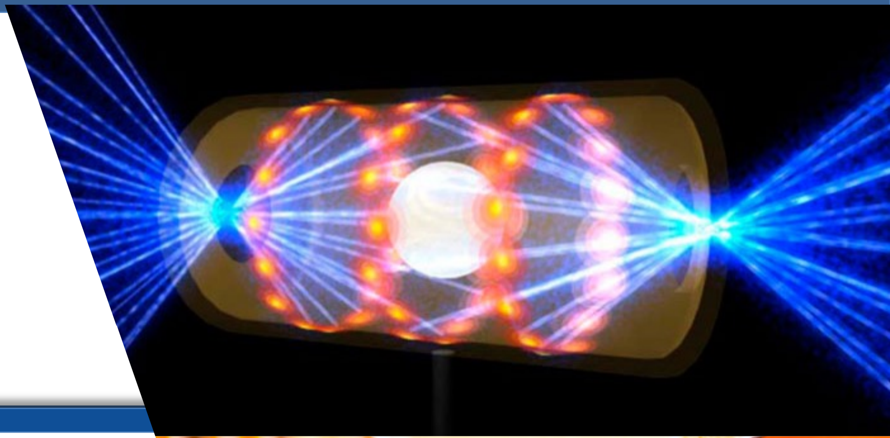
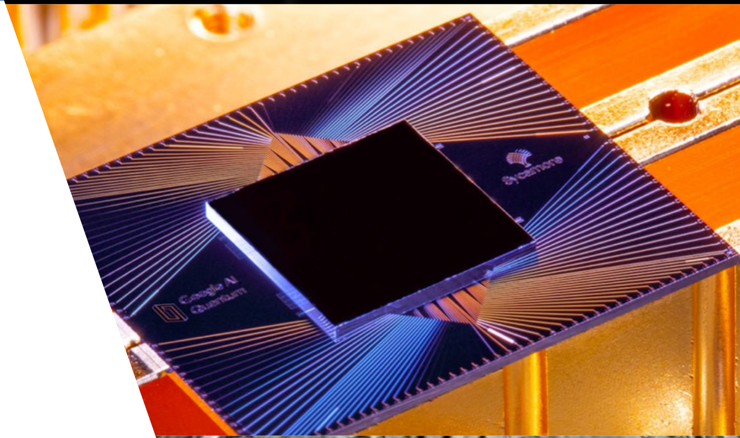
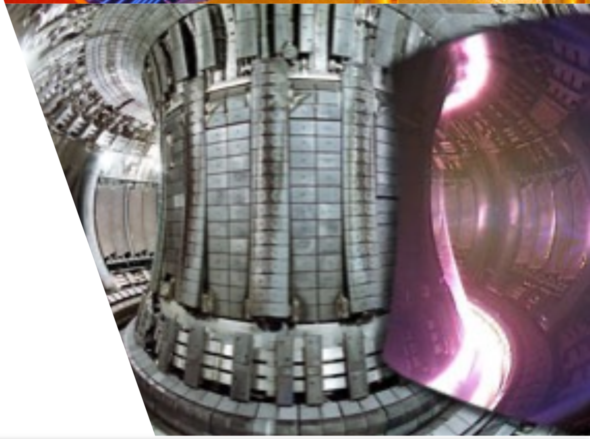
Exploration of Quantum Computing for Fusion Energy Science Applications







I. Joseph, M. D. Porter [1], Y. Shi[2], B. Evert[3],
A. R. Castelli, Y. Cho, V. I. Geyko, F. R. Graziani,
S. B. Libby, R. Minich, I. Novikau, Y. J. Rosen, J. L. Dubois
E. A. Sete[3], M. Reagor[3], A. F. Brown[4], V. Tripathi[4], D. Lidar[4]
Lawrence Livermore National Laboratory
[1]*Sandia National Laboratories,* [2]*University of Colorado Boulder,*
[3]*Rigetti Computing,* [4]*University of Southern California*

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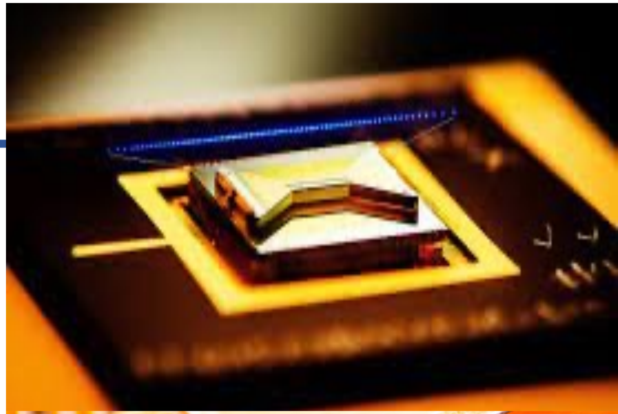
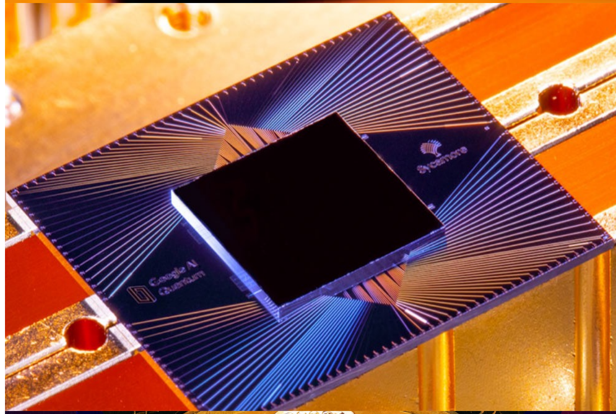
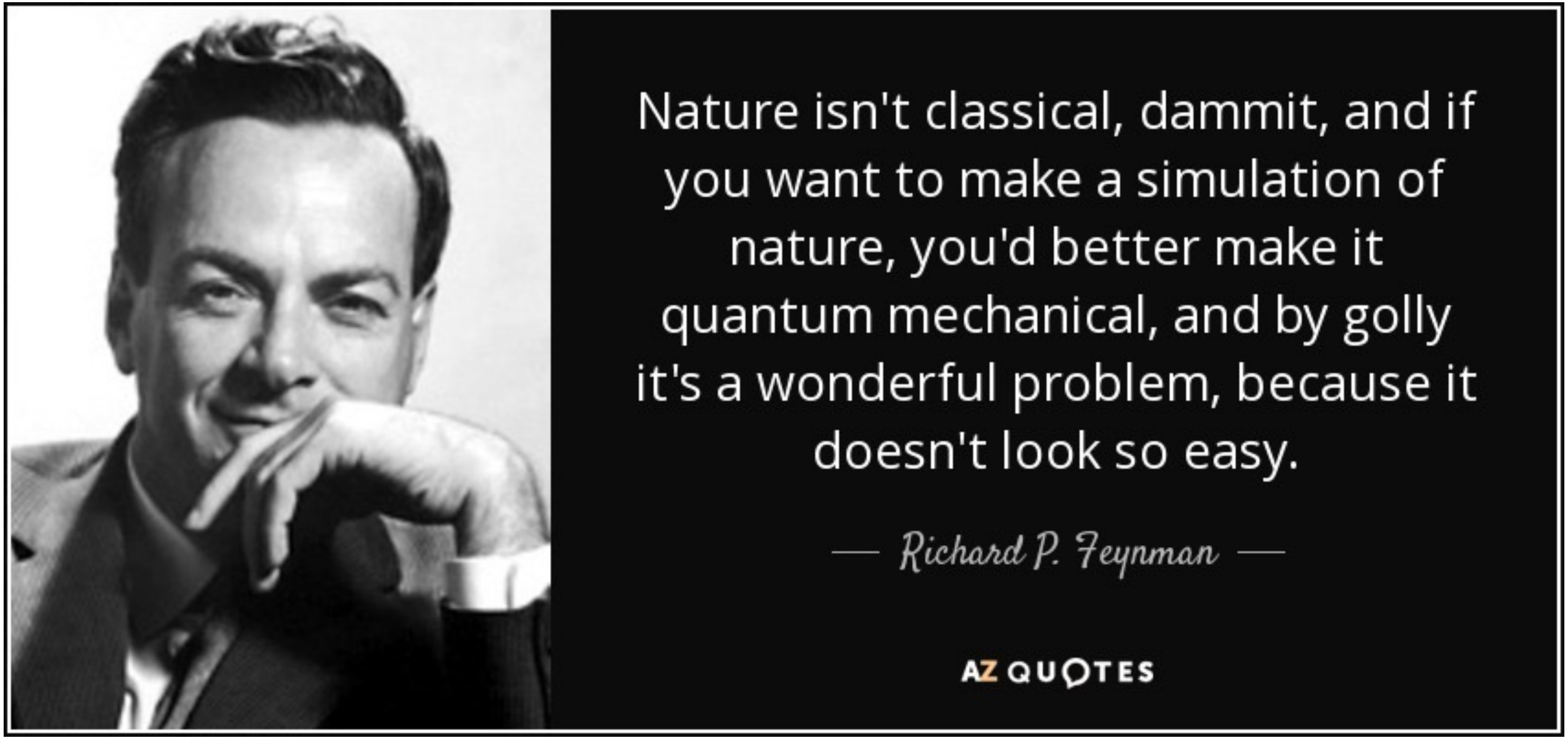
Quantum computing may be a game-changer for fusion and science in general





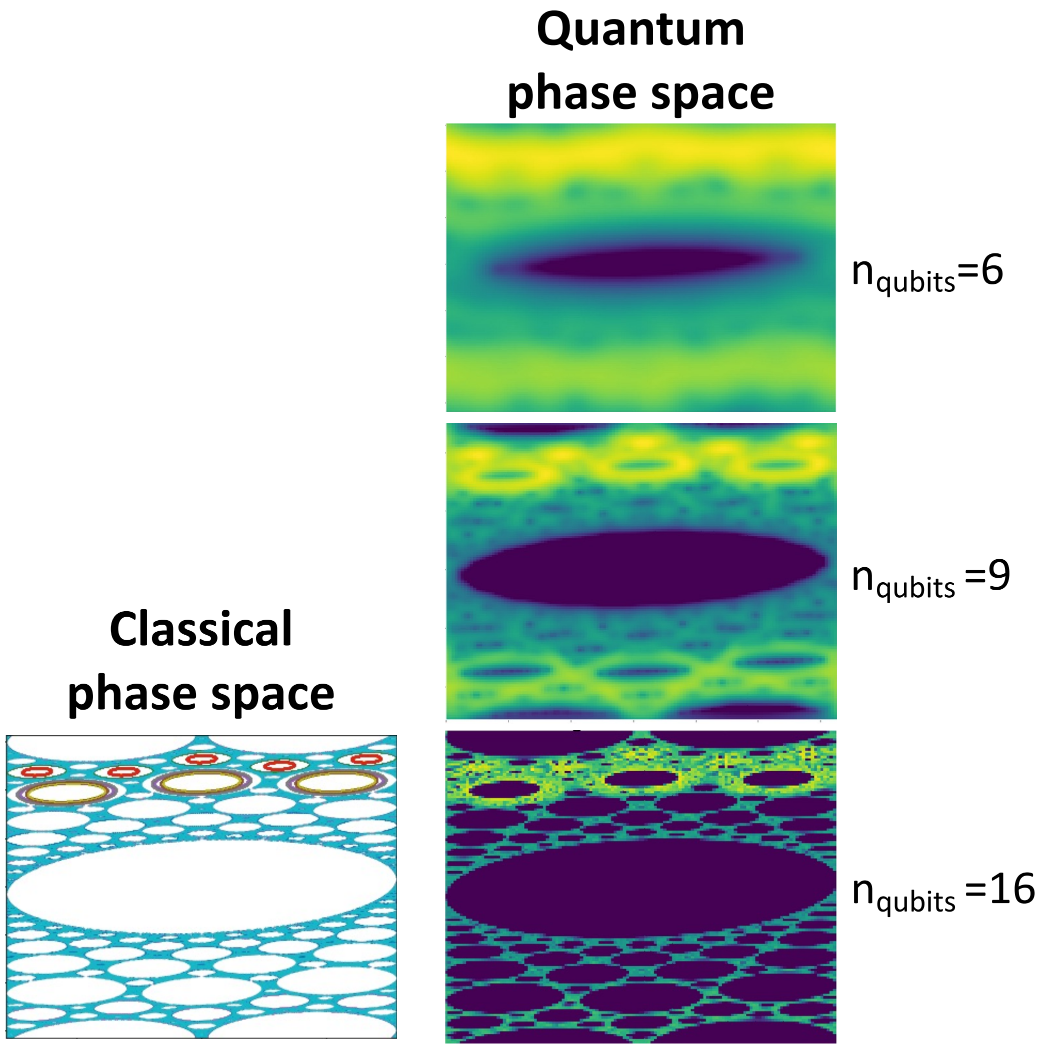
- **Polynomial to exponential gains in memory and computational power**
  - Exponential speedup for the Fourier transform, linear solvers, factoring integers, …
  - Quadratic speedup for unstructured search, optimization, sums & integrals, …
- **Great progress has been made on quantum hardware & technology**
  - Multiple platforms: ion traps, neutral atom traps, superconducting circuits, NMR, …
  - Google, IBM, & others now claim to have achieved **quantum supremacy …**
- **But, we are still in the Noisy Intermediate-Scale Quantum (NISQ) era**
  - Many qubits, but no error correction
  - 1% error rate per gate → can only perform ~100 gate operations

The key insight …

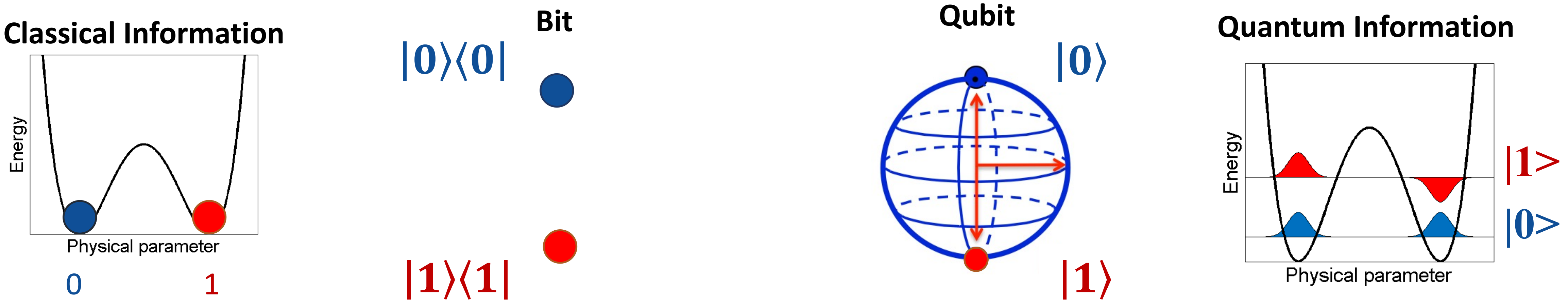


Outline: Quantum Computing for Fusion Energy Sciences

- **Intro to Quantum Computing**
  - Qubits
  - Quantum Algorithms
- **Quantum Simulation Algorithms**
  - Linear
  - Nonlinear
- **Testing Quantum Hardware Platforms**
  - Error Mitigation
  - Error Utilization
- **Conclusions & Outlook**



The qubit is the simplest complex Hilbert space



- **Pure State:** wavefunction $\psi \in \mathbb{C}^2$ is a normalized superposition of the basis states $|0\rangle$ and $|1\rangle$

$$\boldsymbol{\psi} = \begin{pmatrix} \cos\theta \;\; e^{-i\phi/2} \; |\mathbf{0}\rangle \\ \sin\theta \;\; e^{+i\phi/2} \; |\mathbf{1}\rangle \end{pmatrix}$$

- **Mixed State:** probability density matrix $\rho = \rho^\dagger \in \mathbb{H}_4 \sim \mathbb{R}^4$ is a mixture of pure states

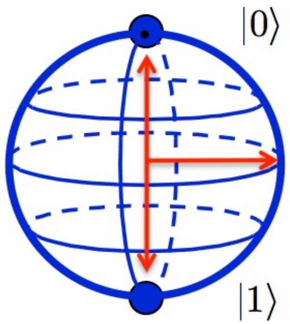
$$\boldsymbol{\rho} = \begin{pmatrix} \rho_{00} |\mathbf{0}\rangle\langle\mathbf{0}| & \rho_{01} |\mathbf{0}\rangle\langle\mathbf{1}| \\ \rho_{01}^{*} |\mathbf{1}\rangle\langle\mathbf{0}| & \rho_{11} |\mathbf{1}\rangle\langle\mathbf{1}| \end{pmatrix}$$

- **PDF:** probability distribution function $f \in \mathbb{R}^2$

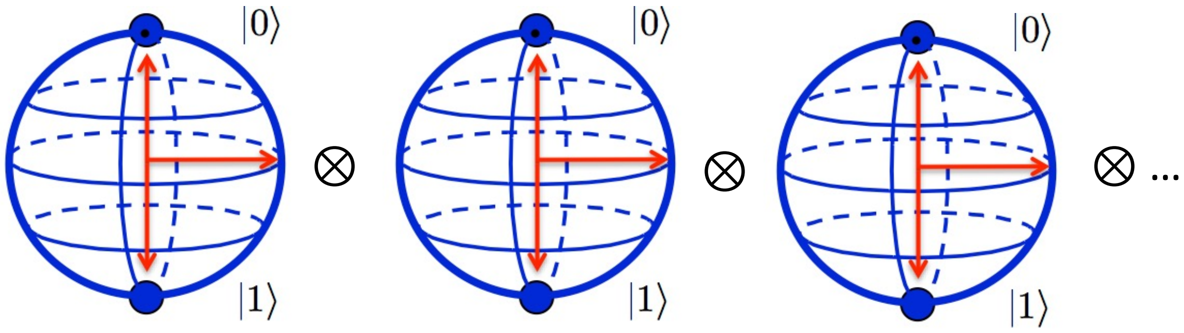
$$\boldsymbol{f} = \mathrm{Diag}(\boldsymbol{\rho}) = \begin{pmatrix} \rho_{00} |\mathbf{0}\rangle\langle\mathbf{0}| & \\ & \rho_{11} |\mathbf{1}\rangle\langle\mathbf{1}| \end{pmatrix}$$

Quantum memory registers are "exponentially large"

Qubit: Dimension 2



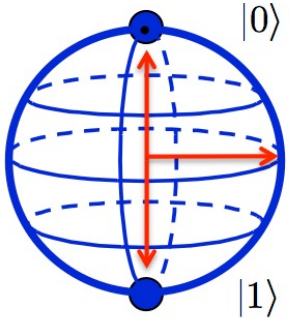
n Qubits → Hilbert Space Dimension: N = 2^n



- **For n qubits, the number of states is N = 2^n**
  - **Pure State:** $\psi \in \mathbb{C}^N$ has $2(N-1)$ real DOFs
  - **Mixed State:** $\rho = \rho^\dagger \in \mathbb{H}_{N\times N}$ has (N^2-1) real DOFs
  - **Classical PDF:** $f \in \mathbb{R}^N$ has $(N-1)$ real DOFs
- **Direct quantum simulation is extremely difficult due to exponentially large Hilbert space!**

Let's use "quantum machines" to simulate quantum physics!

Qubit: Dimension 2



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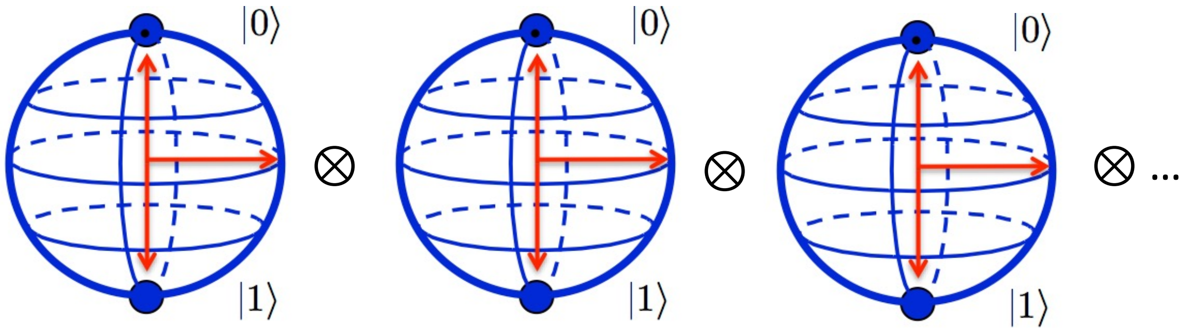
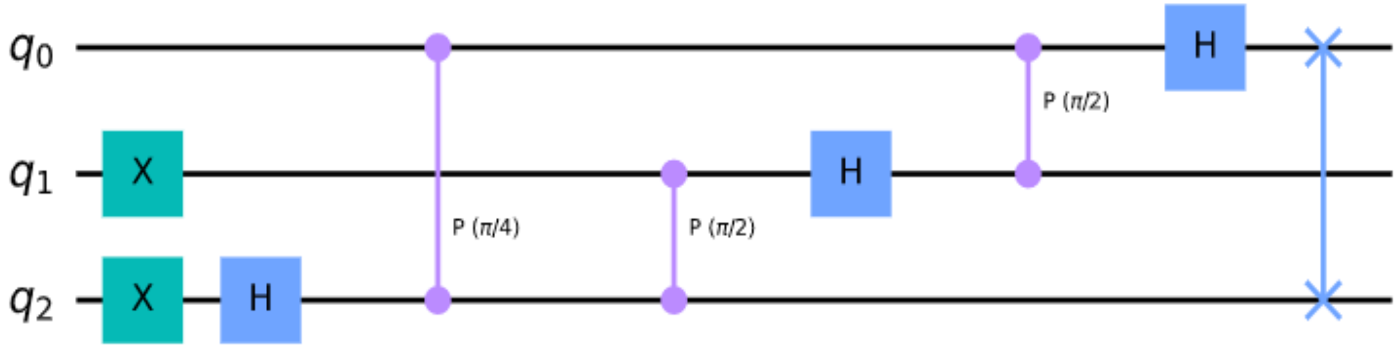


- **A brief history of quantum algorithms:**
  - **Early-1980's:** Turn the challenge into an opportunity — Feynman, Manin, Bennett & Brassard
  - **Mid-1990's:** Factoring integers, unstructured search, quantum counting — Shor, Grover, Brassard, Hoyer, Tapp
  - **Late-1990's:** Efficient simulation algorithms based on Trotter-Suzuki decompositions — Lloyd & Abrams
  - **Early 2000's:** Linear solver algorithms – Harrow Hassidim & Lloyd, Ambianis, Childs Kothari & Somma, …
  - **2015-present:** Accelerated linear solver, linear diff eq & simulation algorithms — Berry, Childs, Low & Chuang

Digital quantum computing model has power and simplicity

- **Quantum states can be transformed efficiently via linear unitary operations**
  - $\psi = \mathbf{U}\psi_0$ where $\mathbf{U} = e^{-i\mathbf{H}t}$ is a unitary $\mathbf{U}\mathbf{U}^\dagger = \mathrm{I}$ evolution operator and $\mathbf{H} = \mathbf{H}^\dagger$ a Hermitian Hamiltonian
  - **This is amazing!** because ψ is an exponentially large vector and $\mathbf{U}$ is a dense exponentially large matrix!

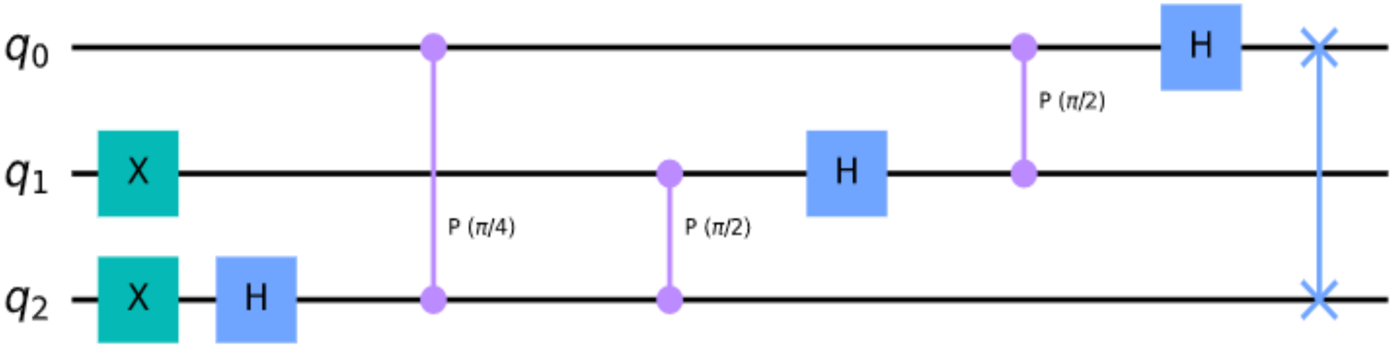


3 qubit FFT

- **While there are a huge number, $N^2 = 2^{2n}$, of unitary operations, they are generated by a small number ~O(n) of basic operations called a "gate set"**
  - Single qubit operations can be achieved efficiently with a few standard gates, e.g. RX and RZ
  - Adding one nontrivial 2-qubit gate, e.g. CNOT or CZ, between nearest neighbors generates the rest

Many useful computations can be performed in O(poly(n)) basic gate operations!

- **The key resource is quantum parallelism: superposition and interference ☺**
  - Any reversible classical computation can also be performed, but typically without a speedup



3 qubit FFT

- **Approximating an arbitrary unitary is exponentially hard ☹**
  - Only certain unitaries can be performed efficiently
  - Initializing all quantum information is exponentially hard
  - Measuring all quantum information is exponentially hard

- **Measuring exponentially small probabilities is hard ☹**
  - Central limit theorem implies direct sampling converges as 1/sqrt(# samples)

Key Limitations

A few essential subroutines power the majority of quantum algorithms

- **Quantum Fourier Transform: Cost of (log N)^2 rather than classical N log N**
  - Phase estimation, factoring integers, and taking discrete logarithms – Peter Shor 1994
  - Powers many Hamiltonian simulation algorithms
  - Hamiltonian simulation powers linear solvers, linear diff. eq. solvers, and variational eigensolvers, etc.

- **Amplitude Amplification: Cost of sqrt(N) rather than classical N**
  - Amplitude amplification first used in Grover's search algorithm – Lov Grover 1996
  - Amplitude estimation & Quantum counting – Brassard, Hoyer, Mosca, Tapp 2000
  - Powers many Monte Carlo and integration algorithms – Heinrich & Novaks 2000, Montanaro 2015

- **Quantum Walks: Cost of N rather than classical N^2**
  - Early models turned into a computational framework – Aharonov, Ambianis, Kempe, Vazirani 2001
  - Graph search, element uniqueness, … – Ambianis, Childs, Kempe
  - Hamiltonian simulation, state preparation – Szegedy 2004, Childs 2010
  - Qubitization, Quantum Signal Processing, Quantum Singular Value Transformation – Low & Chuang 2017

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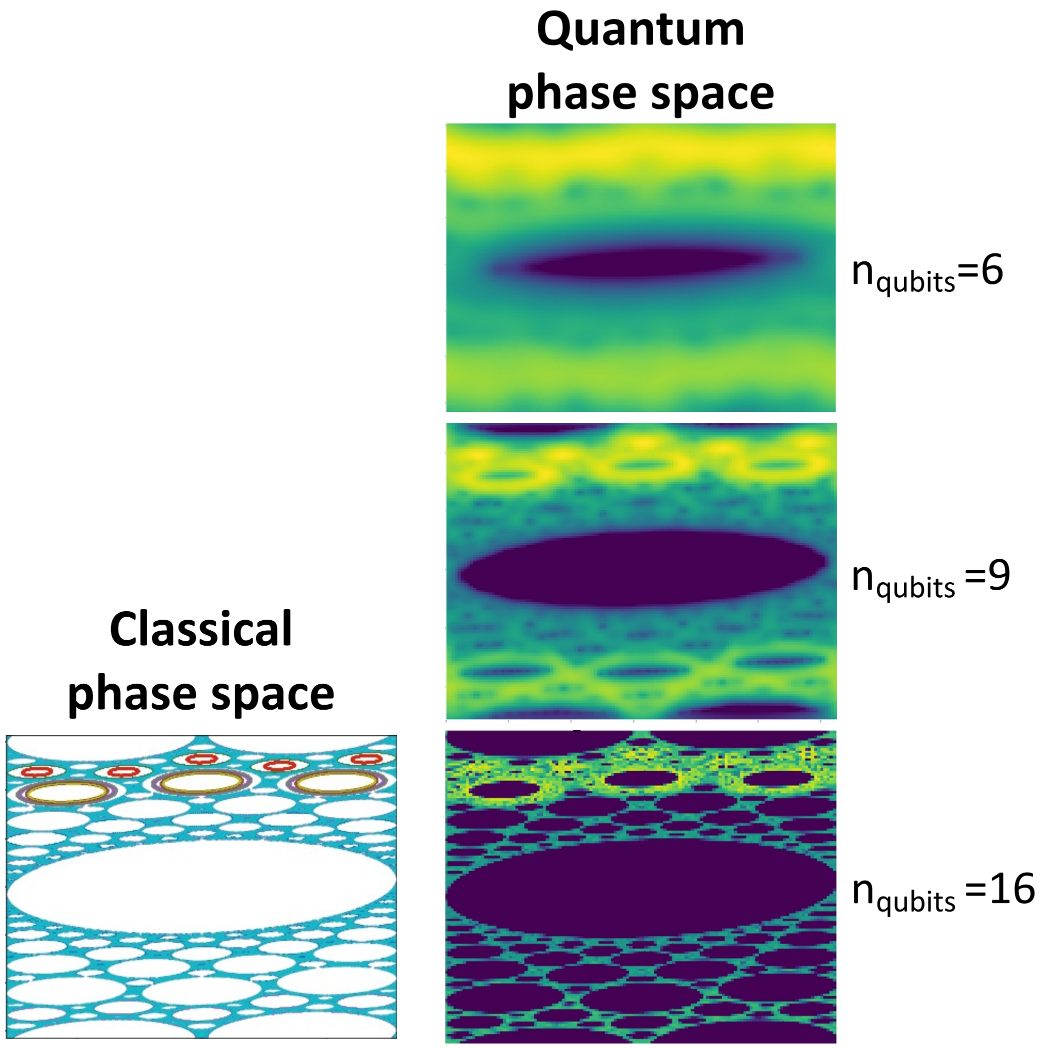


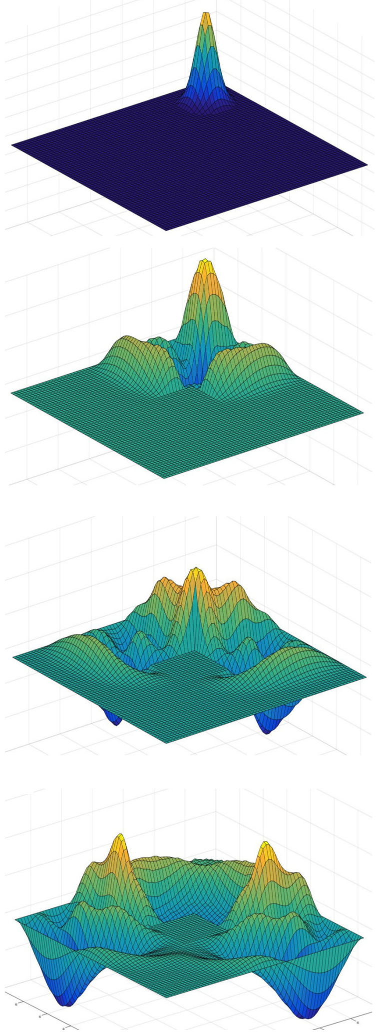
Hamiltonian simulation can speed up the solution of linear PDEs

- **Simple PDEs, e.g. Poisson or wave equation, have simple/sparse Hamiltonians and can typically be solved with exponential speedup**
  - — The output is a wavefunction that encodes the solution
  - — And a few robust physical observables $<O_1>$, $<O_2>$, $<O_3>$

$$|\psi\rangle = \sum_x \psi_x |x\rangle$$

- **However, outputting the data $\{\psi_x\}$ to a classical register, requires an exponential amount of work & reduces speedup to quadratic at best [1,2]**
  - — The same problem occurs for nontrivial initial condition and/or source functions

- **"Hidden Spectral Problem": if you promise there is a basis in which the solution is exponentially sparse, then we can get exponential speedup**
  - — Like doing "**X-ray crystallography**"



P. Costa, S. Jordan, A. Ostrander
Phys. Rev. A 99, 012323 (2019)

[1] Costa et al PRA 2019, [2] Montanaro & Pallister PRA 2016

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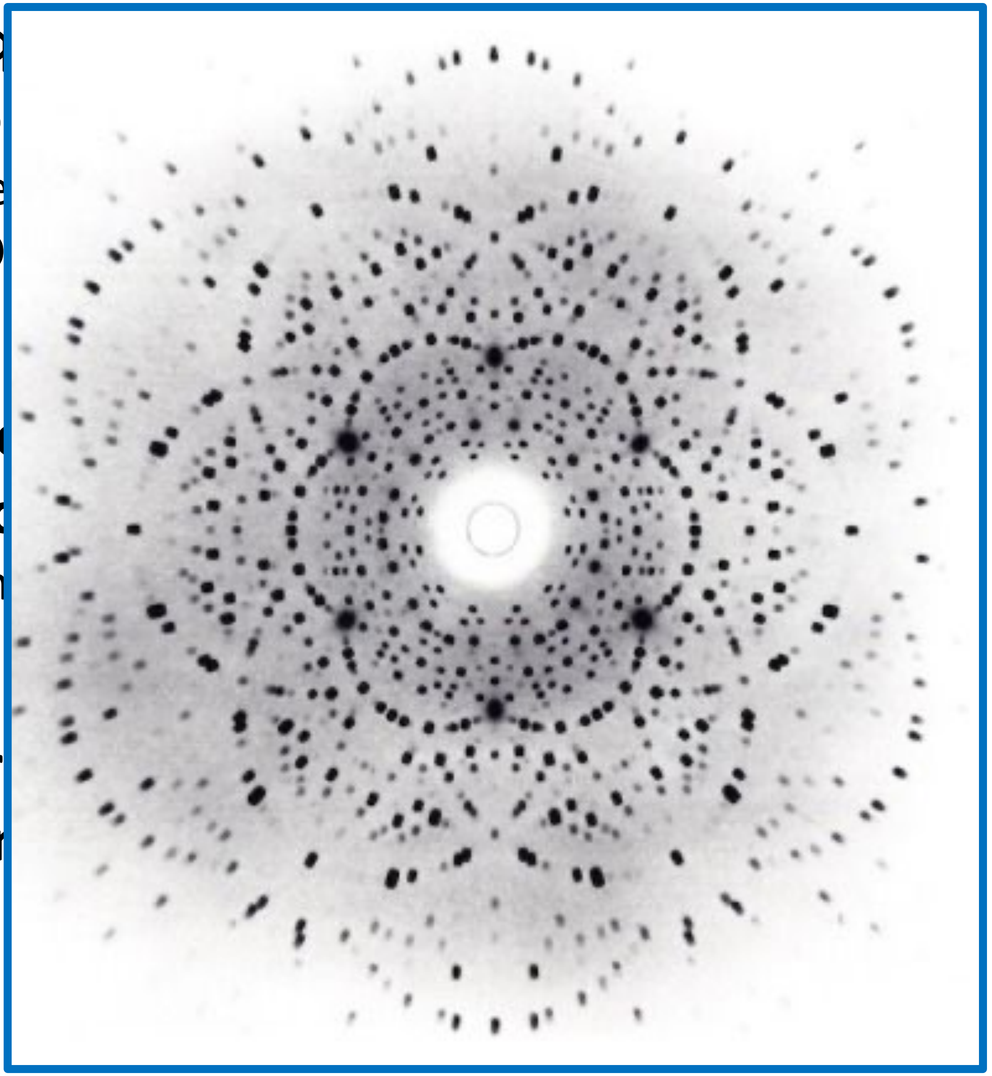

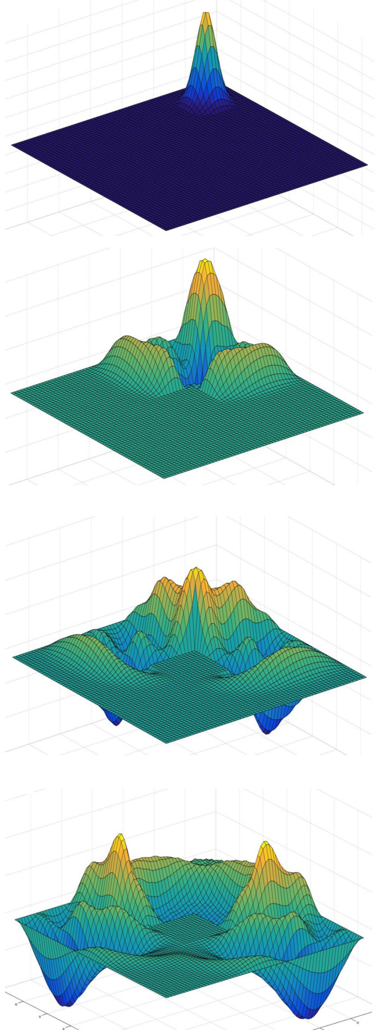

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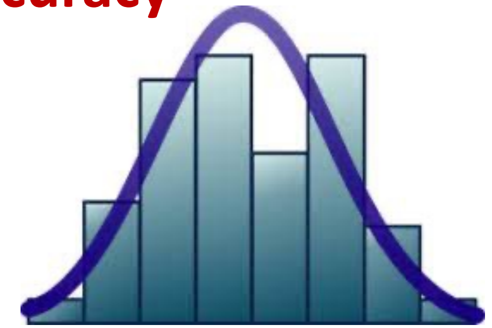
Amplitude Estimation yields up to quadratic speedup for output

- **Central limit theorem: direct sampling requires computational cost ~ 1/accuracy^2**
  - Classical randomized Monte Carlo algorithms can also often provide an exponential speedup over Eulerian methods



- **Amplitude estimation only requires computational cost ~ 1/accuracy**

	function space	deterministic	randomized	quantum
	L_p^N, $2 \le p \le \infty$	1	$n^{-1/2}$	n^{-1}
Holder class	$F_d^{k,\alpha}$	$n^{-(k+\alpha)/d}$	$n^{-(k+\alpha)/d-1/2}$	$n^{-(k+\alpha)/d-1}$
Sobolev class	$W_{p,d}^k$, $2 \le p \le \infty$	$n^{-k/d}$	$n^{-k/d-1/2}$	$n^{-k/d-1}$

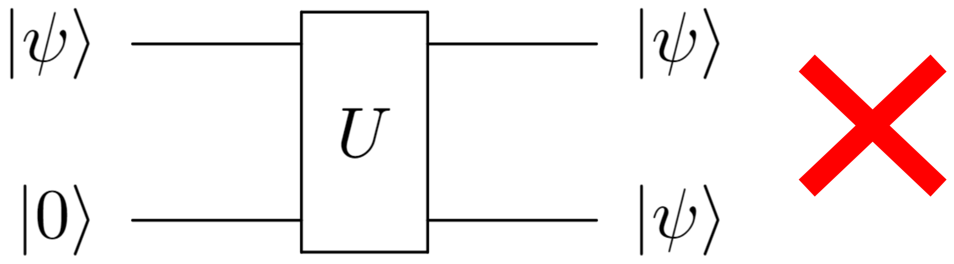
Convergence [1] of error with number of function calls n

- **Relative to deterministic algorithms, speedups increase for high dimensions $d \to \infty$** and for **solutions that are not smooth $k, \alpha \to 0$**
  - **Key Assumption:** location of discontinuities are unknown → ***stochastic / randomized functions***

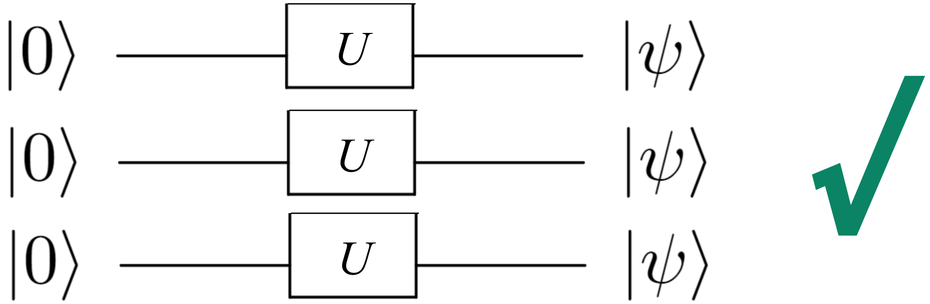
[1] Heinrich & Novak 2001 arXiv:quant-ph/0105114

The No-Cloning Theorem fundamentally limits the ability of a quantum computer to efficiently compute nonlinear functions

- **No-Cloning Theorem:**
  An unknown quantum state cannot be copied
  — The only way to do this is to measure all components and prepare an identical state from scratch



- **If a state preparation process is reproducible, we can form multiple replicas of the state**
  — A fault-tolerant quantum computer can run the same quantum program to create identical outputs



- **Iterative algorithms that require nonlinear operations are exponentially costly [1]**
  — If each iteration needs 2 replicas, then the next iteration needs 4 replicas, and T iterations needs **2^T replicas**

[1] S. K. Leyton, T. J. Osborne, arXiv:0812.4423 (2008)

How about embedding a nonlinear differential equation within a larger linear system?

- **Quantization is a natural embedding for Hamiltonian systems**
  - Dissipation can be included by embedding the system within a much larger ideal system [1]

- **Exact Koopman-von Neumann (KvN) [2] and Carleman [3] approaches**
  - The conservation of the probability distribution function (PDF) is a perfect embedding of a nonlinear system … in an infinite-dimensional system of equations
  - Carleman embedding [4] is a complex analytic form of Koopman [2] that works well near fixed points

- **Special classes of PDEs may have more efficient types of embedding**
  - PDEs that are reducible to ODEs can be embedded using the KvN approach for ODEs [4]: Hamilton-Jacobi equation, advection equation

- **Integrable systems also have special types of embedding**

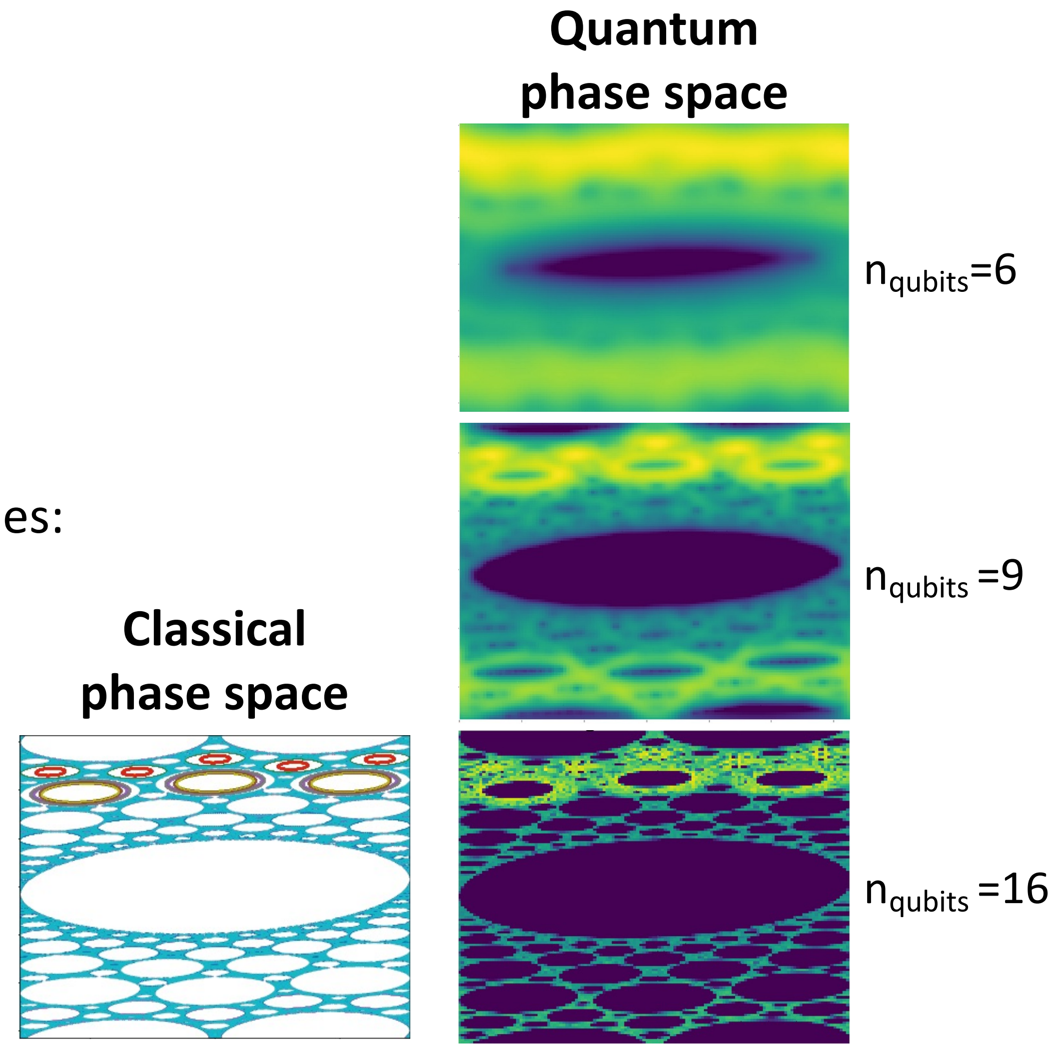
[1] J. Yepez 2002, S. Lloyd 2020 [2] I. Joseph 2020, 2023 [3] Jin-Peng Liu 2021 [4] S. Jin & N. Liu 2022

Approach # 1: Quantize the dynamics $i\hbar\partial_t\psi = \mathbf{H}\psi$

- **Point Example: Quantum Sawtooth Map***
  - Model for chaotic wave-particle interactions
  - Converges to classical result as # of qubits increases

- **Advantages**
  - Quantum version may be the more accurate physical model
  - Many quantum algorithms for quantum simulation
  - Quantum algorithms can efficiently calculate classical quantities: Lyapunov exponent* & diffusion coefficient

- **Disadvantages**
  - **Quantum ≠ Classical:** interference, diffraction, & tunneling
  - Semiclassical limit requires **very large** quantum numbers
  - Non-Hamiltonian systems, e.g. with dissipation, require embedding in a much larger ideal system



*G. Benenti, et al., Quantum Info. Proc. **3**, 273 (2004)

Approach # 2: Nonlinear dynamics acts linearly on function spaces

- **Consider a set of nonlinear Diff Eq's** $dz/dt = V(z,t)$ **with initial conditions** $z_0 \coloneqq z(t=0)$

Lagrangian picture $\quad \partial_t z\big|_{z_0} = +V \cdot \nabla z \quad \xleftrightarrow{\text{chain rule}} \quad \partial_t z_0\big|_{z} = -V \cdot \nabla z_0$

- **The advection equation expresses the evolution of a scalar function:** $\theta(z,t)$

Koopman evolution $\quad \partial_t \theta\big|_{z_0} = +V \cdot \nabla \theta \quad \xleftrightarrow{\text{chain rule}} \quad \partial_t \theta\big|_{z} = -V \cdot \nabla \theta \quad$ Eulerian picture

- **The Liouville equation expresses conservation of probability:** $f(z,t)$

$\partial_t f\big|_{z_0} = +\nabla \cdot (Vf) \quad \xleftrightarrow{\text{chain rule}} \quad \partial_t f\big|_{z} = -\nabla \cdot (Vf) \quad$ Perron-Frobenius evolution

Semiclassical wavefunction yields efficient unitary representation [1]

- Since quantum algorithms act naturally on wavefunctions, consider the "semiclassical" ansatz

$$\psi(z,t) = \sqrt{f(z,t)}e^{i\theta(z,t)}$$

- Where $f(z,t)$ evolves as a PDF and the phase $\theta(z,t)$ evolves as a scalar field with a source

$$\partial_t \theta\Big|_z = -V \cdot \nabla\theta + L(z,t)/\hbar$$

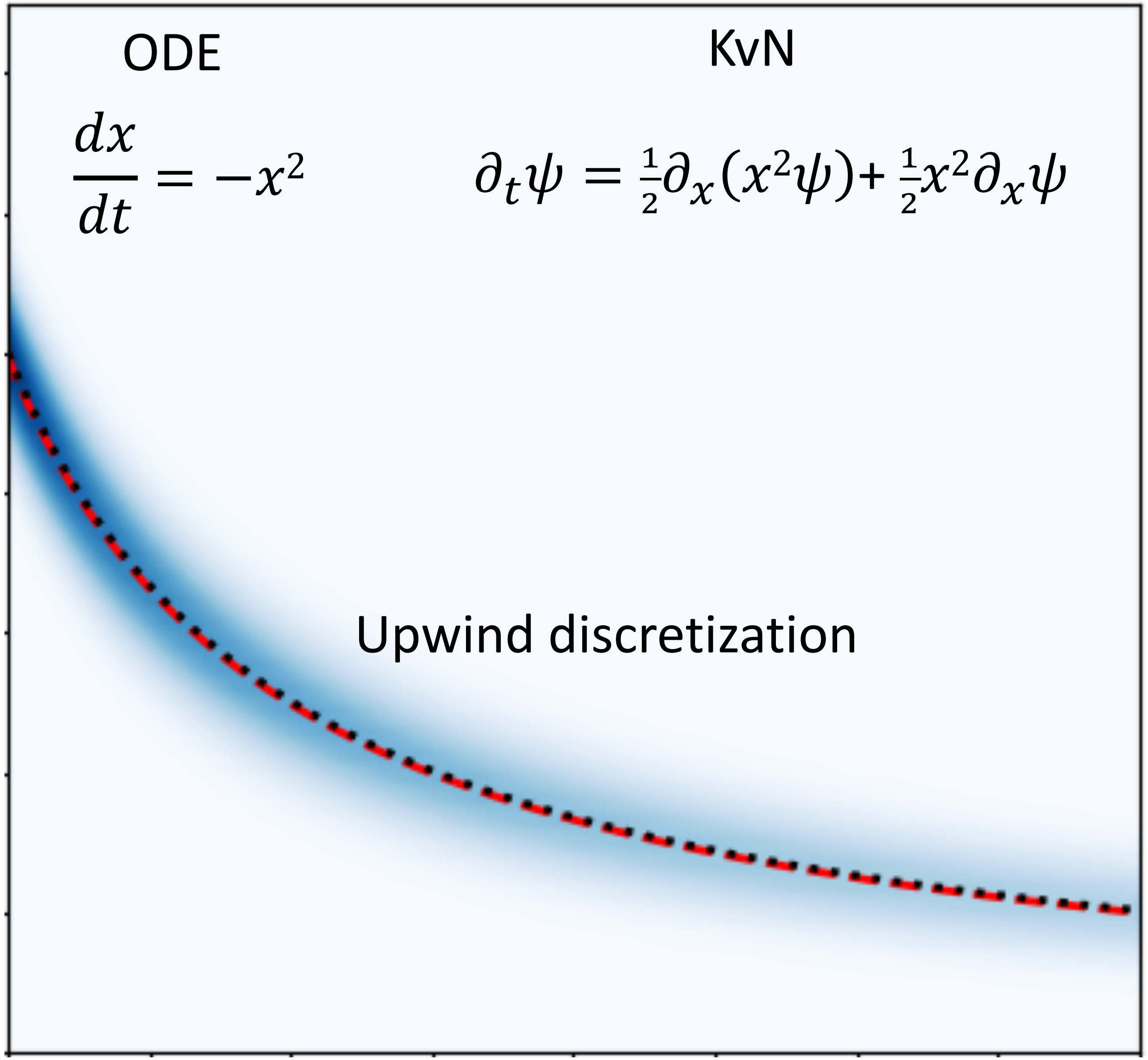
- Inserting the definitions leads to the generalized **Koopman-von Neumann equation [1-2]**

$$\boxed{i\hbar\partial_t\psi\Big|_z = -i\hbar(V \cdot \nabla\psi + \nabla \cdot V\psi)/2 - L\psi}$$

- The **classical Lagrangian** $L(z,t) = p \cdot \partial_p H - H(x,p)$ agrees with Feynman's prescription for the path integral and leads to the **semiclassical Koopman-van Hove equation** [2]

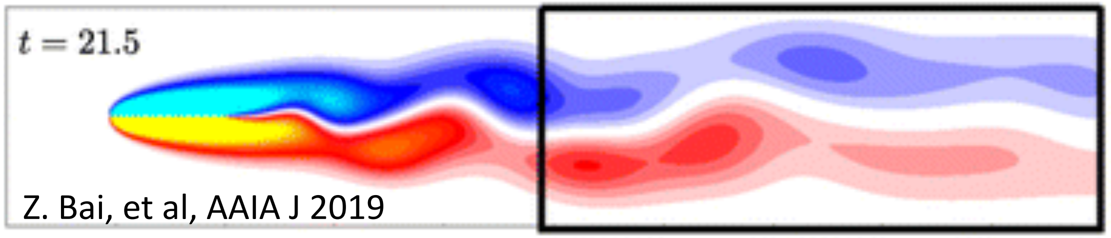
[1] I. Joseph, Phys. Rev. Research **2**, 043102 (2020)
[2] I. Joseph, J. Phys A: Math. Theor. **56** 484001 (2023)

Choice of numerical advection operator is important for accuracy



Killer App? Use quantum machine learning to develop reduced-order models for native quantum simulation / data

- **Quantum machine learning [1] and principle component analysis [2] are potentially powerful techniques**
  - But, they have the I/O problem of getting the database of information in and out



Z. Bai, et al, AAIA J 2019

$$|\psi\rangle = \sum_x \psi_x |x\rangle$$

- **Quantum algorithms for reduced-order modeling of native quantum simulation or experimental data [3] could be the killer app!**
  - Quantum data assimilation [4] and closure of dynamical systems [5]

    qDMD: quantum Dynamic Mode Decomposition

    qSINDy: quantum Sparse Identification of Nonlinear Dynamics

[1] P. Rebentrost PRL 2014, M. Schuld PRA 2016, J. Biamonte, Nature Phys 2017 [2] S. Lloyd, Nature Phys., 2014
[3] B. Kiani PRA 2022 [4] D. Giannakis PRE 2019, D. Freeman PNAS 2023 [5] D. Freeman arXiv:2208.03390

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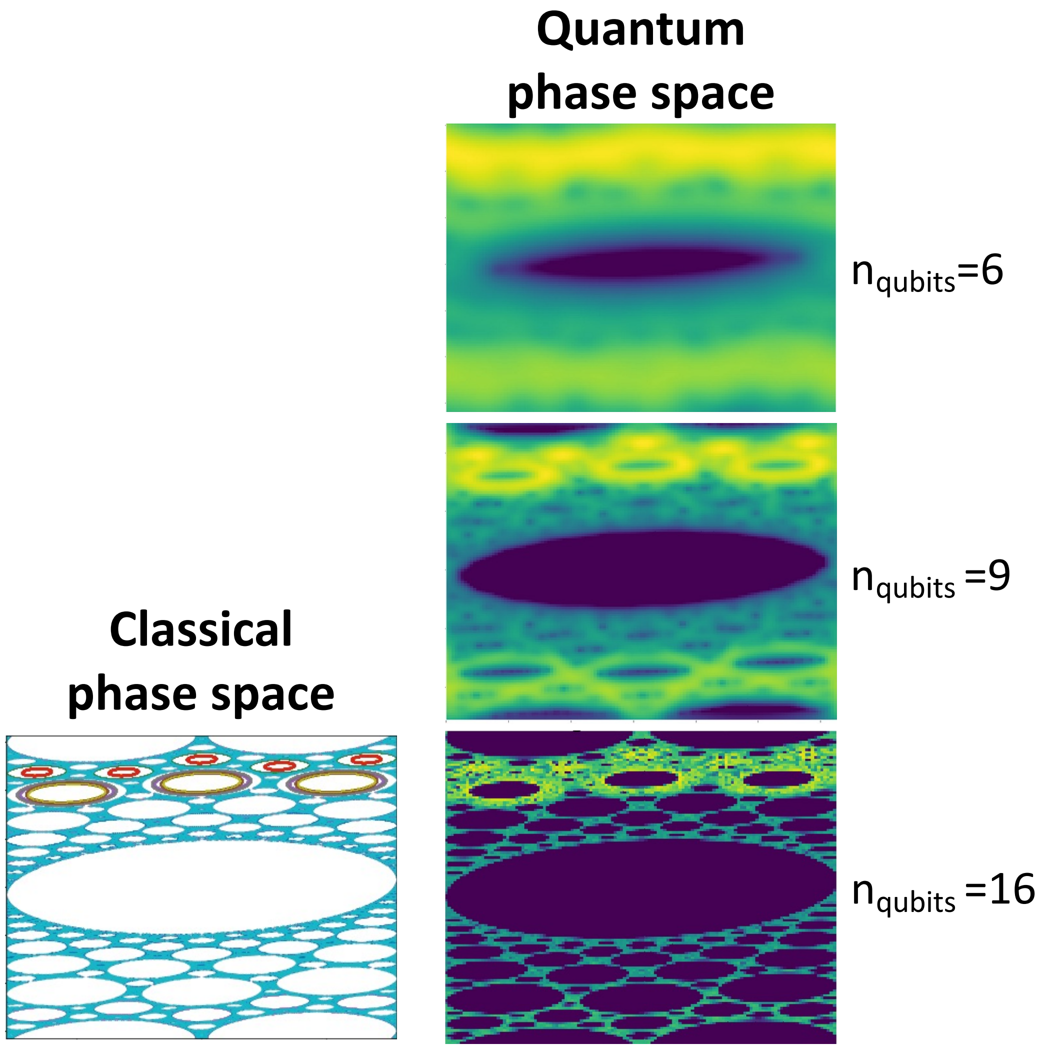
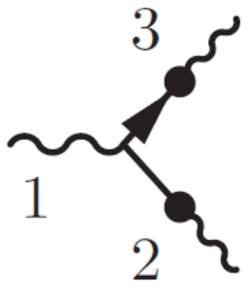


First plasma application: simulating three-wave interactions [1]

- **Cubic couplings are ubiquitous in plasmas, fluids, & nonlinear media**
  - Examples: nonlinear optics, laser-plasma interactions, weak turbulence, gauge theory, lattice QED …
  - Interaction Hamiltonian

$$H_I = igA_1A_2^\dagger A_3^\dagger - ig^*A_1^\dagger A_2A_3$$

$$\omega_1 = \omega_2 + \omega_3$$
$$\mathbf{k}_1 = \mathbf{k}_2 + \mathbf{k}_3$$

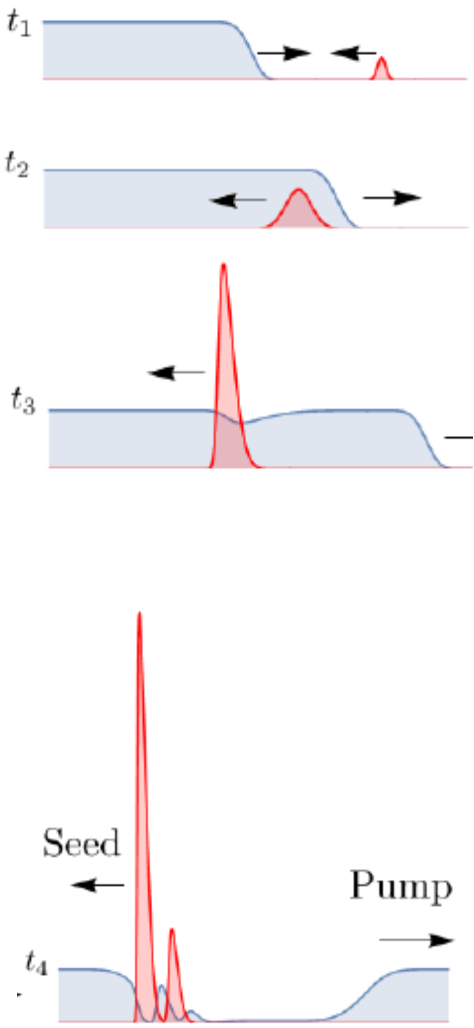


  - Envelope equations for resonant interactions

$$d_tA_1 = -g^*A_2A_3 \quad d_tA_2 = g^*A_1 A_3^\dagger \quad d_tA_3 = g^*A_1 A_2^\dagger$$

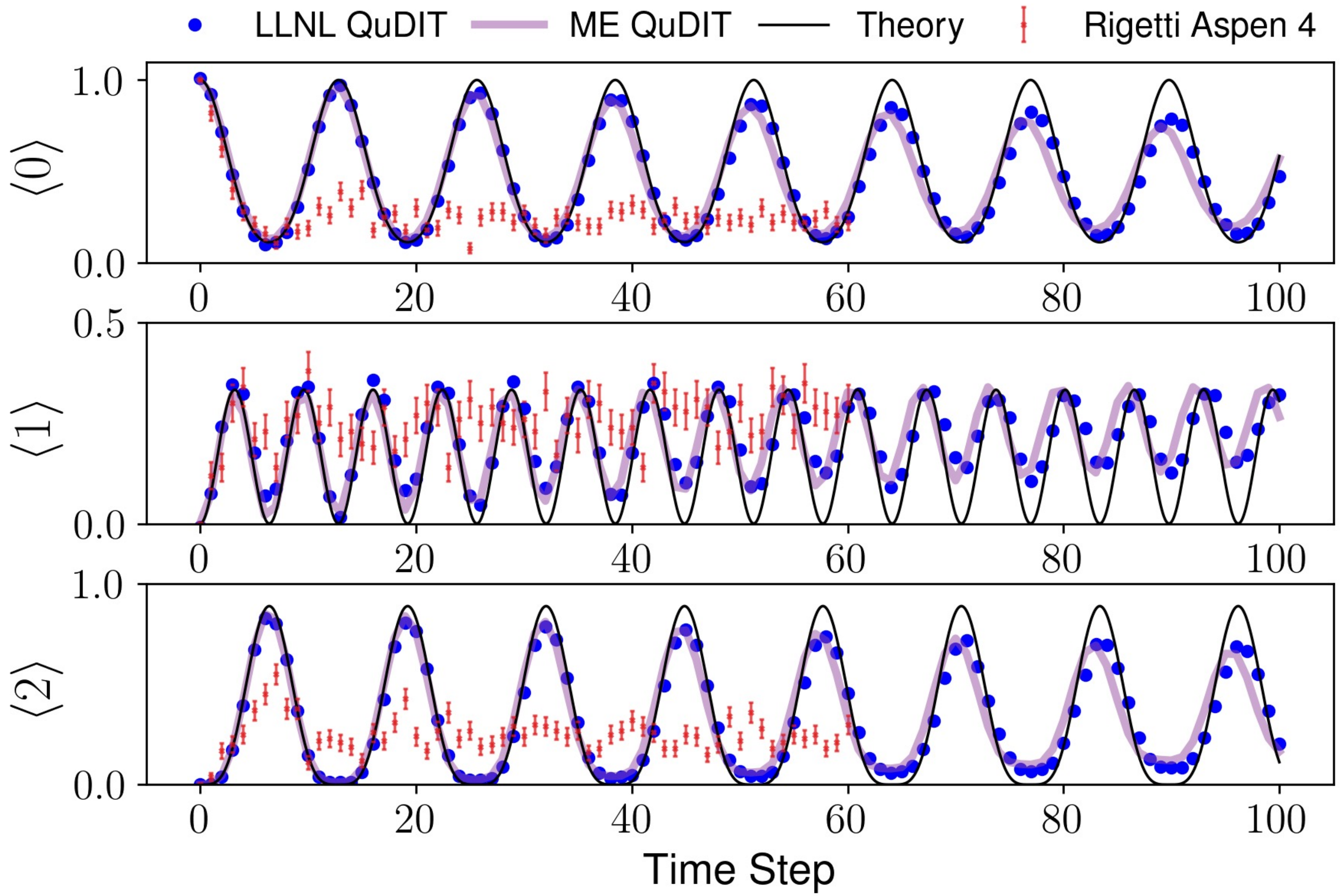
  - Quantized version $\left[A_j, A_k^\dagger\right] = \delta_{jk}$

- **Developed a new quantum algorithm for simulating 3-wave dynamics [1]**
  - Transform to action-angle variables
  - Evolve a sparse tridiagonal Hamiltonian system



[1] Y. Shi, A. R. Castelli, X. Wu, et al, Phys. Rev. A 103, 062608 (2021)

Optimal control approach to 3-wave yields ~10x improvement on LLNL QuDIT [1]



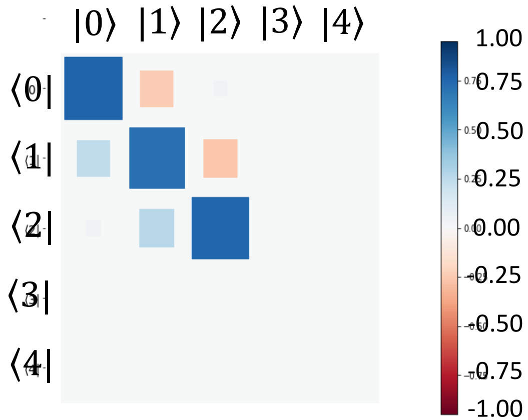
- Results of **LLNL QuDIT** (**blue**) are close to **analytic solution** (**black**) & match **Lindblad Master Equation (ME)** simulation (**purple**)
- Results of **Rigetti Aspen-4 platform** (**red**) perform well for first ~9 time-steps, but use **17x as many gates per step**
- On both platforms, decay and dephasing noise limit the fidelity after ~100 gate repetitions
- Combining gates into single control pulse improves long-term fidelity

[1] Y. Shi, A. R. Castelli, X. Wu, et al, Phys. Rev. A 103, 062608 (2021)

Optimal control approach compresses many standard gates into one

- Optimal control pulse c(t) generates the desired unitary transformation $\mathbf{U}(T)$ for a single time step of length T

$$\mathbf{U}(T) = \mathcal{T}e^{-i\int_0^T (\mathbf{H}_0 + c(t)\mathbf{H}_c)dt}$$

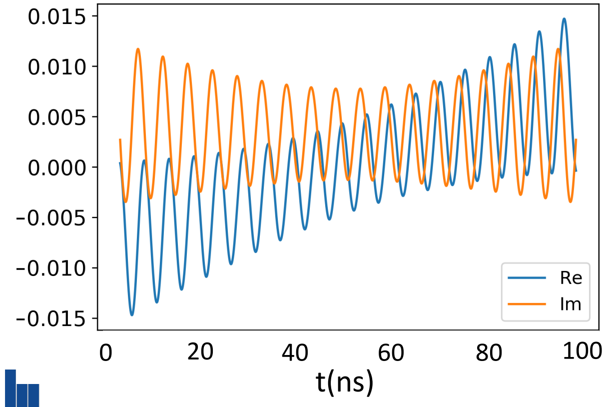


- Although the dynamics is nontrivial, populations achieve the desired levels by the end of the pulse

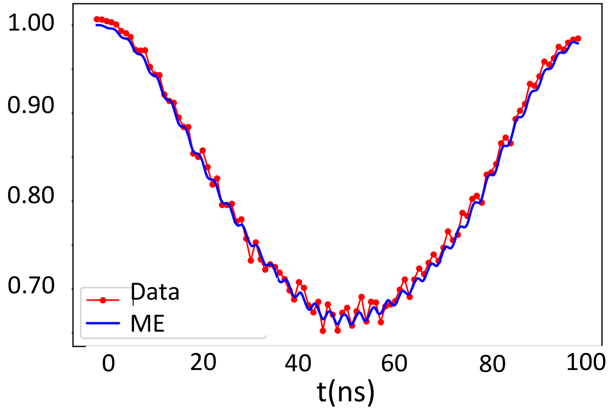
- Density matrix evolution is well-described by an experimentally calibrated decoherence model: the **Lindblad Master Equation (ME)**

$$\partial_t \boldsymbol{\rho} = \frac{1}{i\hbar}[\mathbf{H}, \boldsymbol{\rho}] + \nu^{jk}\left(\mathbf{L}_k\, \boldsymbol{\rho}\, \mathbf{L}_j^\dagger - \frac{1}{2}\{\mathbf{L}_j \mathbf{L}_k^\dagger, \boldsymbol{\rho}\}\right)$$

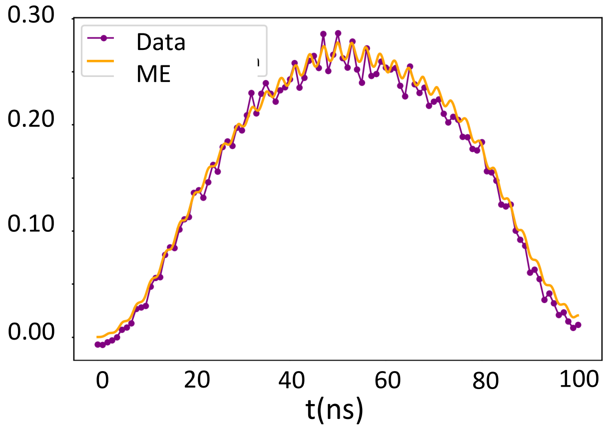
$c(t)$



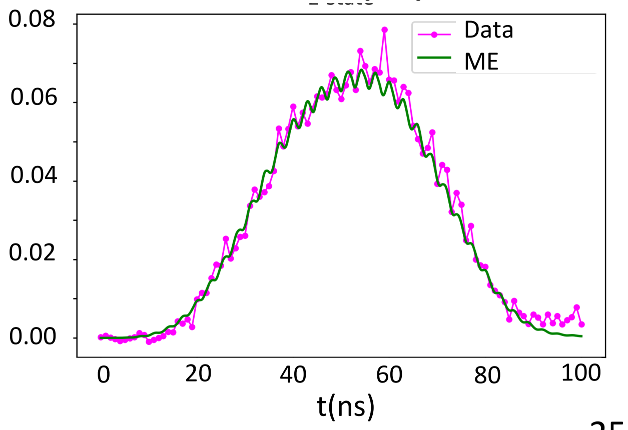
0 state pop.



1 state pop.

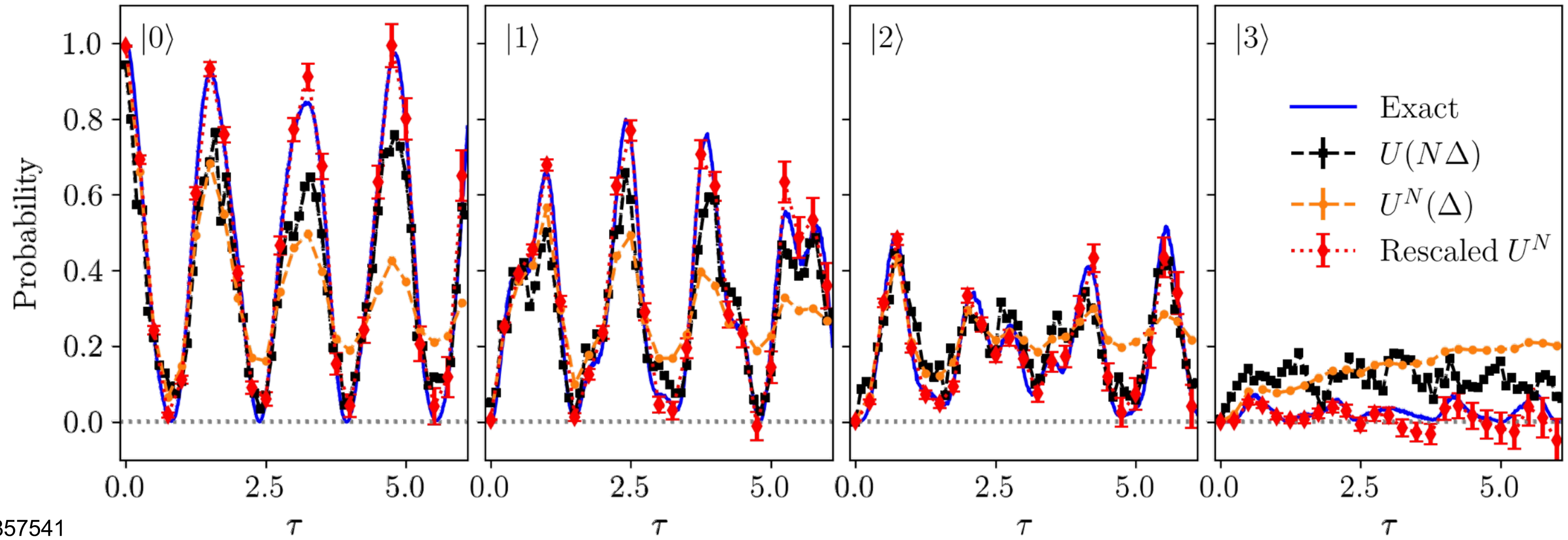


2 state pop.



We now improved the performance of the Rigetti platform for a chaotic 3-wave and 4-wave mixing problem using error mitigation

- **Fast-forwarding:** Directly compiling $U(N\Delta t)$ rather than using $U^N(\Delta t)$ results in fewer gates
- **Randomized compilation[1] :** suppresses *coherent errors*, turning them into *incoherent errors*
  - Compile $U(\Delta t)$ to multiple equivalent circuits, select randomly for each time step
- **Rescaling**[2]: probability P to extract signal S from incoherent noise using ansatz $P = Se^{-\gamma G} + 1/2^n$
  - Signal decay rate γ calibrated with cycle benchmarking



[1] PRA **94**.052325
[2] PRR **4**, 033140

The quantum sawtooth map (QSM) is the most efficient chaotic system to simulate on a quantum computer [1]

- **Classical sawtooth map depends on kicking strength K**

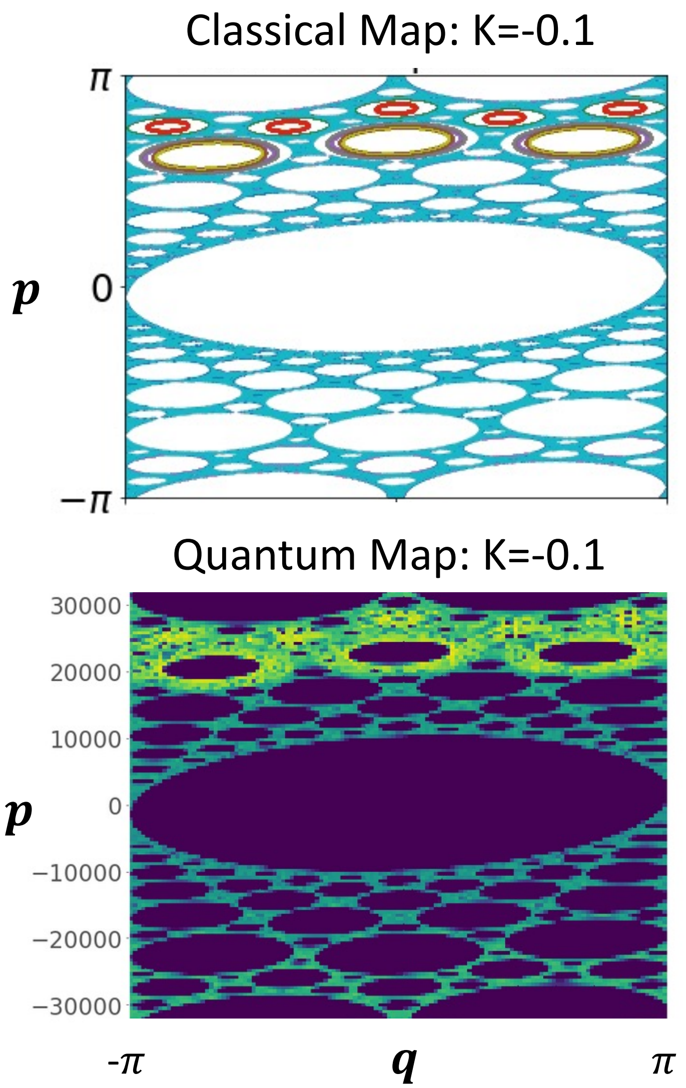
$$H_{saw} = \frac{1}{2}p^2 - \frac{1}{2}Kq^2 \sum_n \delta(t-n) \qquad \text{for } q \bmod 2\pi$$

- **Quantum sawtooth map also depends on $\hbar$**
  - Map eigenvalues of p to n qubits that represent $N = 2^n$ states
  - $\hbar$ is quantized in order to match periodicity in p

$$\Delta p = 2\pi = \hbar N \qquad \hbar = 2\pi/N$$

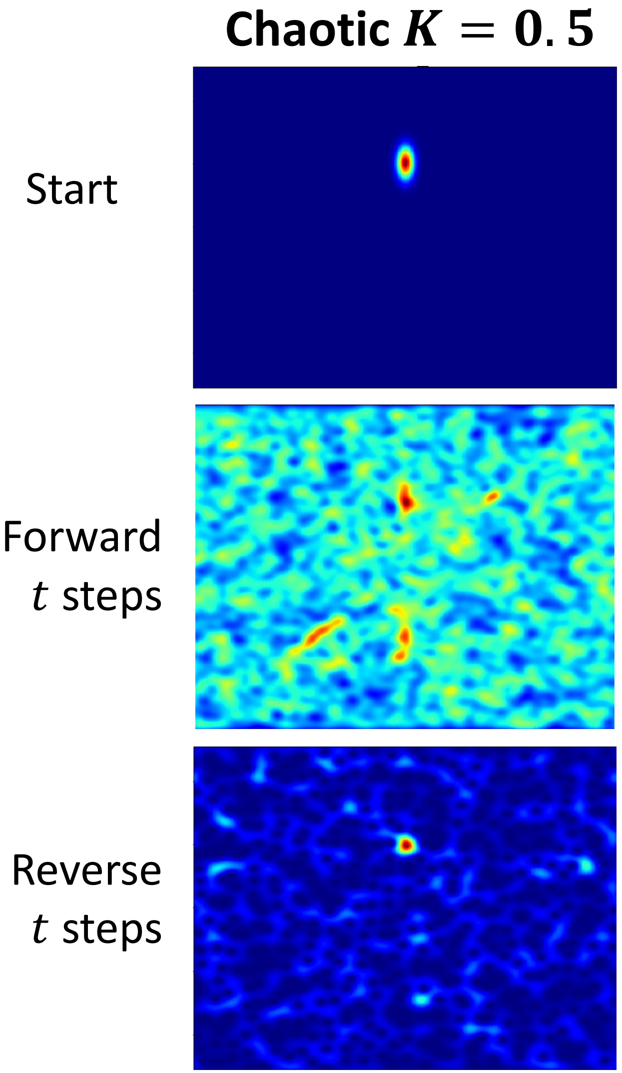
  - Quantum propagator has four stages:

$$U_{QSM} = \hat{\mathcal{T}} e^{-i\int H_{saw} dt/\hbar} = U_{kin}(\hbar)\, U_{QFT}^{-1}\, U_{pot}(K/\hbar)\, U_{QFT}$$



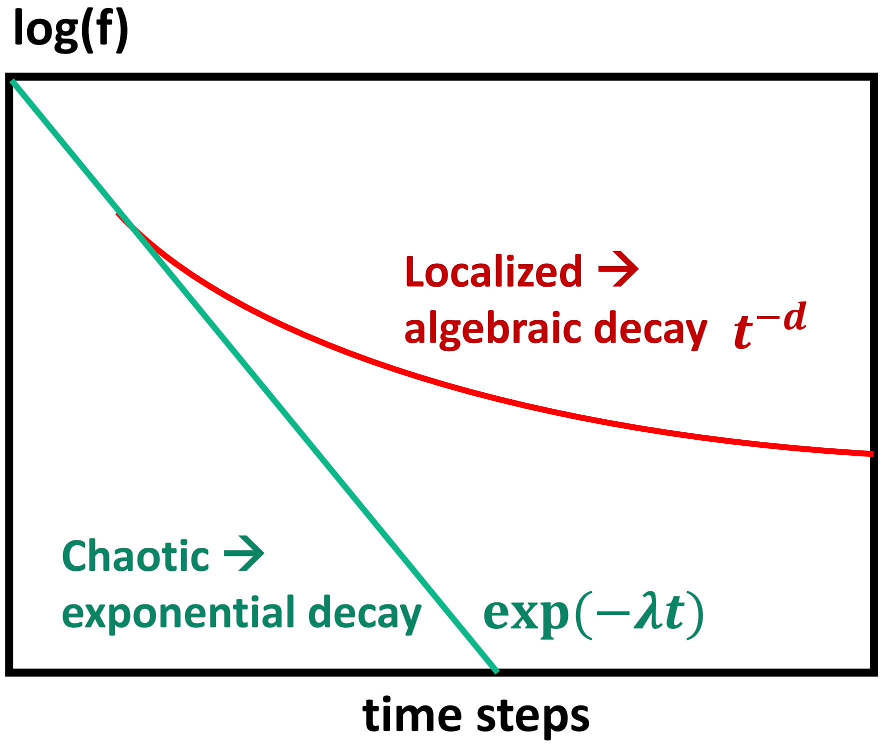
[1] G. Benenti, et al, PRL 87 227901 (2001)

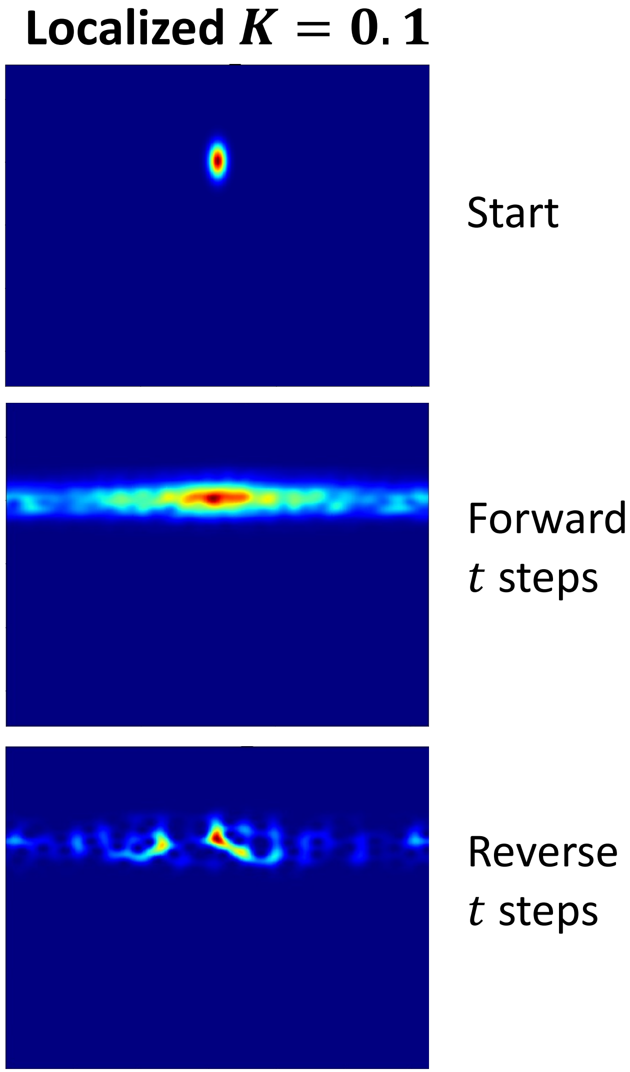
Noisy quantum computers can efficiently compute key signatures of chaos: Lyapunov rate λ = exponential separation of trajectories [1,2]



Simply measure the fidelity

$$f = \left|\langle \psi_{\text{actual}} | \Psi_{\text{target}} \rangle\right|^2$$



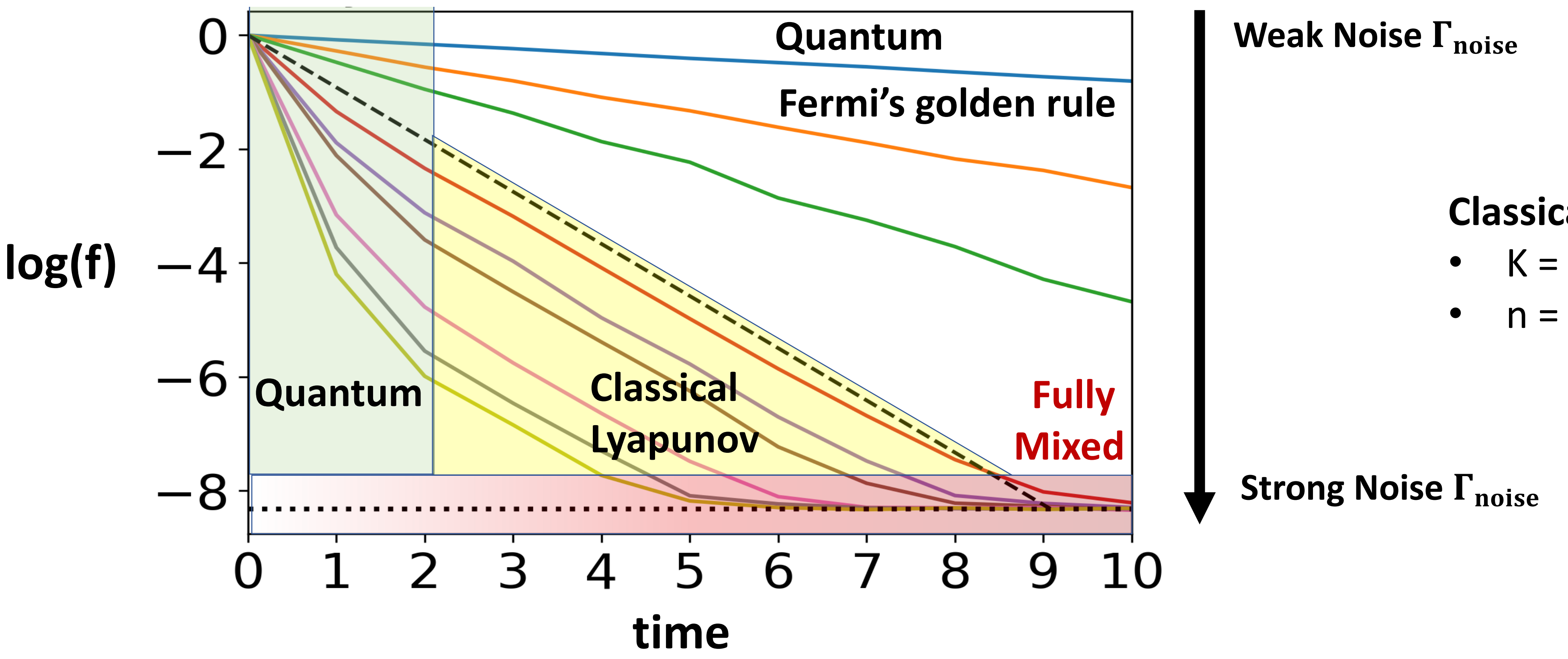


[1] G. Benenti, et al., Quantum Info. Proc. **3**, 273 (2004)
[2] Ph. Jacquod, et al., Adv. Physics **58**, 67 (2009)

Semiclassical theory predicts that fidelity has two components that decay at different rates*

*M. D. Porter, I. Joseph, Quantum **6**, 799 (2022)

$$f(t) \approx f_{\text{Quantum}} e^{-\Gamma_{\text{noise}} t} + f_{\text{Classical}}\, e^{-\lambda_{\text{Lyap}} t} + 1/N$$

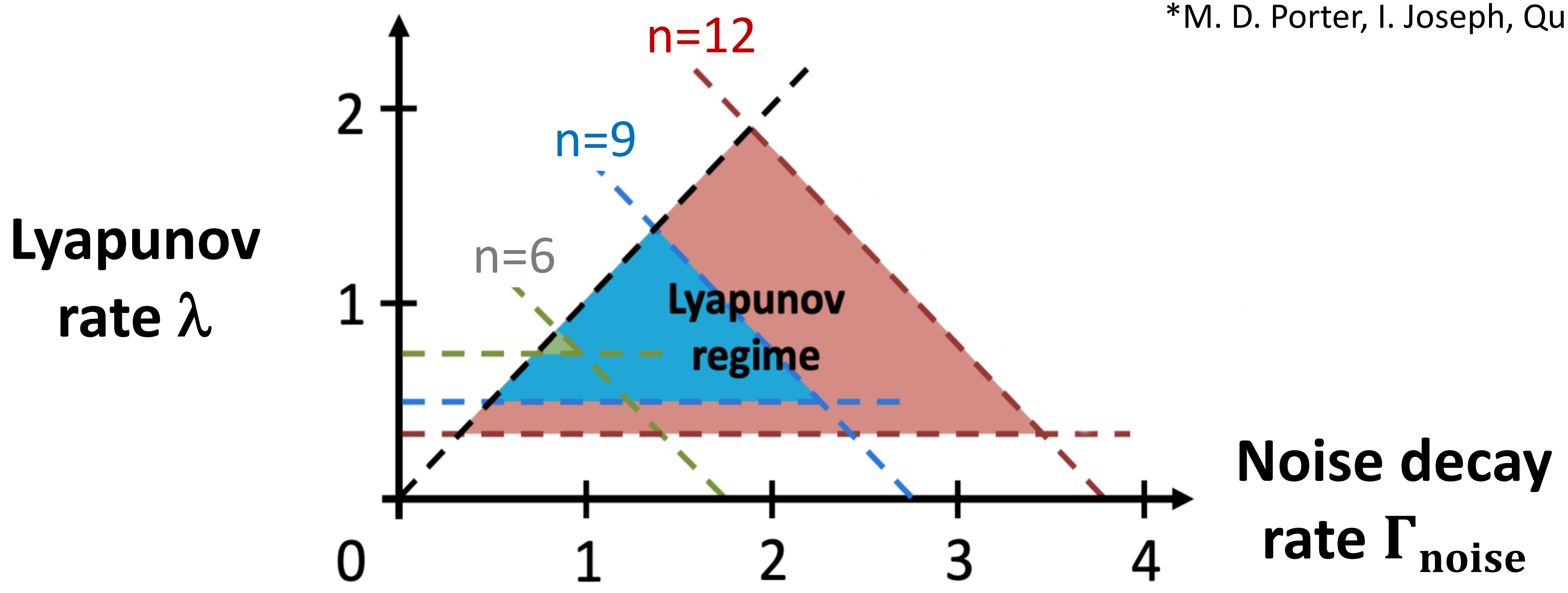


Classical simulation

- K = 0.9
- n = 12 qubits

Fidelity phase diagram determines whether the Lyapunov rate can be observed*

*M. D. Porter, I. Joseph, Quantum **6**, 799 (2022)



Key Limitations

- Dynamics must be chaotic
- Lyapunov rate < noise decay rate
- Overall decay rate cannot be too fast
- Noise cannot be too strong or too weak

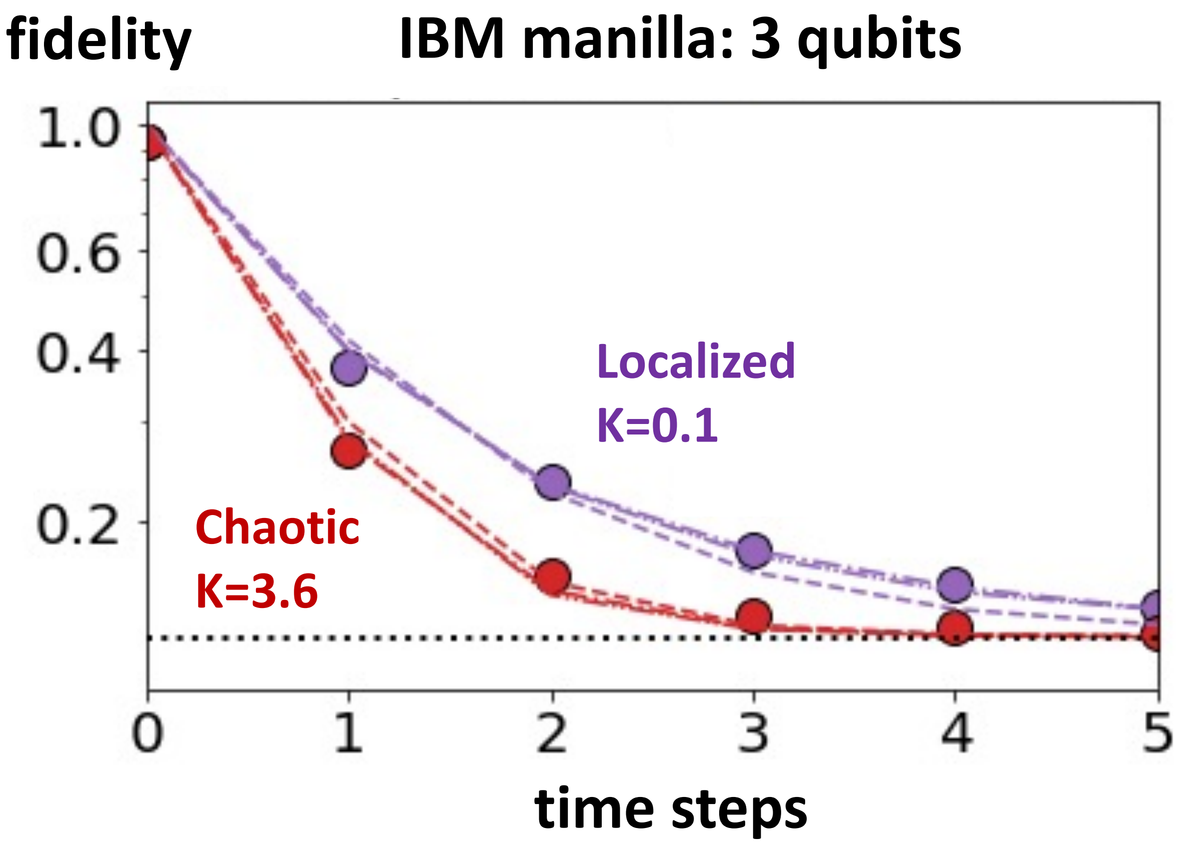
Key Requirements

- At least **6 qubits**
- Noise must be reduced by **10-100x**
- Depends on architecture
  - Parallelization, layout, etc.

We performed the first gate-based quantum simulation proving that fidelity depends on dynamics in addition to gate-count*

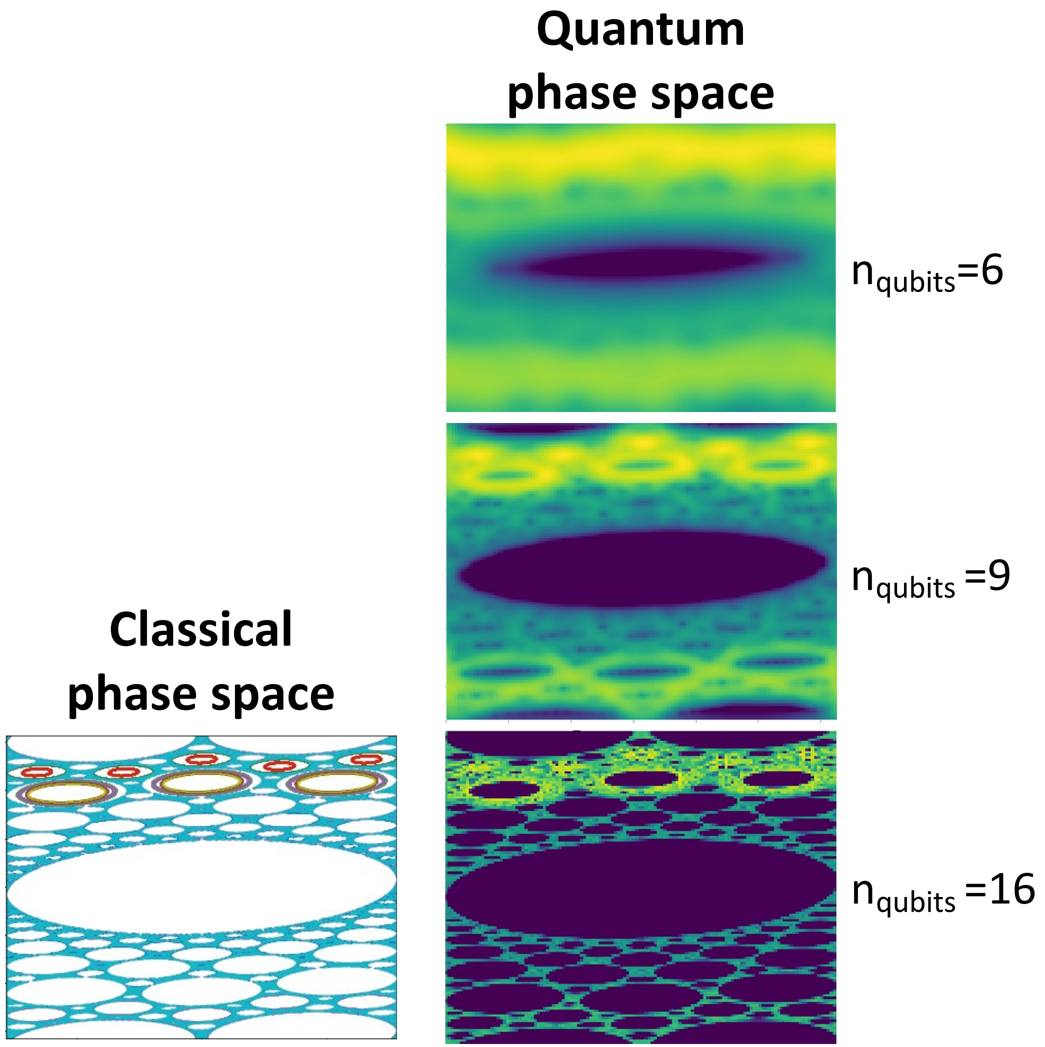
*M. D. Porter, I. Joseph, arXiv:2206.04829

- **Decay rate is faster for chaotic dynamics with same # of gates**
  - Only single-qubit rotation angles change
- **Saturates at low and high values of K**
  - Increases during the transition to chaos, but does not keep increasing with Lyapunov rate
- **Chaos generates delocalized entangled states that are more sensitive to noise**
  - Actual error rates are 3 – 5x larger than reported
  - Lindblad decoherence model infers 3x larger dephasing rate $1/T_2^*$



Outline: Quantum Computing for Fusion Energy Sciences

- **Intro to Quantum Computing**
  - Qubits
  - Quantum Algorithms
- **Quantum Simulation Algorithms**
  - Linear
  - Nonlinear
- **Testing Quantum Hardware Platforms**
  - Error Mitigation
  - Error Utilization
- **Conclusions & Outlook**



Conclusions & Outlook

- **Quantum computing holds great promise for accelerating scientific discovery**
  - Efficient Fourier transforms, sparse linear solvers, sparse Hamiltonian simulation, variational eigensolvers, …
  - Chemistry, materials science, high-energy physics, nuclear physics, …, **fusion energy science!**

- **Quantum simulation of the PDF of nonlinear dynamical systems can achieve exponential speedup over Eulerian methods and up to quadratic speedup over Monte Carlo methods**
  - Simulations of fluids, plasmas, molecular dynamics, finance, ecology, epidemiology, …
  - Quadratic speedup attained for high dimension and lack of smoothness
  - Exponential speedup for end-to-end app's likely requires problems with special structure

- **Algorithms that utilize noise have potential for near-term quantum advantage**
  - Simulate open system dynamics with an open quantum system
  - Passive and active error mitigation, e.g. quantum optimal control, are under extensive development
  - Decoherence controls the **"information confinement time"**

I. Joseph, Y. Shi, M. D. Porter, et al, Phys. Plasmas **30** 010501 (2023)

Quantum Computing for Fusion Energy Science Applications

I. Joseph (LLNL), M. D. Porter (Sandia), Y. Shi (U Colorado Boulder), B. Evert (Rigetti), et al.

- **Quantum computing holds great promise for accelerating scientific discovery**
  - Efficient Fourier transforms, sparse linear solvers, Hamiltonian simulation, variational eigensolvers, …
  - Chemistry, materials science, high-energy physics, nuclear physics, …, **fusion energy science!**

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  - Simulate open system dynamics with an open quantum system
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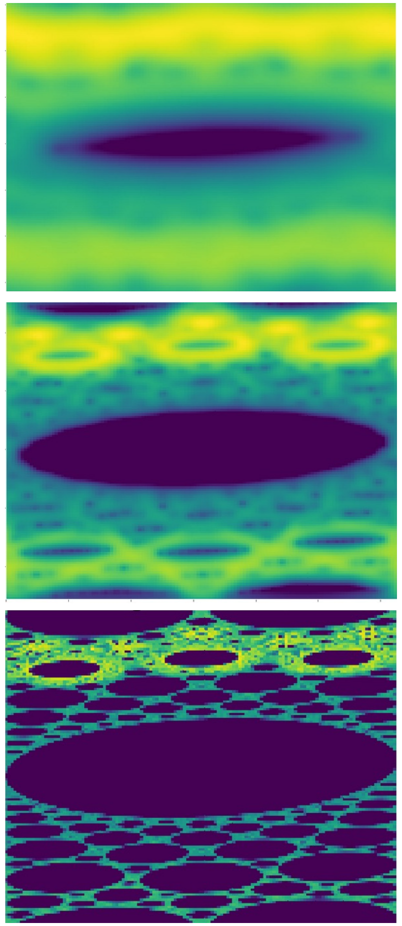
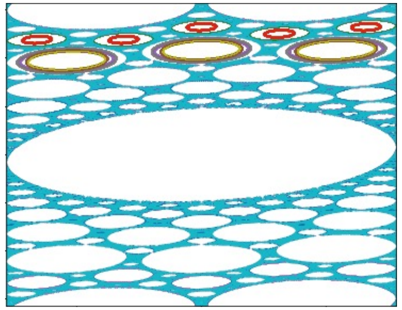
  - Decoherence controls the **"information confinement time"**

Quantum phase space



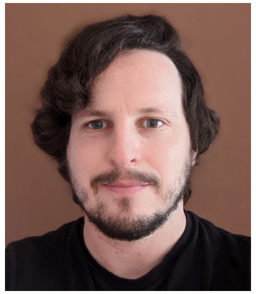
Classical phase space



I. Joseph, Y. Shi, M. D. Porter, et al, Phys. Plasmas **30** 010501 (2023)

Our team consists of experts in MFE, HEDS and QIS

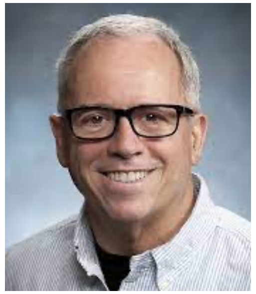
- **Core Team**
  - **MFE:** Ilon Joseph (PI), Vasily Geyko, *Jeff Parker (FY20)*
  - **HEDS:** Frank Graziani, Stephen Libby, Yuan Shi (U Colorado Boulder)
  - **QIS:** Jonathan DuBois, Al Castelli, Max Porter (Sandia), Gabriel Woolls (Caltech/Berkeley)


Al Castelli


Jonathan DuBois

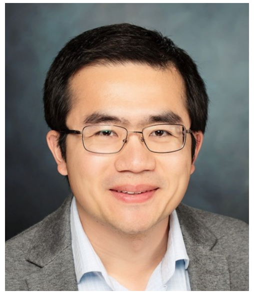

Vasily Geyko


Ilon Joseph


Frank Graziani


Steve Libby


Max Porter


Yuan Shi


Gabriel Woolls

- **LLNL Collaborators**
  - **Quantum Coherent Device Physics Group:** Kristi Beck (formerly IonQ), Yujin Cho, Yaniv Rosen, Xian Wu (now at Rigetti)
  - **NACS:** Roger Minich, Kyle Wendt, Sofia Quaglioni; **CASC:** Anders Petersson, Stephanie Gunther
  - **Students:** Jessica Tucker (SJSU), Chris Yang (Caltech, SSGF Fellowship)

- **External Collaborators**
  - Robin Blume-Kohut (Sandia), Denys Bondar (Tulane), Frank Gaitan (LPS), Cesare Tronci (U. Surrey, Tulane), R. Tyler Sutherland (Quantinuum)

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Quantum information science (QIS) may soon lead to game-changing capabilities for science in general

- **Quantum Sensing:** improves measurement sensitivity
  — Heisenberg limit for noise/signal ratio scales as 1/N instead of 1/sqrt(N)

Quantum-Enhanced Advanced LIGO Detectors in the Era of Gravitational-Wave Astronomy

M. Tse *et al.* Phys. Rev. Lett. **123**, 231107 (2019)

- **Quantum Communications:** secure information transfer
  — Intrinsically parallel data transfer / data compression

China Demonstrates Quantum Encryption By Hosting a Video Call

A. Nordrum, IEEE Spectrum (2017-10-03)

- **Quantum Computing:** polynomial or exponential gains in effective memory and computational power
  — Fourier transform, linear solvers, Hamiltonian simulation, …
  — **Today = Noisy Intermediate-Scale Quantum (NISQ) era**

Quantum supremacy using a programmable superconducting processor

F. Arute, *et al.* Nature. 127, 180502 (2019)

Strong Quantum Computational Advantage Using a Superconducting Quantum Processor

Yulin Wu, *et al.* Phys. Rev. Lett. 127, 180501 (2021)

Phase-Programmable Gaussian Boson Sampling Using Stimulated Squeezed Light

Han-Sen Zhong, *et al.* Phys. Rev. Lett. 127, 180502 (2021)

Semiclassical wavefunction yields efficient unitary representation [1]

- Since quantum algorithms act naturally on wavefunctions, consider a "semiclassical" ansatz

$$\psi(z,t) = \sqrt{f(z,t)}e^{i\theta(z,t)}$$

- Assume that the phase evolves as a scalar with a source

$$\partial_t \theta\Big|_z = -V\cdot\nabla\theta + L(z,t)/\hbar \qquad \partial_t\theta|_{z_0} = +V\cdot\nabla\theta - L(z,t)/\hbar$$

  - For classical dynamics, the **classical Lagrangian** $L(z,t) = p\cdot\partial_p H - H(x,p)$ is the natural choice because it agrees with Feynman's prescription for the path integral & has special Hamiltonian structure [2]

- Inserting the definitions leads to the **"Koopman-van Hove" equation** [1-3]

$$i\hbar\partial_t\psi\Big|_z = -i\hbar(V\cdot\nabla\psi + \nabla\cdot V\psi)/2 - L\psi$$

$$i\hbar\partial_t\psi\Big|_{z_0} = +i\hbar(V\cdot\nabla\psi + \nabla\cdot V\psi) + L\psi$$

[1] I. Joseph, Phys. Rev. Research 2, 043102 (2020)
[2] C. Tronci, I. Joseph, J. Plasma Phys. 87, 835870402 (2021)
[3] I. Joseph, arXiv:2306.01865 (2023)

Quantum algorithms for differential equations come in many flavors

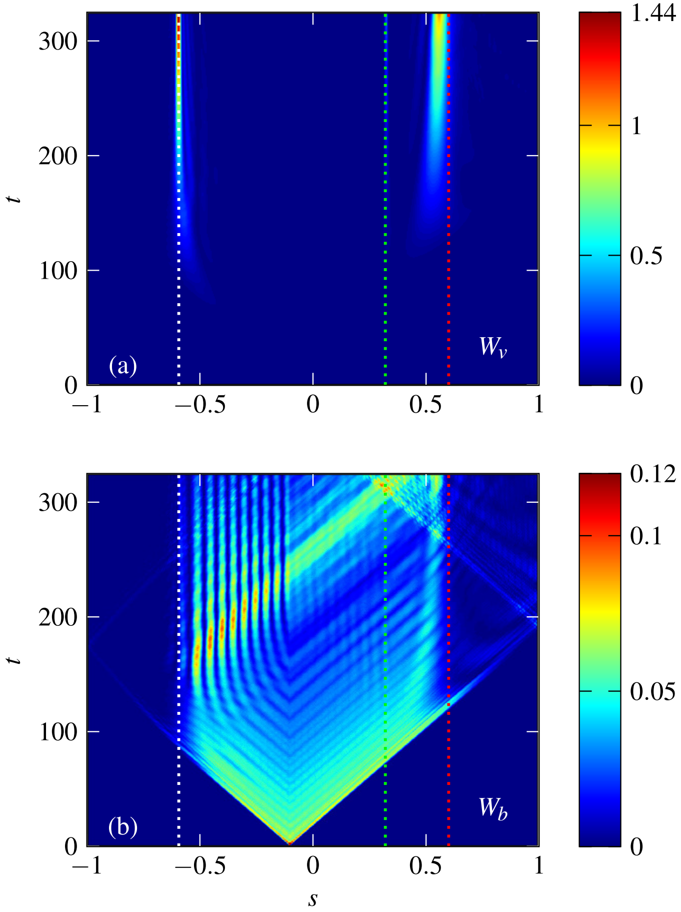
- **Linear vs. Nonlinear**
  - For sparse Hamiltonians, quantum computers can exponentially speed up linear operations
  - Koopman & Carleman: Nonlinear systems can be embedded within an infinite-dimensional linear system
- **Deterministic vs. Stochastic**
  - Amplitude estimation can quadratically speed up Monte Carlo sums and integrals = observable estimation
  - Quantum walks can quadratically speed up the mixing time of Markov chains = time to solution
- **Variational Algorithms and Quantum Machine Learning**
  - Classical computer can efficiently perform nonlinear operations that drive a quantum computer
  - Quantum machine learning can potentially avoid the use of classical computers altogether except for I/O
- **Discrete vs. Continuous Variable computation for classical PDEs & quantum field theory**
  - Uses a quantum field theory as the computational basis
  - Classical limit is a classical field theory, i.e. a set of PDEs such as Maxwell's equations

Speedup requires exploiting special structure and/or sparsity

- **Trotter-Suzuki & Lie group decompositions [1] work well for specific Hamiltonians**

$$e^{n(A+B)} \approx \prod_{j=1}^{n} e^{B/2} e^{A} e^{B/2} = e^{-B/2} \left(\prod_{j=1}^{n} e^{B} e^{A}\right) e^{B/2}$$

- **Black box simulation methods work well for sparse Hamiltonians**
  - — "Efficiently row-computable sparse" matrices
  - — Linear Combination of Unitaries (LCU) [2]; spectral methods [3]
- **Quantum signal processing (QSP) & qubitization [4], eigenvalue & singular value transformation [5] use block-encoded Hamiltonians**
  - — Block encoding allows non-unitary operations to be performed!



I. Novikau, E. Startsev, I. Dodin
Phys. Rev. A **105**, 062444 (2022)

[1] S. Lloyd 1996 [2] D. Berry 2017 [3] A. Childs 2021 [4] G. Low & I. Chuang 2017 [5] A. Gilyen 2019

Sparse linear evolution can be solved using black-box methods

- **Choose a basis for finite-dimensional numerical discretization**
  - **Possible choices of basis functions $\phi_n(z)$**
    - **Spectral [1,2]** e^{inz}, **orthogonal polynomials** $H_n(z)$, etc., …
    - **Finite difference & finite element:** local orthogonal polynomials
    - **Carleman linearization [3,4]:** polynomials z^k
    - **Reproducing Kernel Hilbert Spaces [2]:** allow pointwise evaluation

$$\psi(z,t) = \sum_n \psi_n(t)\phi_n(z)$$

$$i\hbar \frac{d}{dt}\psi_n = \sum_m H_{nm}\psi_m$$

- **If the evolution is unitary, use the quantum Hamiltonian simulation algorithm (QHSA) [1,2]**

$$\psi(t) = \mathbf{U}_{approx}\psi(0) \approx \mathrm{T}\, e^{-i\int \mathbf{H}dt/\hbar}\,\psi(0)$$

- **Otherwise, use the quantum linear differential equation solver algorithm (QLDA) [3,4]**
  - Uses **quantum linear solver algorithm (QLSA)** to propagate forward for small timesteps Δt

$$1 = \alpha + \beta \qquad (1 + i\alpha\mathbf{H}\Delta t/\hbar)\psi(t+\Delta t) \approx (1 - i\beta\mathbf{H}\Delta t/\hbar)\psi(t)$$

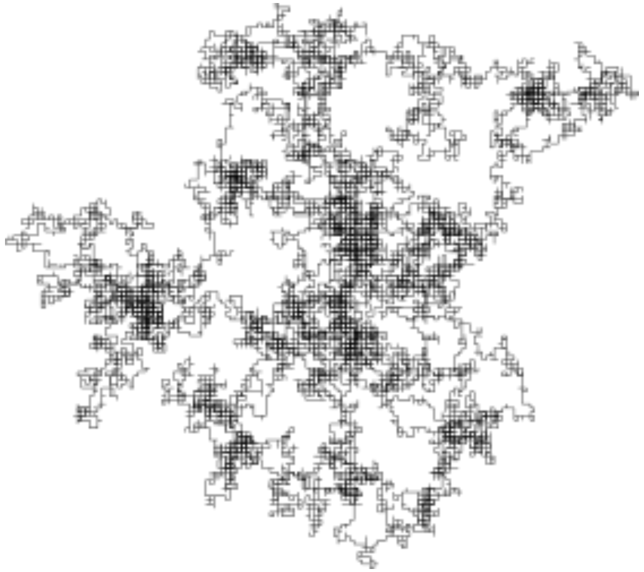
semi-implicit time splitting

[1] I. Joseph, Phys. Rev. Research 2, 043102 (2020)
[2] D. Giannakis, A. Ourmazzi, P. Pfeffer, et al., arXiv:2012.06097 (2022)
[3] Jin-Peng Liu, H.Ø. Kolden, H.K. Krovi, et al., PNAS 118, e2026805118 (2021)
[4] A. Engel, G. Smith, S. P. Parker, Phys. Plasmas 28, 062305 (2021)

Quantum walks yield up to quadratic speedup for solving stochastic differential equations (SDEs)

- **Quantum walks can speedup random walks [1] and Hamiltonian simulation [2]**
  - **Quadratic** speedup of the **mixing time** of Markov processes [1]

- **Quantum algorithms for sums and integrals [3] are based on quantum walks & accelerate the solution of SDEs [4] and Monte Carlo algorithms [5]**
  - Algorithm for turbulent mixing rate and turbulent reaction rate [6]
  - Algorithm for diffusion, Navier-Stokes [7], and radiation-hydrodynamics

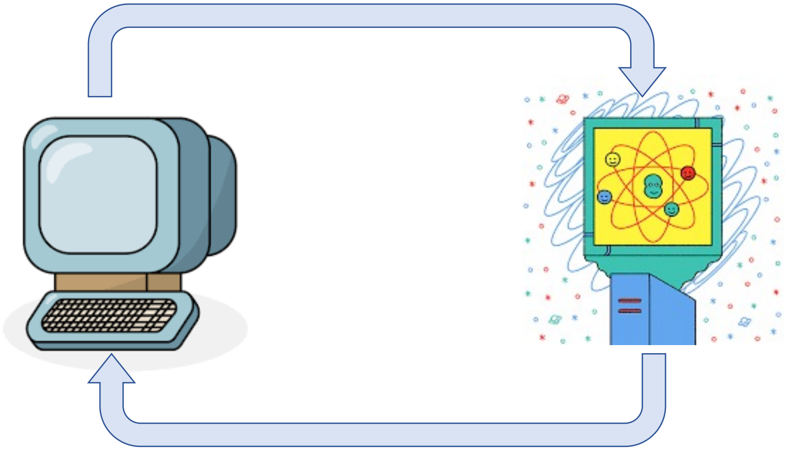


- **Also leads to new methods for solving multi-level SDEs [8]**
  - Algorithms for finance, Monte-Carlo collision operators, …

[1] M. Szegedy, FOCS 2004 [2] A. Childs, Comm. Math. Phys. 2010
[3] S. Heinrich & E. Novaks, 2001 [4] B. Kacewicz, J. Complexity 2004 [5] A. Montanaro, PRSA 2015
[6] F. Gaitan, Nature Phys. 2021 [7] G. Xu, et al AIAA J. 2018 [7] D. An, et al, Quantum 2021

Approach #3: Hybrid classical-quantum variational algorithms

- **Let a classical computer do the nonlinear work …**
  - **The classical computer iteratively solves a nonlinear optimization problem using standard techniques**
    The parameters to be optimized are encoded within the quantum program that will be run by the quantum computer
  - **At each step, the quantum computer evaluates a computationally challenging cost function**
    e.g. based on a Hamiltonian with many degrees of freedom



[1] M. Lubasch, et al, PRA 2015 [2] I. Joseph, et al, Phys. Plasmas 2023

Approach #3: Hybrid classical-quantum variational algorithms

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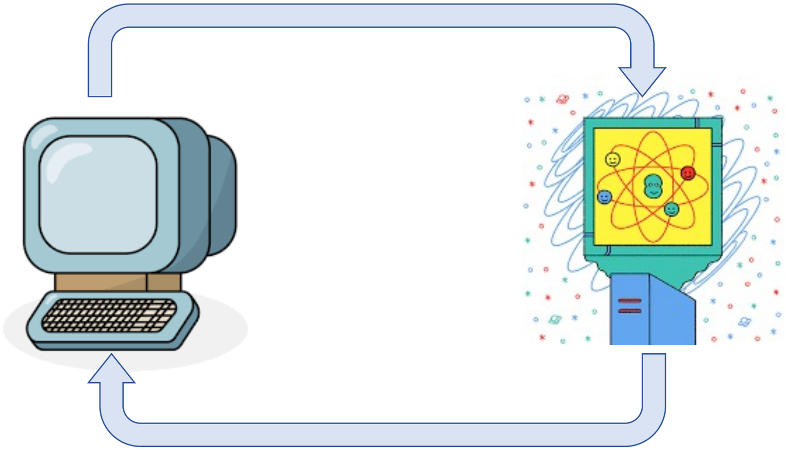
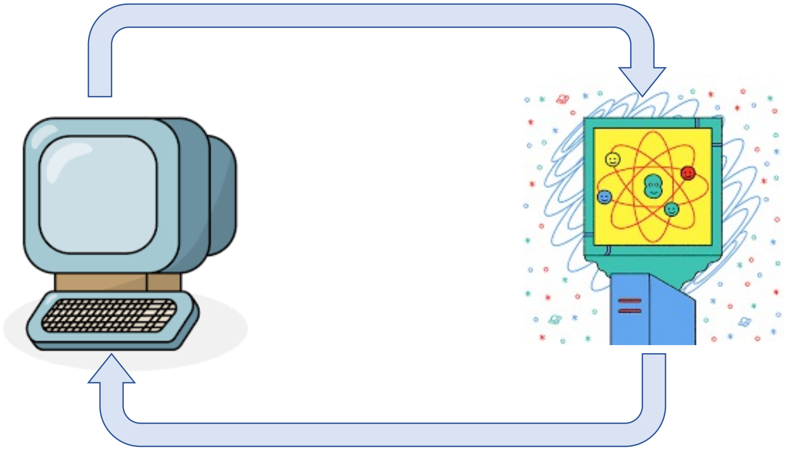


- **Complete data exchange generically only admits up to quadratic speedup**
- **Perhaps a high-order linear quantum model interacting with a low-order nonlinear classical reduced model can obtain exponential improvement [2]?**

[1] M. Lubasch, et al, PRA 2015
[2] I. Joseph, et al, Phys. Plasmas 2023

Variational algorithms have a few key steps …

- **For each time step, iterate until convergence [1]:**
  - Prepare initial ansatz
  - Solve equations using Hamiltonian simulation
  - Measure cost function and, potentially, gradients of the cost function
  - Execute step of classical optimization algorithm
  - Update ansatz



[1] M. Lubasch, et al, PRA 2015 [2] L. Bittel & M. Kliesch, PRL 2021

Variational algorithms have a few key steps … and a few key limitations

- **For each time step, iterate until convergence [1]:**
  - Prepare initial ansatz
  - Solve equations using Hamiltonian simulation
  - Measure cost function and, potentially, gradients of the cost function
  - Execute step of classical optimization algorithm
  - Update ansatz

NASA Earth Observatory: Himalayas

- **Optimization landscape may have intrinsic difficulties such as …**
  - Many local maxima and minima
  - Barren plateaus with little information on the gradient of the cost function

- **NP-complete optimization problems may not have any quantum advantage at all [2]**

[1] M. Lubasch, et al, PRA 2015

[2] L. Bittel & M. Kliesch, PRL 2021

PDEs are naturally encoded in the Continuous Variable (CV) model of quantum computing

- **Digital quantum computers are actually made out of quantum fields**
  - Photons, electrons, ions, atoms, …
- **Quantum field theory (QFT) is the quantum counterpart of classical field theory (PDEs)**
  - In the large number limit, quantum fields approach a classical field
- **The Continuous Variable (CV) model of quantum computation uses quantum fields directly**
  - The CV model has similarities with the analog model of classical computation
  - Average position and phase are CV
- **The CV model allows one to emulate PDEs and QFTs with basic QFTs: Dirac, Photon, …**
  - Similar to a "Wind Tunnel" or "Optics Experiment": works well for the task at hand, but not likely one can control everything perfectly

[1] Arazzola **[2] Shi Jin & Nana Liu** **[3] Vahala**

Amplitude estimation of physical observables[1–3] is up to quadratically more efficient than best classical methods

- **Expectation value $\langle \mathcal{O} \rangle = \sum_x \mathcal{O}(x) f(x)$ can be found by simulating a reversible classical computation of**

$$\phi(x) := \mathcal{O}^{1/2}(x)\psi(x) \qquad \phi'(x) := \sqrt{1 - |\phi(x)|^2} \qquad |\phi\rangle := \sum_x \phi(x)\,|x\rangle \,/\, \|\phi\|$$

- **Add an ancillary qubit to $|\psi\rangle$ and compute a state proportional to $|\phi\rangle$**

$$\mathcal{R}_\phi \,|\psi\rangle\,|0\rangle := \sum_{x=1}^{N} |x\rangle \left(\phi'(x)\,|0\rangle + \phi(x)\,|1\rangle\right)/N^{1/2} = \cos(\theta)\,|\phi'\rangle\,|0\rangle + \sin(\theta)\,|\phi\rangle\,|1\rangle$$

- **Amplitude estimation of the ancillary $|1\rangle$ state probability yields $\sin^2(\theta) = \langle \mathcal{O} \rangle / N$ with complexity $\sim Q_H/\epsilon$**

[1] D. S. Abrams and C. P. Williams, arXiv:quant-ph/9908083 (1999)
[2] S. Heinrich and H. Novak, *Proc. 4th Int. Conf. on Monte Carlo and Quasi-Monte Carlo Methods, Hong Kong 2000*, Springer-Verlag (2002)
[3] A. Montanaro, Proc. R. Soc. London, Ser. A 471, 20150301 (2015)

Motivation: Can we simulate chaotic dynamics on near-term universal quantum devices?

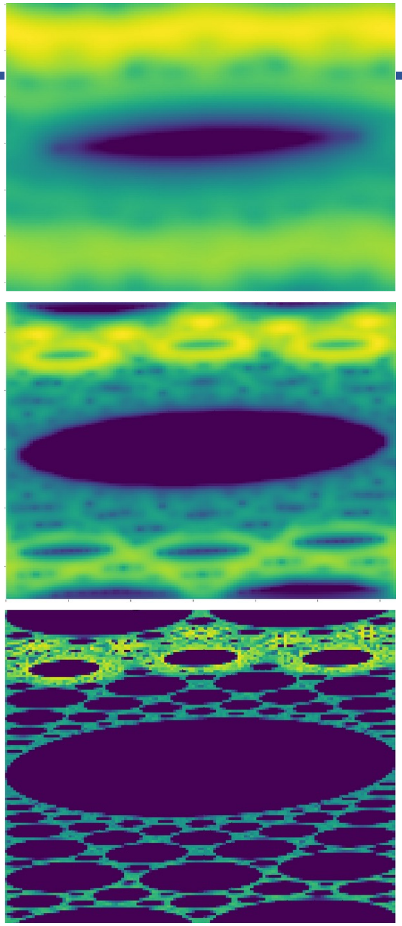
- **Interesting quantum simulations usually contain chaotic regions**
  - Quantum chaotic simulations are important for many body localization, black hole information scrambling, classical chaos, …
- **Efficient detection of quantum chaos can come from quantum-classical correspondence**
  - Quantum systems recover classical limit at small $\hbar$, but require many qubits
  - Quantum fidelity decay of perturbed Hamiltonian evolution can reveal classically chaotic or regular dynamics[1,2]
  - For chaotic dynamics, quantum fidelity can decay at the rate of the Lyapunov exponent λ, which measures the exponential divergence of classical trajectories[3]
- **Quantum maps allow efficient simulation of chaotic dynamics[4]**
  - A quantum map decaying at the Lyapunov rate may be the most resource-efficient signature of quantum chaos

Quasiprobability (Husimi Q)

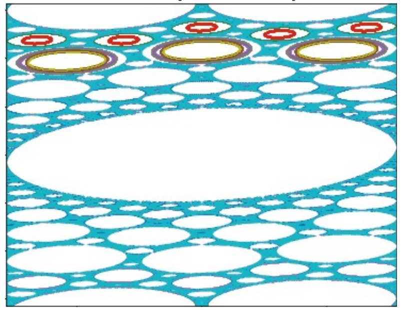
n_{qubits}=6

n_{qubits} =9

n_{qubits} =16



Classical phase space



[1]A. Peres, *PRA* 30.4 (1984) 1610
[2]Ph. Jacquod et al., *Advances in Physics* 58.2, 67-196 (2009)
[3]R. A. Jalabert, H. M. Pastawski, *PRL* 86.12, 2490 (2001)
[4]G. Benenti et al., *PRL* 87.22, 227901 (2001)

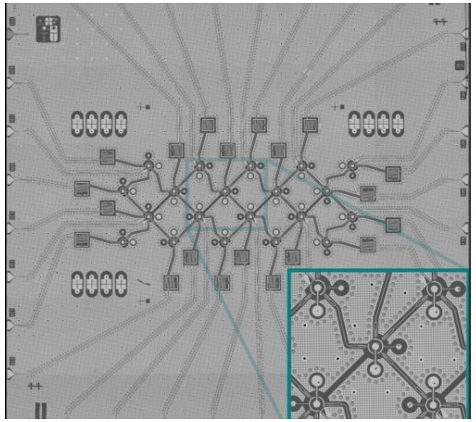
To date, we've used superconducting hardware platforms & are starting to use ion traps

- **IBM-Quantum Experience**
  — Open but limited access to 5 qubit devices with relatively good fidelity

IBM-Q
Eagle
127 qubits

- **Rigetti Quantum Cloud Services**
  — Rigetti-LLNL-USC Collaboration

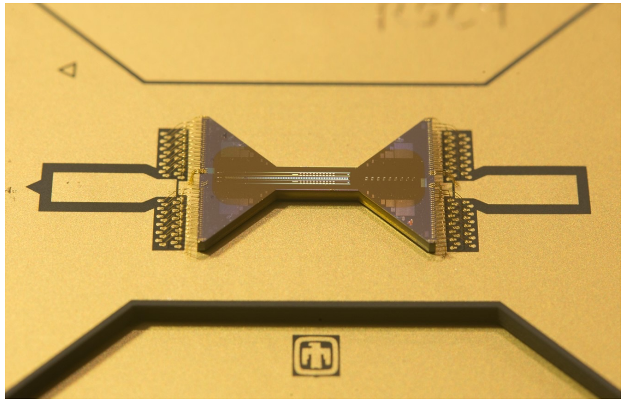
Rigetti
20 qubit device
(Aspen-M series have ~80 qubits)

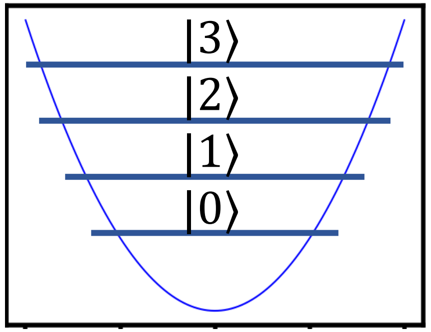


- **LLNL Quantum Design and Integration Testbed (QuDIT)**
  — Open access to 3-level and 4-level qudits rather than 2-level qubits

- **Sandia QSCOUT ion trap**

Sandia
Peregrine
6 qubits



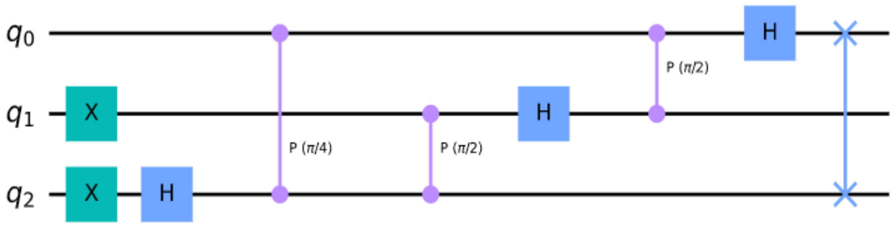


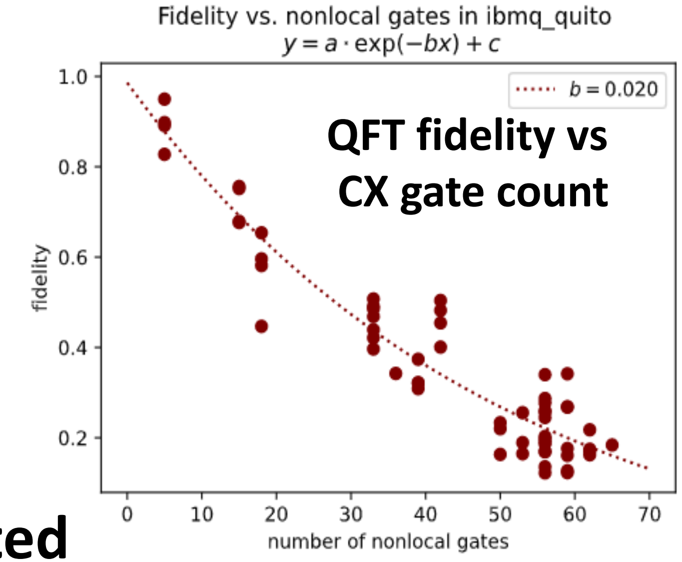
LLNL
Quantum Design & Integration Testbed (QuDIT)
~ 6 qubits

Lack of error-correction limits fidelity of present-day calculations

- **"Fidelity" is the figure of merit:** $F = \left|\langle\psi_{\text{expected}}|\psi_{\text{actual}}\rangle\right|^2$
  - — Single qubit gate fidelity (IBM-Q): 99.9% --> 700 useful operations before 50%
  - — Two qubit gate fidelity (IBM-Q): 99.5% --> 140 useful operations before 50%
  - — State preparation & measurement (SPAM): 95% --> error at beginning and end

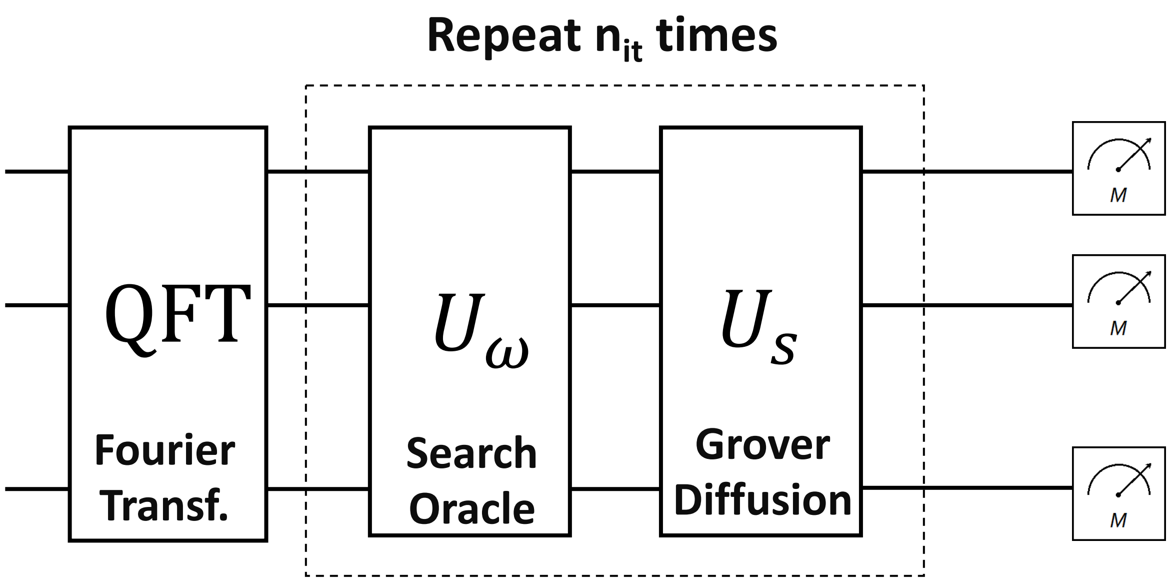
QFT circuit for 3 qubits

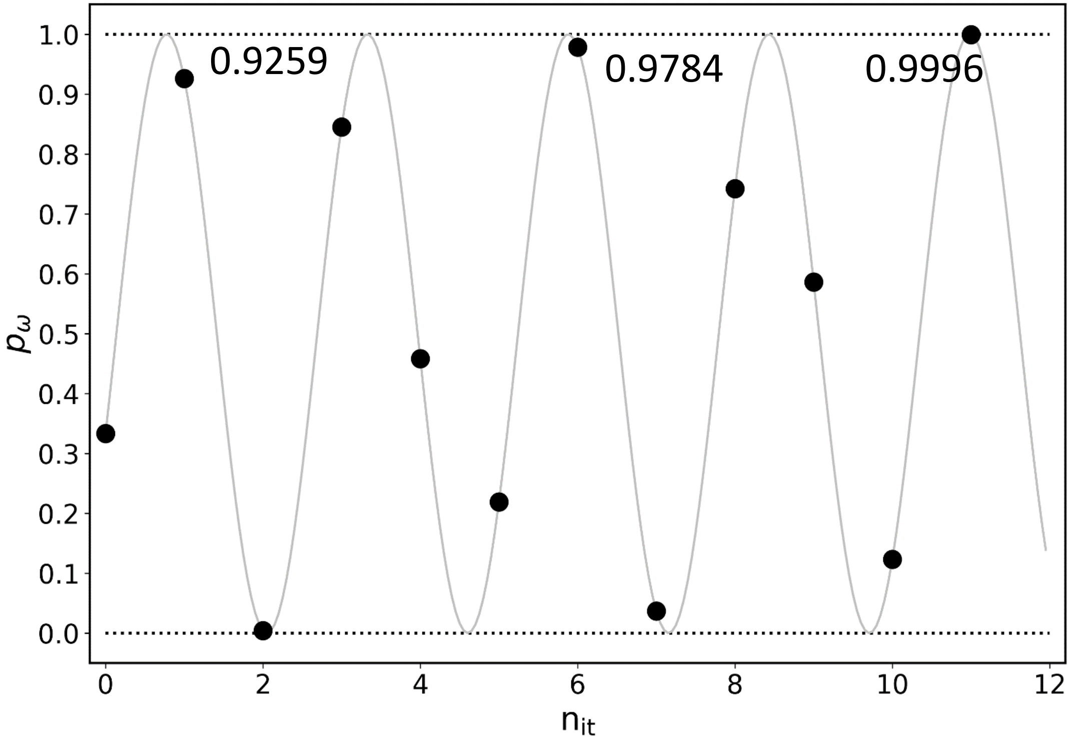




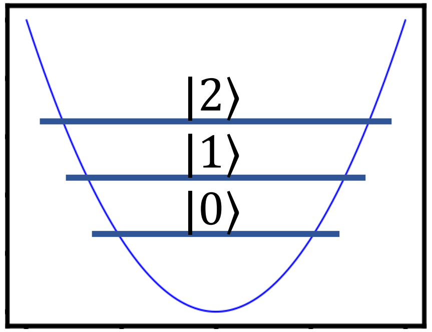
- **Infidelity for realistic calculations is ~2-5x worse than expected**
  - — Fidelity does not always decay at an exponential rate
  - — Coherent gate errors are important and need to be corrected for
  - — Coherent errors can be much more damaging to intended calculations

Grover's search algorithm can be modified to directly work on LLNL's 3-level QuDIT



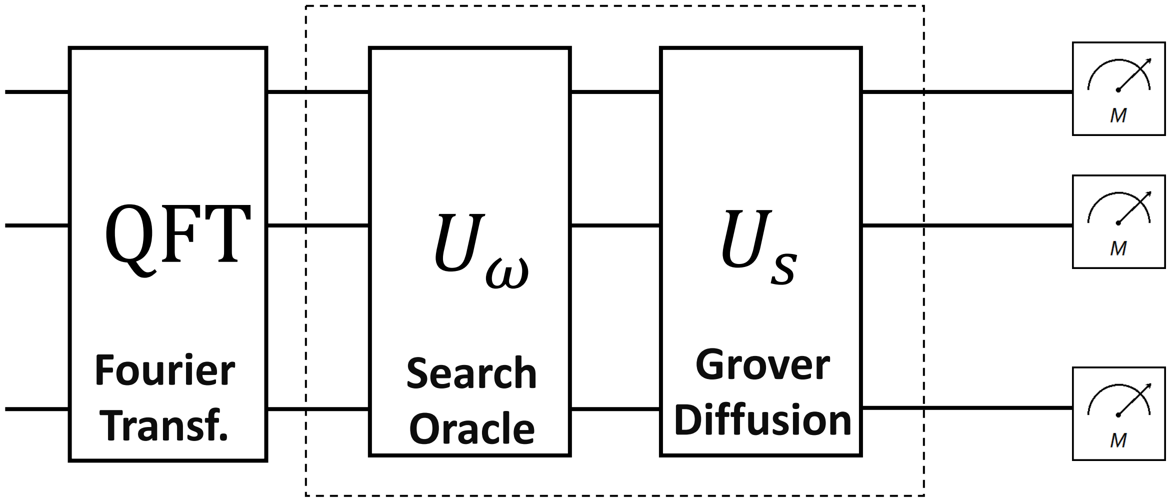


- Search on 3 items has a **92.6% success probability** on the first iteration
- Compare to 2-qubits: search on 4 items has 100% success on 1st iteration

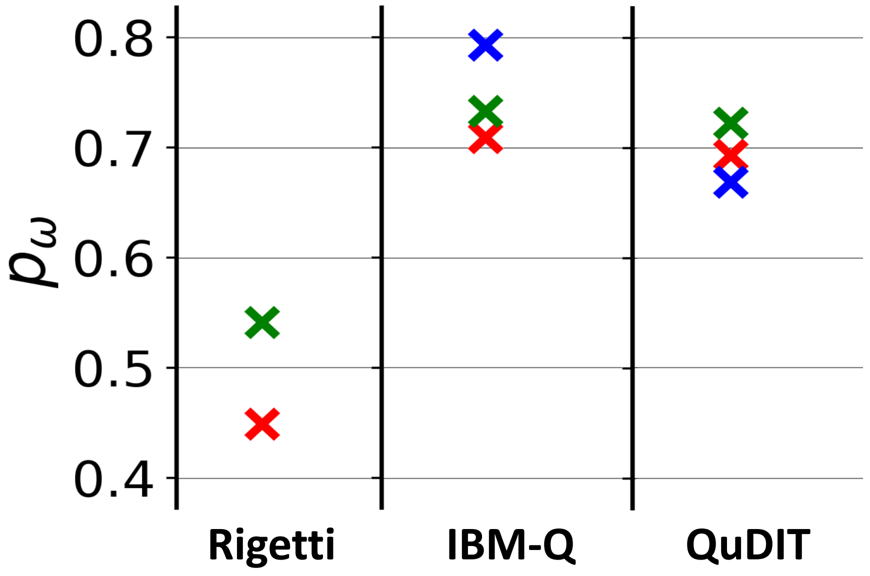


The performance of Grover's search can be improved using optimal control [1]

Repeat n_{it} times



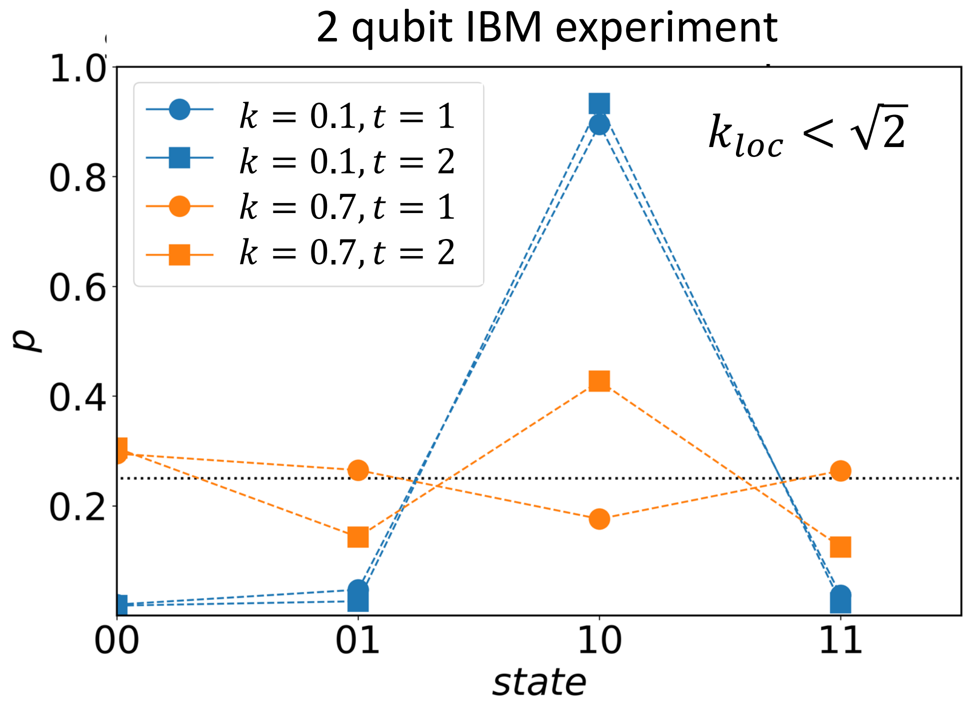
Expt. fidelity after 11 iterations

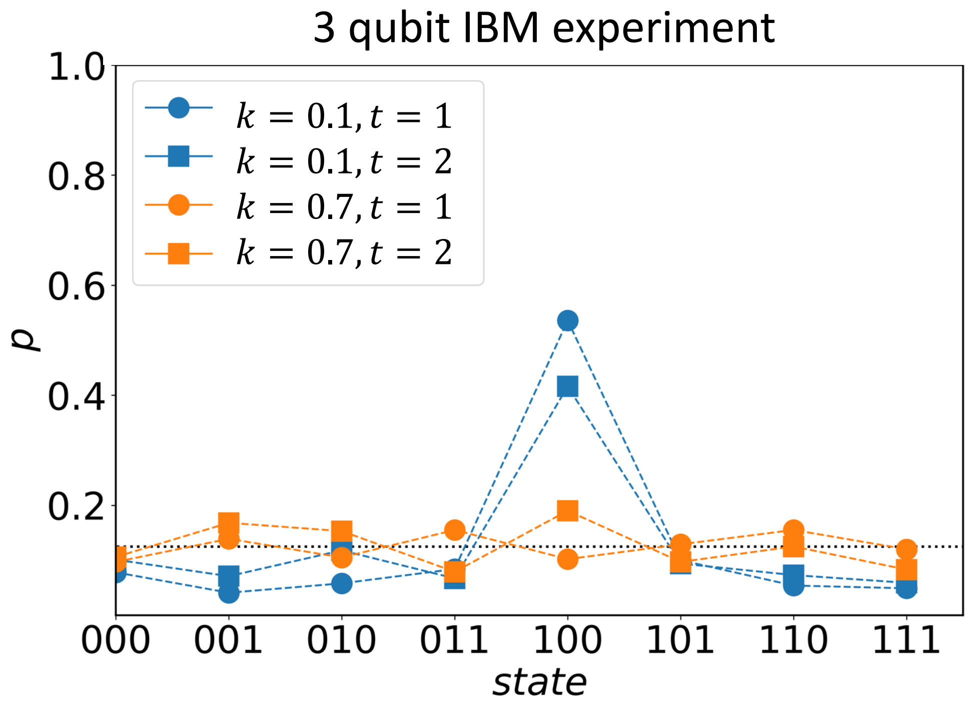


- **Tests on IBM-Q, Rigetti, and LLNL QuDIT demonstrate reasonably good performance for 1-11 iterations**
  - Optimal control effectively improves hardware performance

[1] V. I. Geyko, et al., "Using Grover's search algorithm to test present state-of-the-art quantum computing platforms" (2023)

The phase transition between diffusive and localized dynamics is clearly observable on IBM-Q





Statistical error $= 1/\sqrt{8{,}192}$ $\sim 1\%$

What about Generalized Eigenvalue Problems (GEVP)?

- **Generalized Eigenvalue Problem:** $$\mathbf{A}v = \lambda \mathbf{B}v$$
  - Assume $\mathbf{A}$ is Hermitian and sparse
  - Assume $\mathbf{B}$ is symmetric positive definite (SPD)
- Any SPD matrix, **B**, has a unique **SPD square root** $\mathbf{B}^{1/2}$
- The problem can be reduced to standard Hermitian form using the transformation

$$u = \mathbf{B}^{1/2}v \qquad \mathbf{H} = \mathbf{B}^{-1/2}\mathbf{A}\mathbf{B}^{-1/2} \quad \Rightarrow \quad \mathbf{H}u = \lambda u$$

- In general, $\mathbf{H}$ will not be sparse and, hence, QPE will not be efficient, unless …
- **For special $\mathbf{B}$**, e.g. diagonal or block diagonal, then both $\mathbf{B}^{-1/2}$ and $\mathbf{H}$ are also sparse

J. B. Parker and I. Joseph arXiv:2002.08497 (2020)

FES Application: MHD plasma stability is a GEVP

- Linear Ideal MHD is routinely used for plasma stability calculations of magnetic confinement fusion experiments and reactor designs

$$\mathbf{F} \cdot \boldsymbol{\xi} = -\omega^2 \rho \boldsymbol{\xi}$$

- **Fundamental Theorem of MHD:** Force operator, $\mathbf{F}(\mathbf{x})$, is a self-adjoint 2nd order differential operator [I. B. Bernstein et al. (1958)]

- Numerical approximations such as finite differences, finite volume, and finite elements in the position, $\boldsymbol{x}$, basis typically lead to a sparse banded matrix for **F** and block-diagonal $\boldsymbol{\rho}$

Hermitian form: $\boldsymbol{u} = \rho^{1/2}\boldsymbol{\xi}$ $\quad \mathbf{H} = \rho^{-1/2}\mathbf{F}\rho^{-1/2}$ ⟹ $\mathbf{H} \cdot \boldsymbol{u} = -\omega^2 \boldsymbol{u}$

Quantum phase estimation can be applied to ideal MHD stability

Is this a route to fast stability calculations for design optimization or feedback control?

J. B. Parker and I. Joseph arXiv:2002.08497 (2020)

Lawrence Livermore National Laboratory