta}_t)\rangle \Longrightarrow U_{\text{trot}}(\tau)\,|\psi(\boldsymbol{\vartheta}_t)\rangle$
- Then, update variational parameters $\vartheta_t \rightarrow \vartheta_{t+\tau}$ by optimizing fidelity cost function

Fidelity cost function $\mathcal{C} = |\,\langle\psi_0|U^\dagger(\boldsymbol{\vartheta}_{t+\tau})U_{\text{trot}}(\tau)U(\boldsymbol{\vartheta}_t)|\psi_0\rangle\,|^2$

Our variational state: $$|\psi(\boldsymbol{\vartheta})\rangle = U(\boldsymbol{\vartheta})\,|\psi_0\rangle = \prod_{l=1}^{\ell}\prod_{i=1}^{N} e^{-i\vartheta_{l,i}A_i}\,|\psi_0\rangle$$

ℓ = number of layers
N = number of parameters per layer
A_i= Hermitian operator (e.g. Pauli matrix)



Return probability to initial state is maximal for optimal parameters $\vartheta_{t+\tau}$

Measure cost function on QPU [3]

[1] Lin, Green, Smith, Pollmann (2020); [2] Barison, Carleo (2021), [3] Berthusen, Trevisan, Iadecola, PPO (2021).

Application to Heisenberg model: choice of ansatz

1D AF Heisenberg model $H_0 = \frac{J}{4}\sum_{i=1}^{M}(X_iX_{i+1} + Y_iY_{i+1} + Z_iZ_{i+1})$

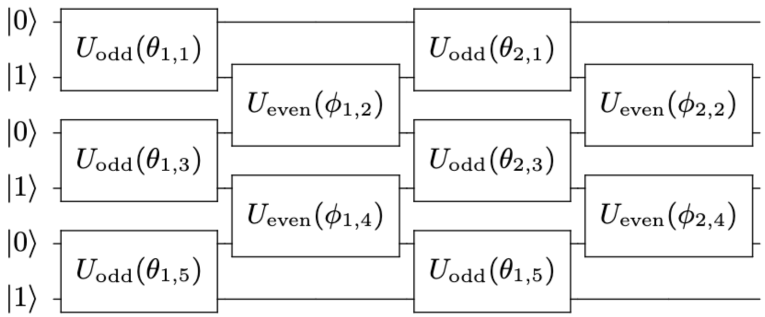
> Start from classical Néel state and time-evolve with H_0: $|\psi(t)\rangle = e^{-iH_0 t}|010101\cdots\rangle$

$$|\psi(\boldsymbol{\vartheta}^{(\ell)})\rangle = \prod_{l=1}^{\ell} U_{\text{even}}(\boldsymbol{\phi}_l)\, U_{\text{odd}}(\boldsymbol{\theta}_l)\, |\psi_0\rangle$$

$$U_{\text{odd}}(\boldsymbol{\theta}_l) = \prod_{j\ \text{odd}} e^{-i\,\theta_{l,j}\,(X_jX_{j+1}+Y_jY_{j+1}+Z_jZ_{j+1})}$$

$$U_{\text{even}}(\boldsymbol{\phi}_l) = \prod_{j\ \text{even}} e^{-i\,\phi_{l,j}\,(X_jX_{j+1}+Y_jY_{j+1}+Z_jZ_{j+1})}$$

Brickwall form of quantum circuit



> Determine depth of layered ansatz $\ell \equiv \ell^*$ to accurately describe $|\psi(t)\rangle$

Required layer numbers versus time

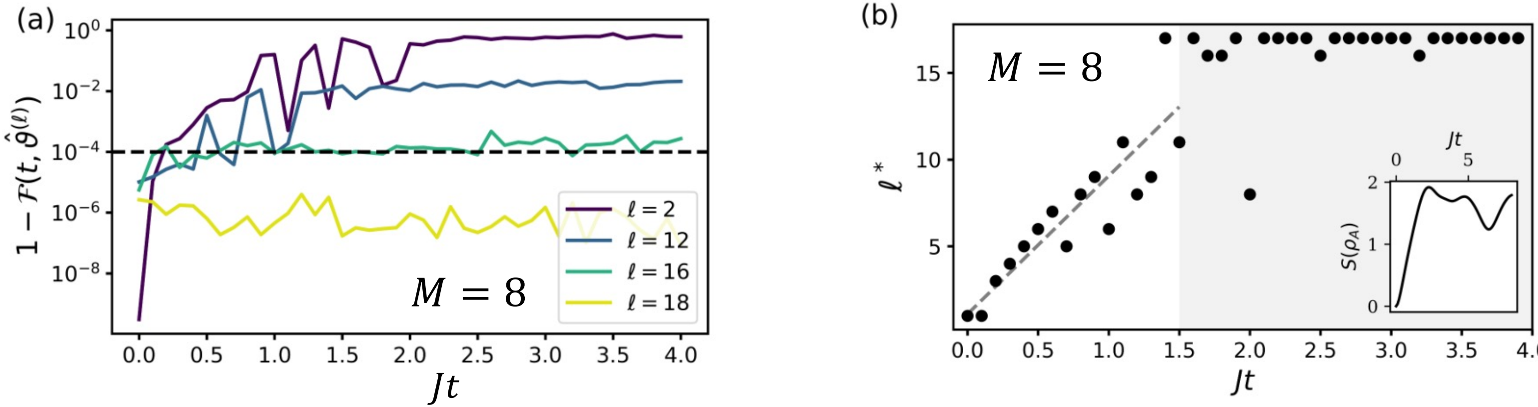
- Start from classical Néel state and time-evolve with H_0: $|\psi(t)\rangle = e^{-iH_0 t}|010101\cdots\rangle$
- Determine depth of layered ansatz ℓ to accurately describe $|\psi(t)\rangle$

Overlap with exact state

$$1 - \mathcal{F}(t, \boldsymbol{\vartheta}^{(\ell)}) = 1 - |\langle\psi(\boldsymbol{\vartheta}^{(\ell)})|\psi(t)\rangle|^2$$

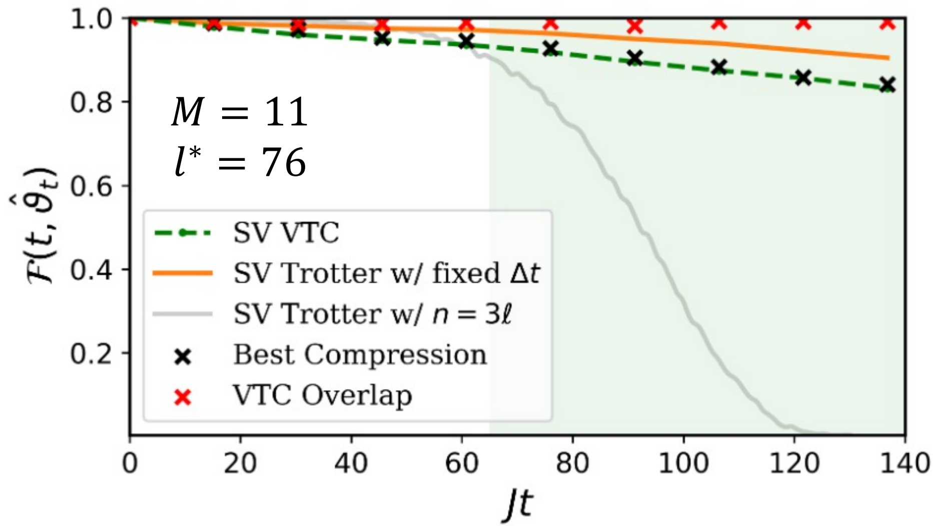
Variational form

$$|\psi(\boldsymbol{\vartheta}^{(\ell)})\rangle = \prod_{l=1}^{\ell} U_{\text{even}}(\boldsymbol{\phi}_l)\, U_{\text{odd}}(\boldsymbol{\theta}_l)\, |\psi_0\rangle$$



Required layer number ℓ to achieve $1 - \mathcal{F} < 10^{-4}$ grows **linearly with time** and then **saturates**.

VTC benchmark on statevector simulator



- VTC approximately follows Trotter with fixed small step size $\Delta t = \frac{0.2}{J}$
- Orange curve has depth $\mathrm{n} = 700$ at t_f
- Grey curve has depth $3\ell = 228$ at all t
- VTC cost function has fixed depth $3\ell = 228$
- Gradient based optimization using L-BFGS-B

Fidelity = Overlap with exact state $\mathcal{F}(t, \hat{\boldsymbol{\vartheta}}_t) = |\langle \psi(\hat{\boldsymbol{\vartheta}}_t) | \psi(t) \rangle|^2$

$$\text{Best Compression} \equiv |\langle \psi(t) | U_{\text{Trot}}(n = \ell) | \psi(\hat{\boldsymbol{\vartheta}}_{t-\tau}) \rangle|^2$$

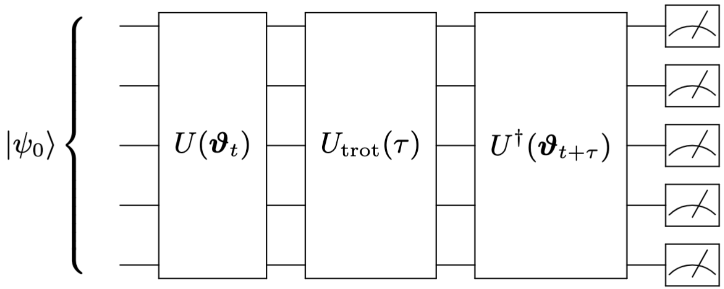
$$\text{VTC overlap} \equiv |\langle \psi(\hat{\boldsymbol{\vartheta}}_t) | U_{\text{Trot}} | \psi(\hat{\boldsymbol{\vartheta}}_{t-\tau}) \rangle|^2$$

VTC allows simulating to arbitrarily long times with high fidelity.

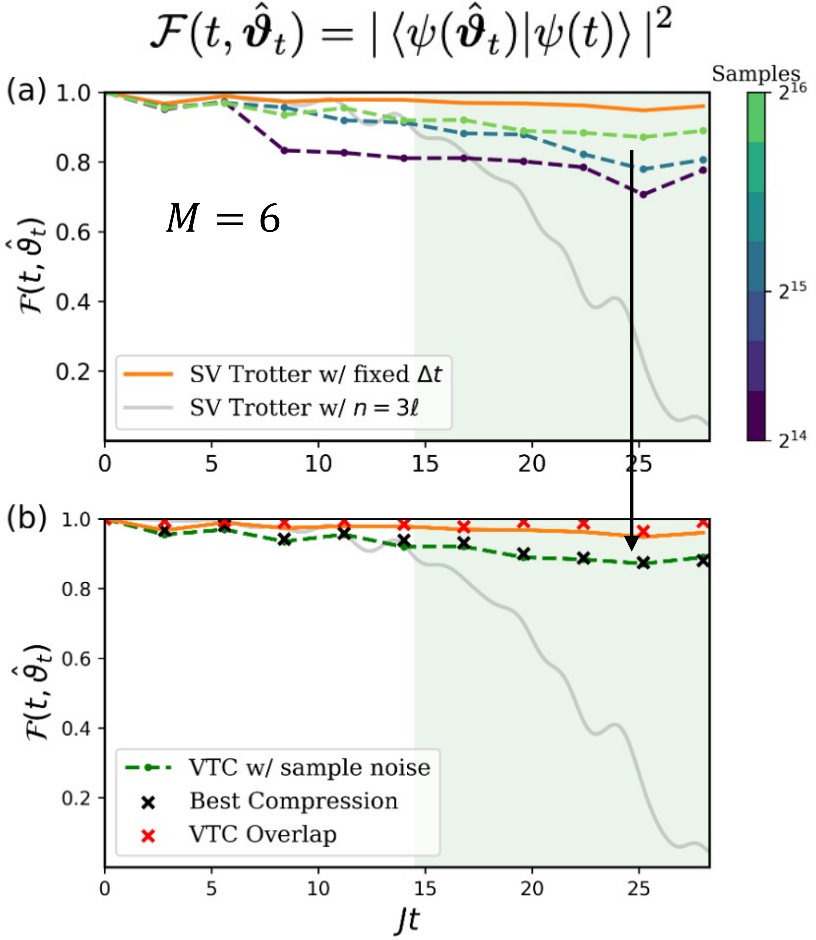
Parameters: $\ell = 76, n = 76$
$\tau = 15.2/J, \Delta t = 0.2/J$

VTC on ideal circuit simulators

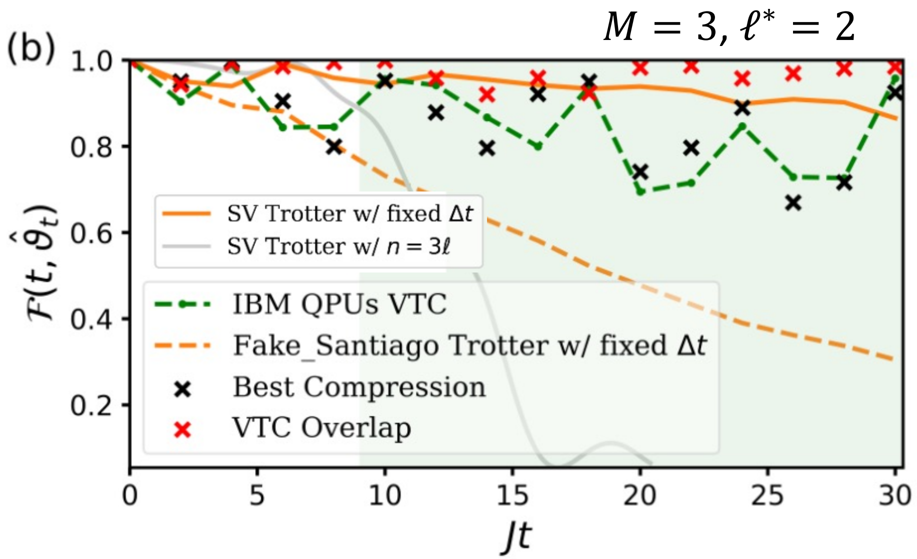
- Double-time contour cost function circuit
- Non-gradient-based optimizer: CMA-ES
- Larger shot numbers increase fidelity
- Single compression step takes few hours



VTC is feasible for noisy cost function.



VTC on IBM hardware

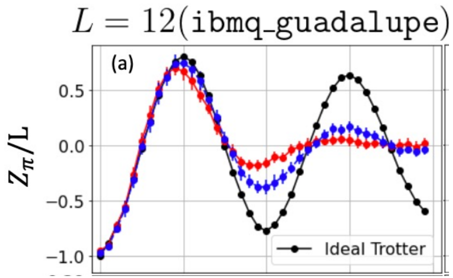


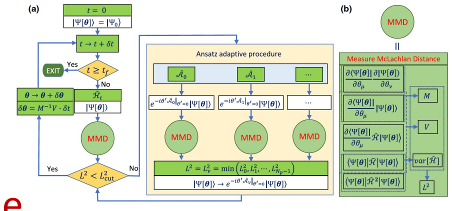
Explicit demonstration of dynamics simulations beyond QPU coherence time

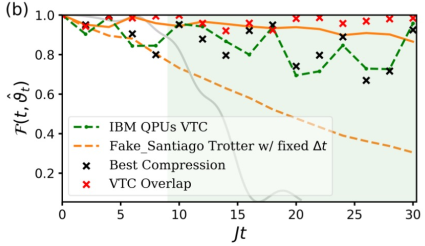
- Cost function evaluation on IBM hardware `ibmq_santiago & ibmq_quito`
- Final fidelity = 0.96, where Trotter fidelity has decayed to < 0.4 already
- 15 compression steps
- Average fidelity $\langle F \rangle = 0.86$
- $\mathcal{M} = 5700$ measurement circuits in total
- Comparable number of measurements for MacLachlan simulations $\approx 10^4$

Summary

- Trotter dynamics simulations with pulse-level control
  - Straightforward to implement even for large systems
  - Error mitigation and pulse-level control boost performance
- Adaptive variational quantum dynamics simulation (AVQDS) framework
  - Orders of magnitude shallower circuits than Trotter simulations
- Explicit demonstration of dynamics simulation beyond QPU coherence time
  - Variational Trotter Compression on IBM hardware for $M = 3$ sites
  - Can simulate out to arbitrary long times with high fidelity







References:

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Thank you for your attention!