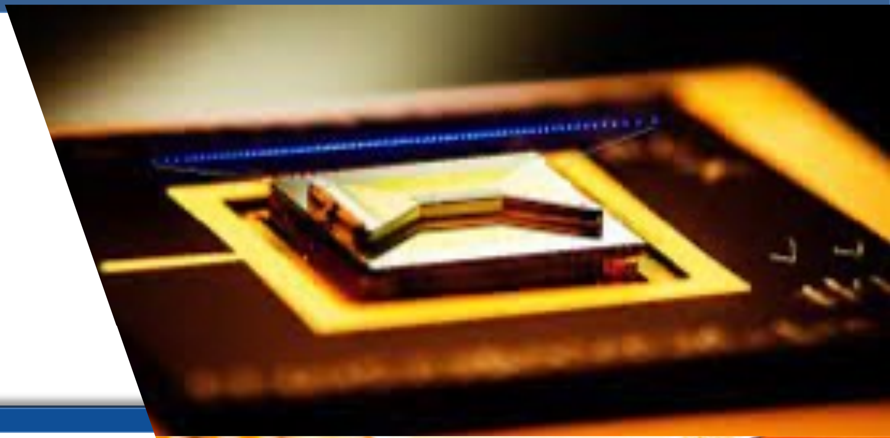
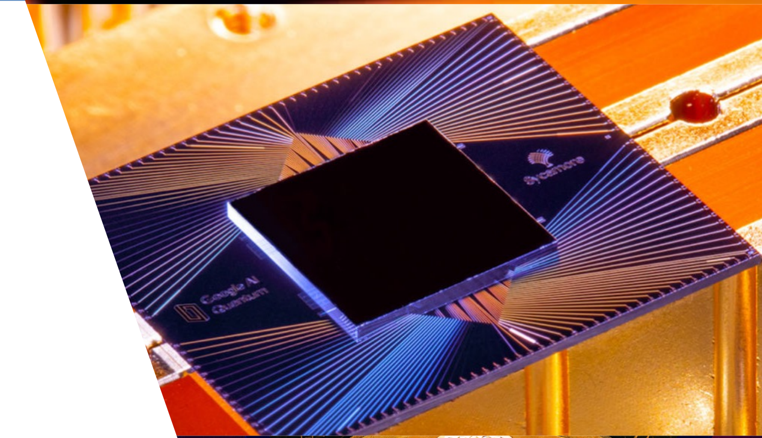
Exploration of Quantum Computing for Fusion Energy Science Applications





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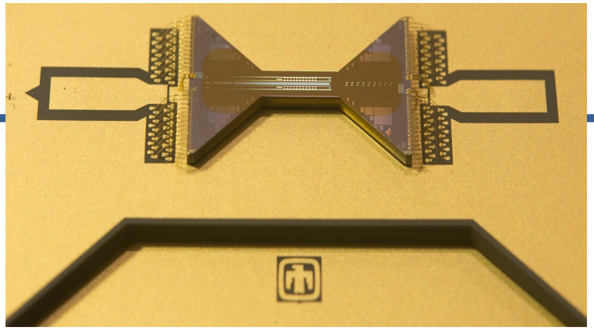
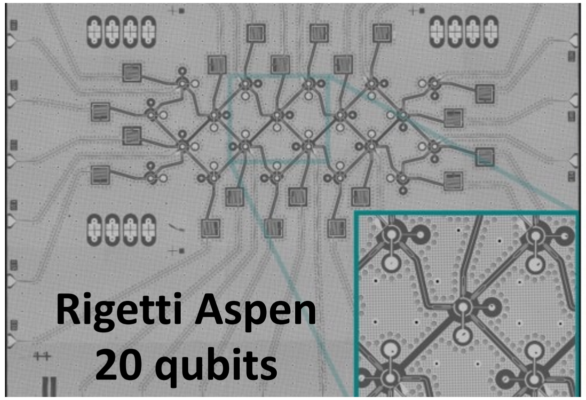
Quantum computing may be a game-changer for fusion and science in general

- **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, …
  - 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

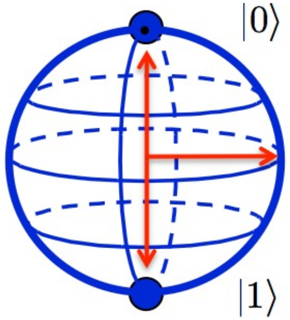
Sandia Peregrine
6 qubit ion trap



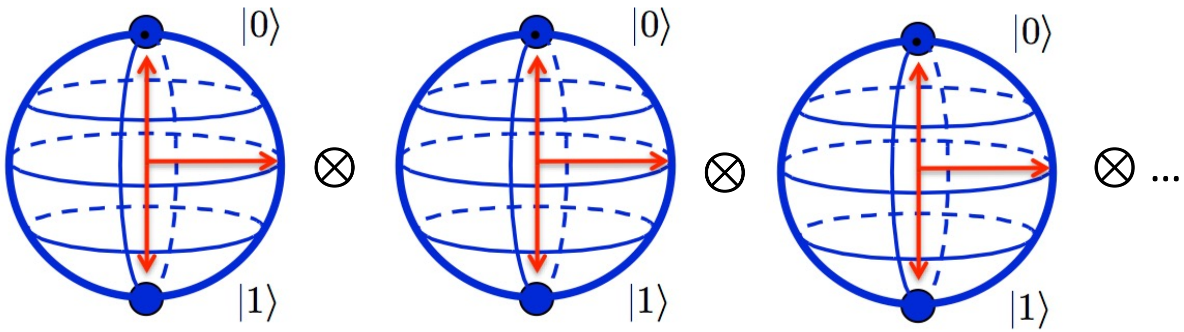


Quantum memory registers are "exponentially large"

Qubit: Dimension 2



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



A few essential subroutines power the majority of quantum algorithms

- **Quantum Fourier Transform:** Cost of $(\log N)^2$ rather than classical $N \log N$
- **Amplitude Amplification:** Cost of sqrt(N) rather than classical N
- **Quantum Walks:** Cost of N rather than classical N^2

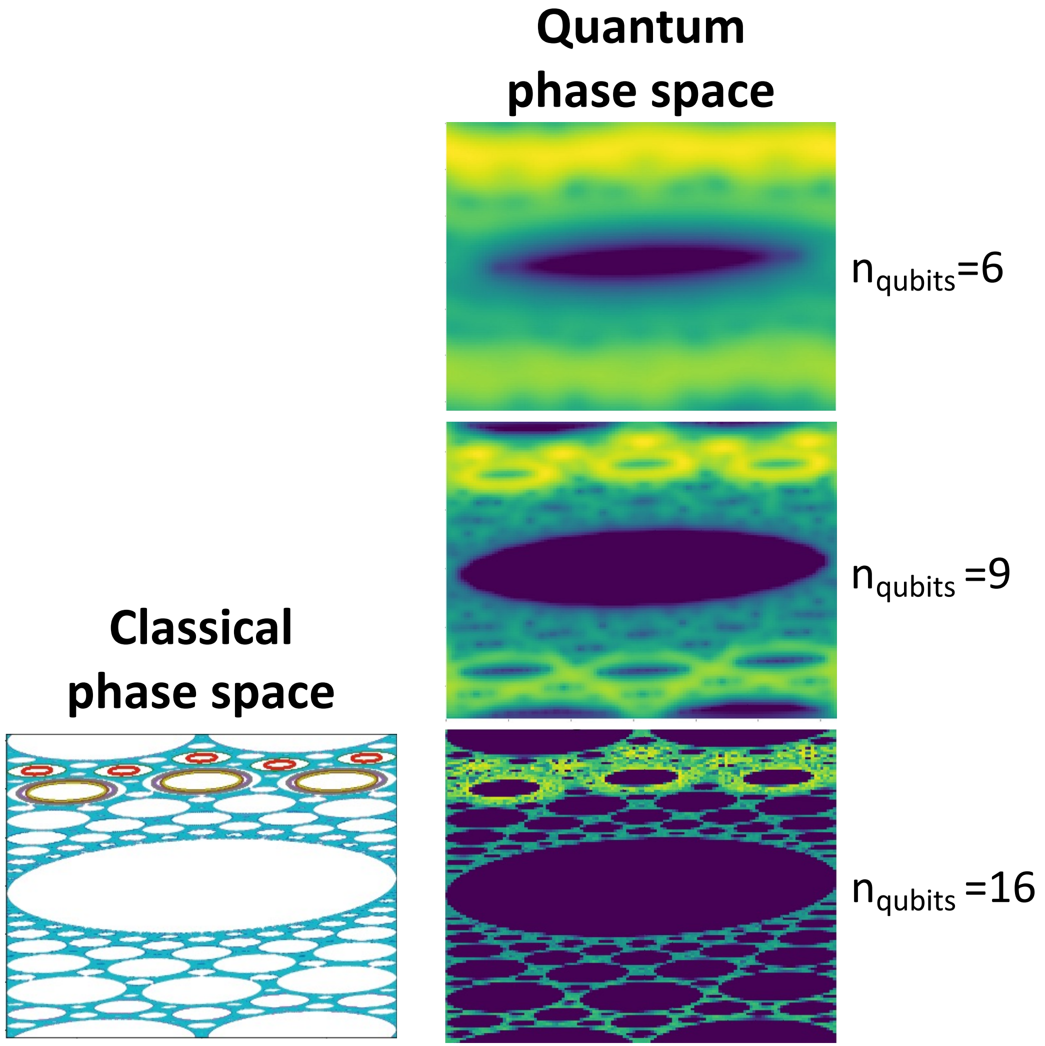
Generic quadratic speedup <= quantum density matrix DOFs / classical PDF DOFs

Outline: Quantum Computing for Fusion Science Applications

- **Quantum Algorithms for Diff Eqs**
  - Linear problems can be solved efficiently
  - Nonlinear problems can be embedded within linear problems

- **Testing Quantum Hardware Platforms**
  - Error mitigation
  - Error exploitation

- **Conclusions & Outlook**



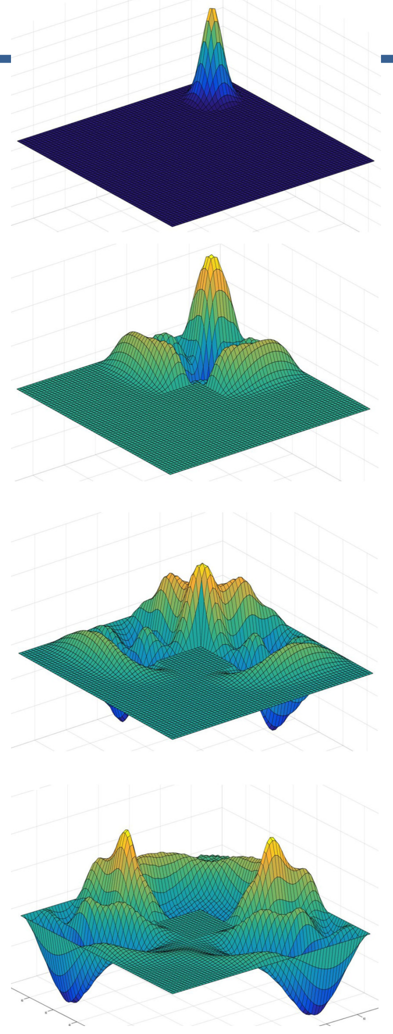
Quantum algorithms for solving linear problems can achieve polynomial to exponential speedup

- **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
  - A few robust physical observables $\langle O_1 \rangle$, $\langle O_2 \rangle$, $\langle O_3 \rangle$

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

- **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 sources

- **"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**"



Costa, Jordan, Ostrander
Phys. Rev. A 2019

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

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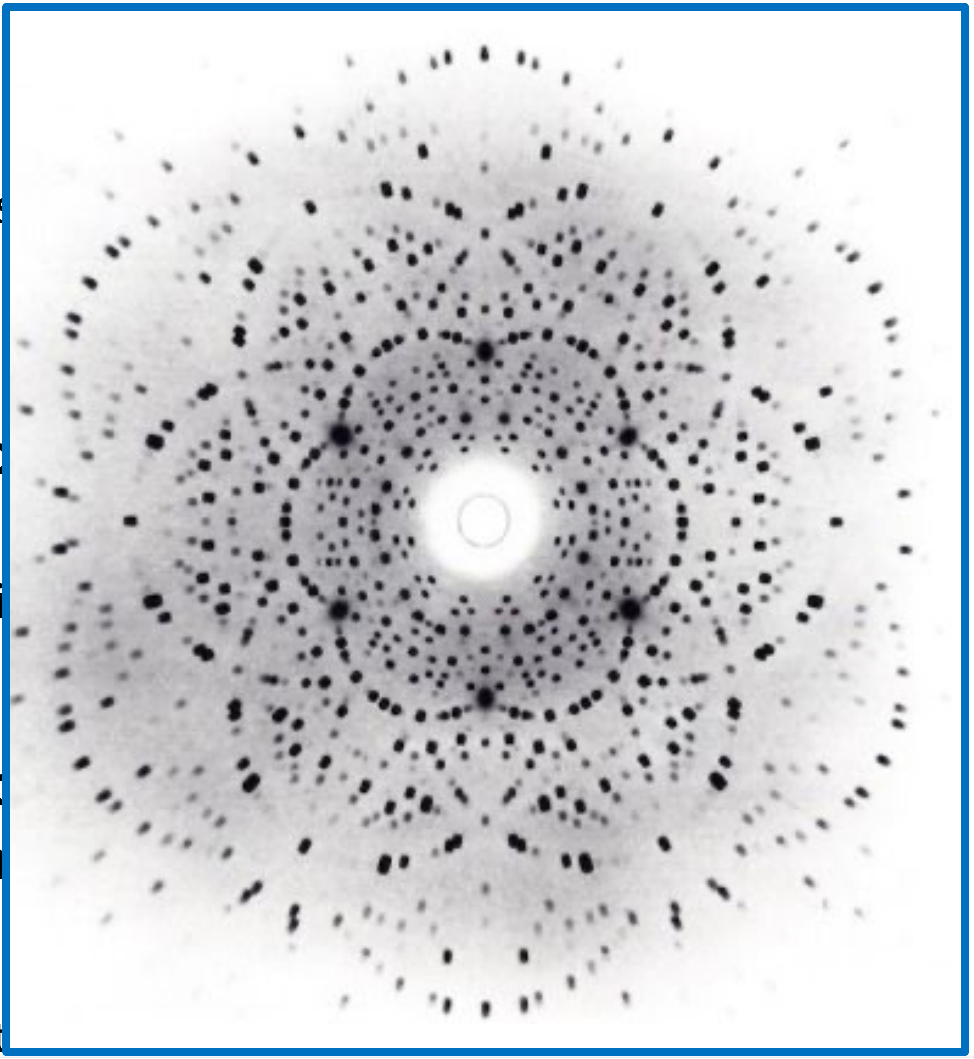

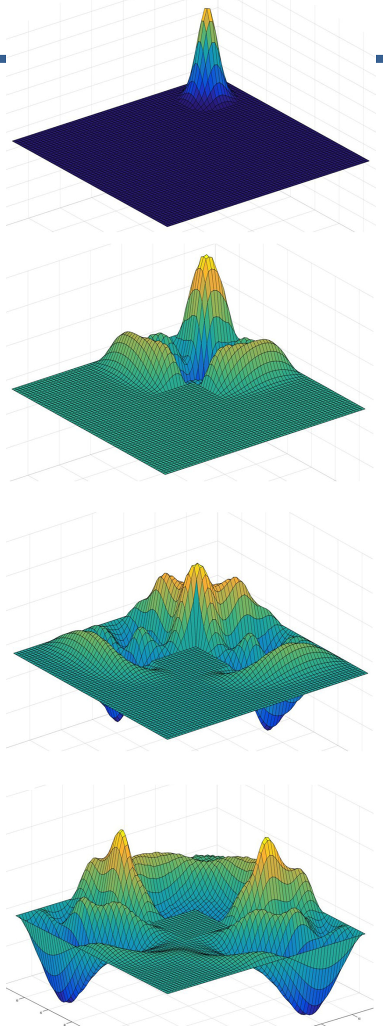

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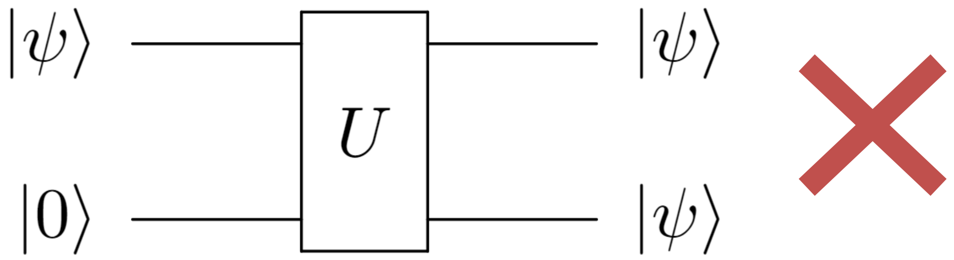
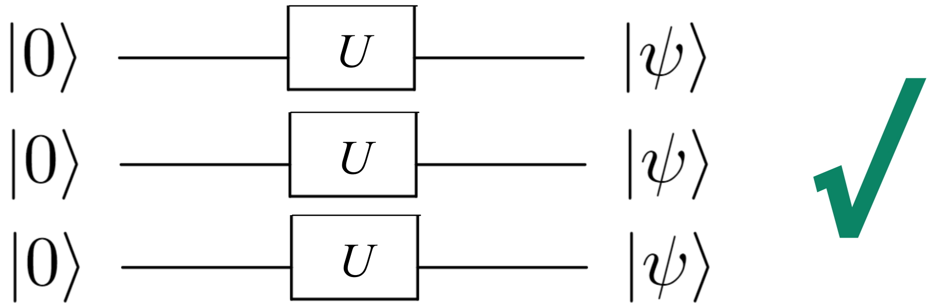
The No-Cloning Theorem fundamentally limits the ability of a quantum computer to efficiently compute nonlinear functions

- **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***
  — If each iteration needs 2 replicas, then the next iteration needs 4 replicas, and T iterations needs **2^T replicas**

*S. K. Leyton, T. J. Osborne, arXiv:0812.4423 (2008)

How about embedding nonlinear Diff Eqs within larger linear systems?

- **Quantization is an approximate 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 law for the probability distribution function (PDF) is a perfect embedding of a nonlinear system … within an infinite-dimensional system of equations for the PDF
  - Carleman embedding is a complex analytic form of KvN [4] that works well near fixed points

- **Special classes of PDEs may have more efficient types of embedding [5]**
  - PDEs that are reducible to ODEs can be embedded using the KvN approach for ODEs: Hamilton-Jacobi equation, advection equation

- **Integrable Diff Eqs also have special types of embedding**

[1] J. Yepez 2002, S. Lloyd 2020 [2] I. Joseph 2020 [3] Jin-Peng Liu 2021 [4] I. Joseph 2023 [5] S. Jin & N. Liu 2022

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

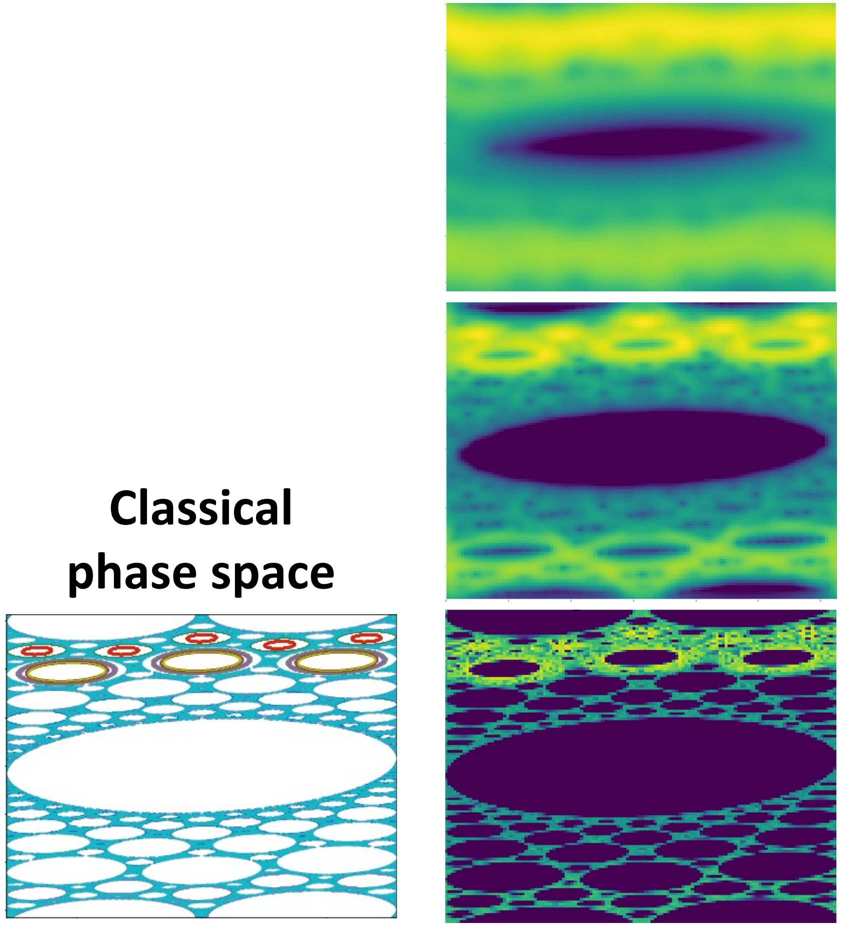
- **Point Example: Quantum Sawtooth Map***
  — Model for chaotic wave-particle interactions
  — Converges to classical result as # of qubits increases

- **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 $\neq$ 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

Quantum phase space

Classical phase space



n_{qubits}=6

n_{qubits} =9

n_{qubits} =16

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

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 $\partial_t z\Big|_{z_0} = +V \cdot \nabla z$ $\xleftrightarrow{\text{chain rule}}$ $\partial_t z_0\Big|_{z} = -V \cdot \nabla z_0$

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

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

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

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

Semiclassical wavefunction yields efficient unitary representation [1-2]

- 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 **"Koopman-van Hove" equation [1-2]**

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

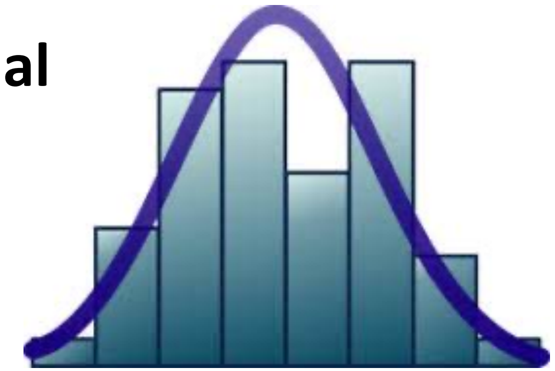
- The **classical Lagrangian** $L(z,t) = p \cdot \partial_p H - H(x,p)$ is the natural choice for semiclassical dynamics because it agrees with Feynman's prescription for the path integral [2]

[1] I. Joseph, Phys. Rev. Research **2**, 043102 (2020)

[2] I. Joseph, arXiv:2306.01865, J Phys A: Math Theor (2023)

Amplitude Estimation provides up to quadratic speedup for output

- **Classical randomized Monte Carlo algorithms also provide an exponential speedup over Eulerian methods**
  - **Central limit theorem:** direct sampling requires computational **cost ~ 1/accuracy²**



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

	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 of error with **number of function calls n**

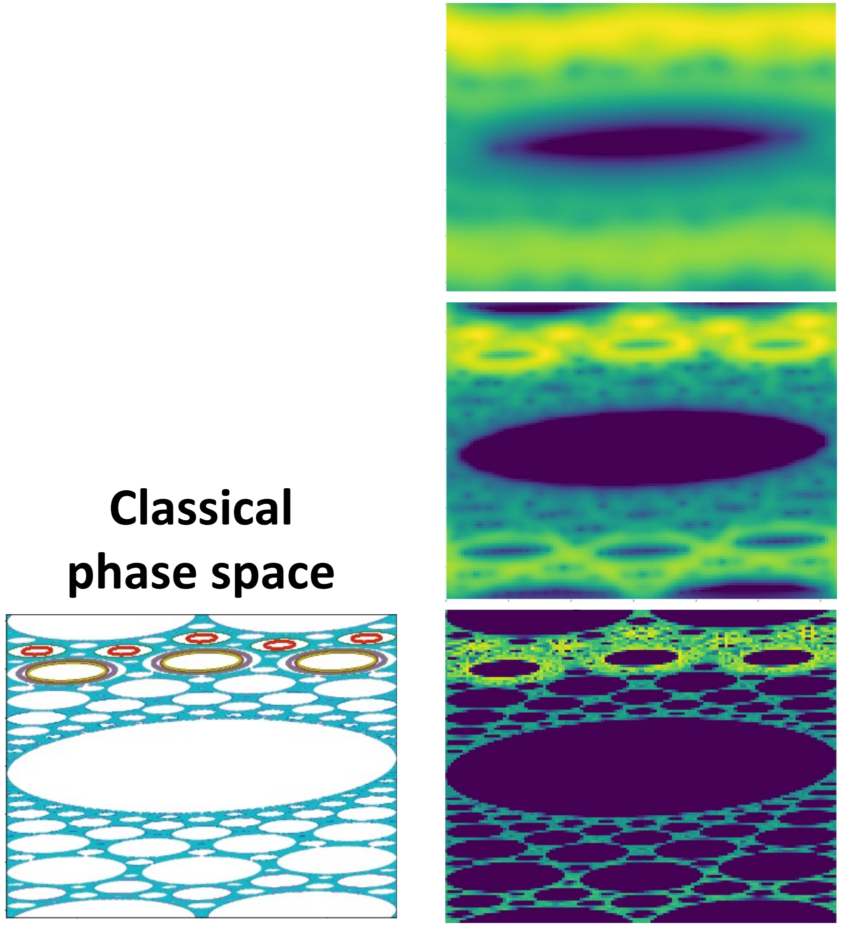
Heinrich & Novak 2001
arXiv:quant-ph/0105114

Outline: Quantum Computing for Fusion Science Applications

- Quantum Algorithms for Diff Eqs
  - Linear problems
  - Nonlinear problems
- **Testing Quantum Hardware Platforms**
  - Error mitigation improves results (Yuan Shi's talk)
  - Errors can be exploited for certain calculations
- Conclusions & Outlook

Quantum phase space

Classical phase space



n_{qubits}=6

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

- **Classical sawtooth map depends on kicking strength $\boldsymbol{K}$**

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

- **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

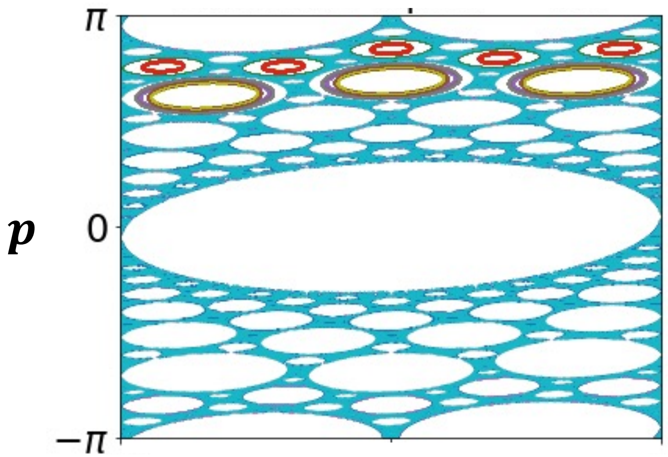
$$\Delta p = 2\pi = \hbar N \qquad\qquad \hbar = 2\pi/N$$

  — Quantum propagator has four stages:

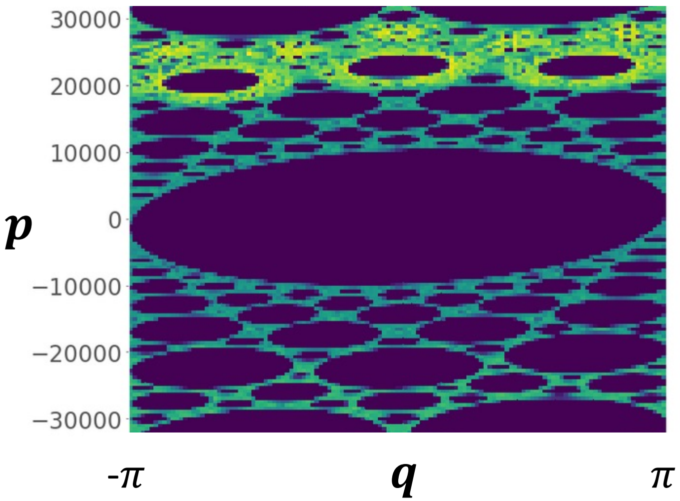
$$U_{QSM} = \hat{\mathcal{T}} e^{-i \int H_{saw} dt/\hbar} = \; U_{kin}(\hbar)\, U_{QFT}^{-1}\, U_{pot}(K/\hbar)\, U_{QFT}$$

*G. Benenti, et al, PRL **87** 227901 (2001)

Classical Map: K=-0.1



Quantum Map: K=-0.1



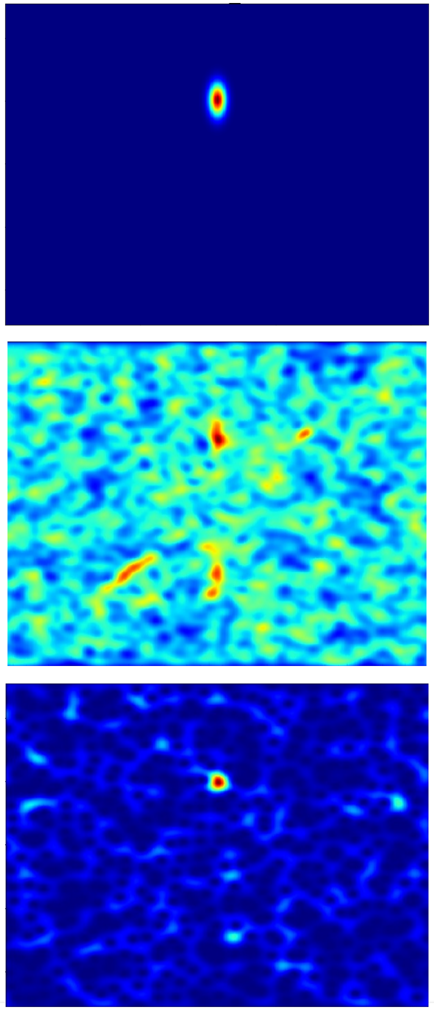
Noisy quantum computers can efficiently compute key signatures of chaos, such as the Lyapunov rate λ = the exponential separation of trajectories*

Chaotic $K = 0.5$

Start

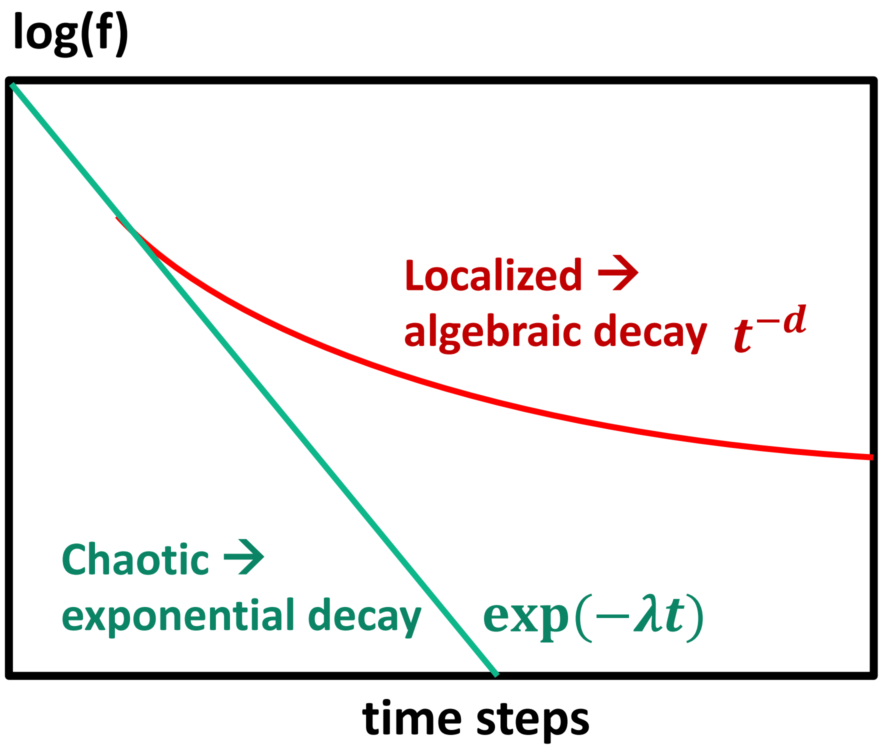
Forward t steps

Reverse t steps



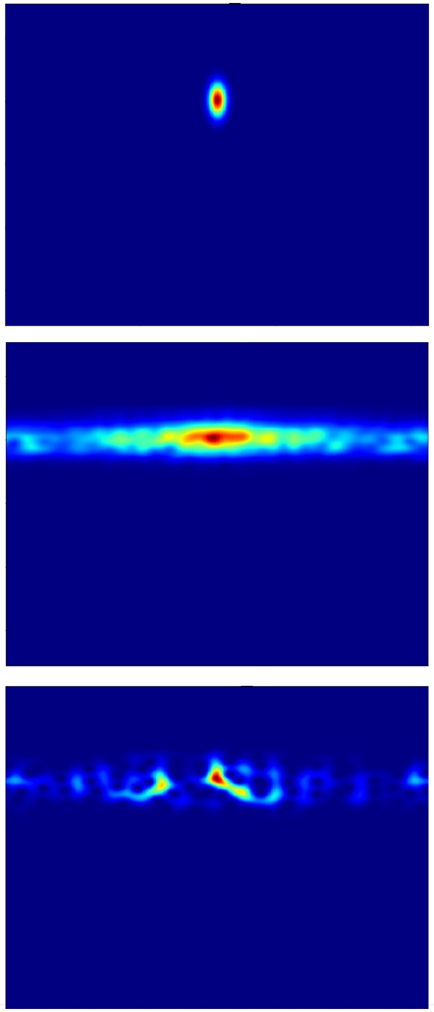
Simply measure the fidelity

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



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

Localized $K = 0.1$



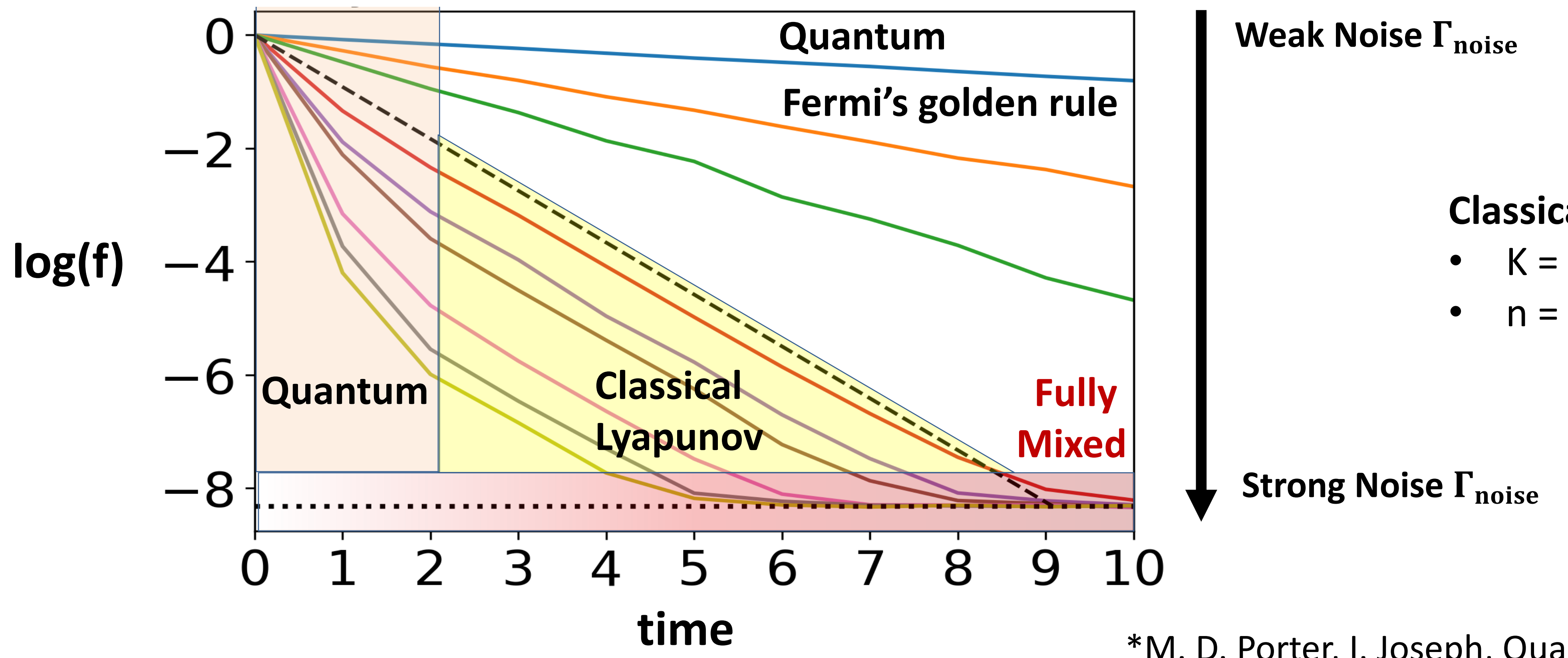
Start

Forward t steps

Reverse t steps

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

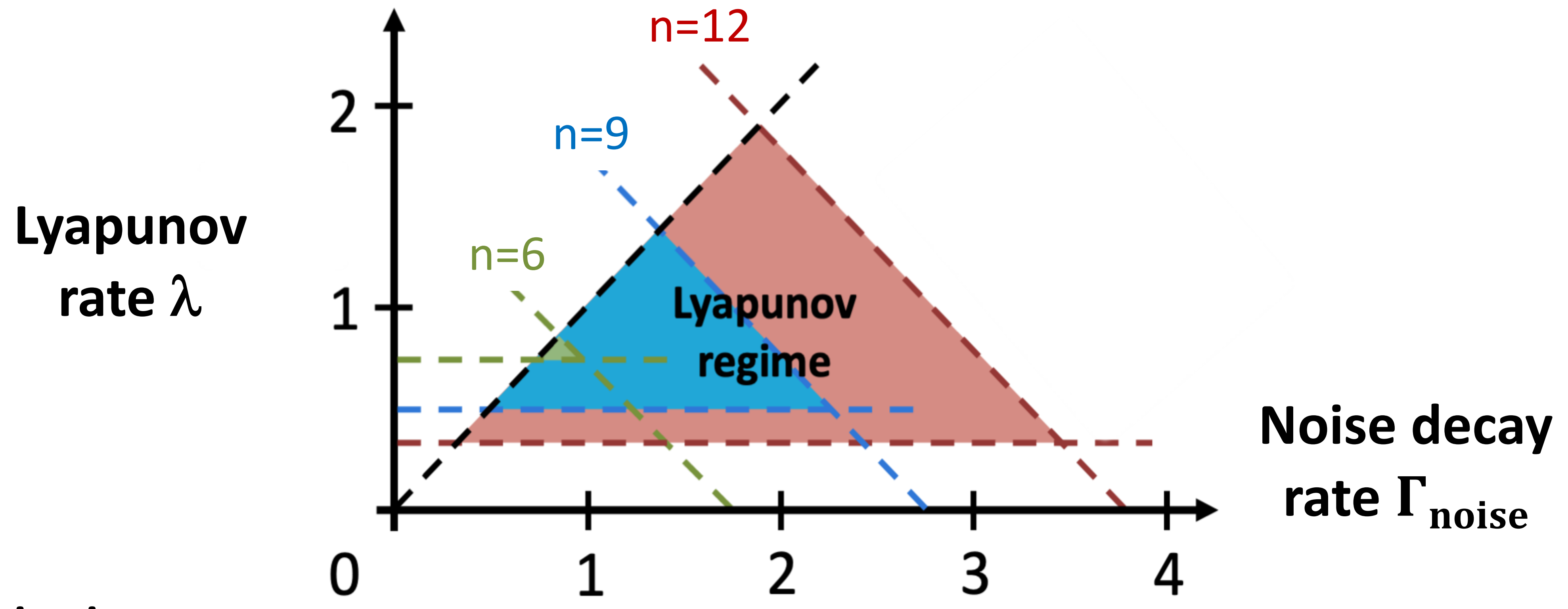
$$f(t) \approx f_{\text{Quantum}} e^{-\Gamma_{\text{noise}} t} + f_{\text{Classical}}\, e^{-\lambda_{\text{Lyap}} t} + 1/N$$



Classical simulation
- K = 0.9
- n = 12 qubits

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

Fidelity phase diagram determines whether the Lyapunov rate can be observed



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.

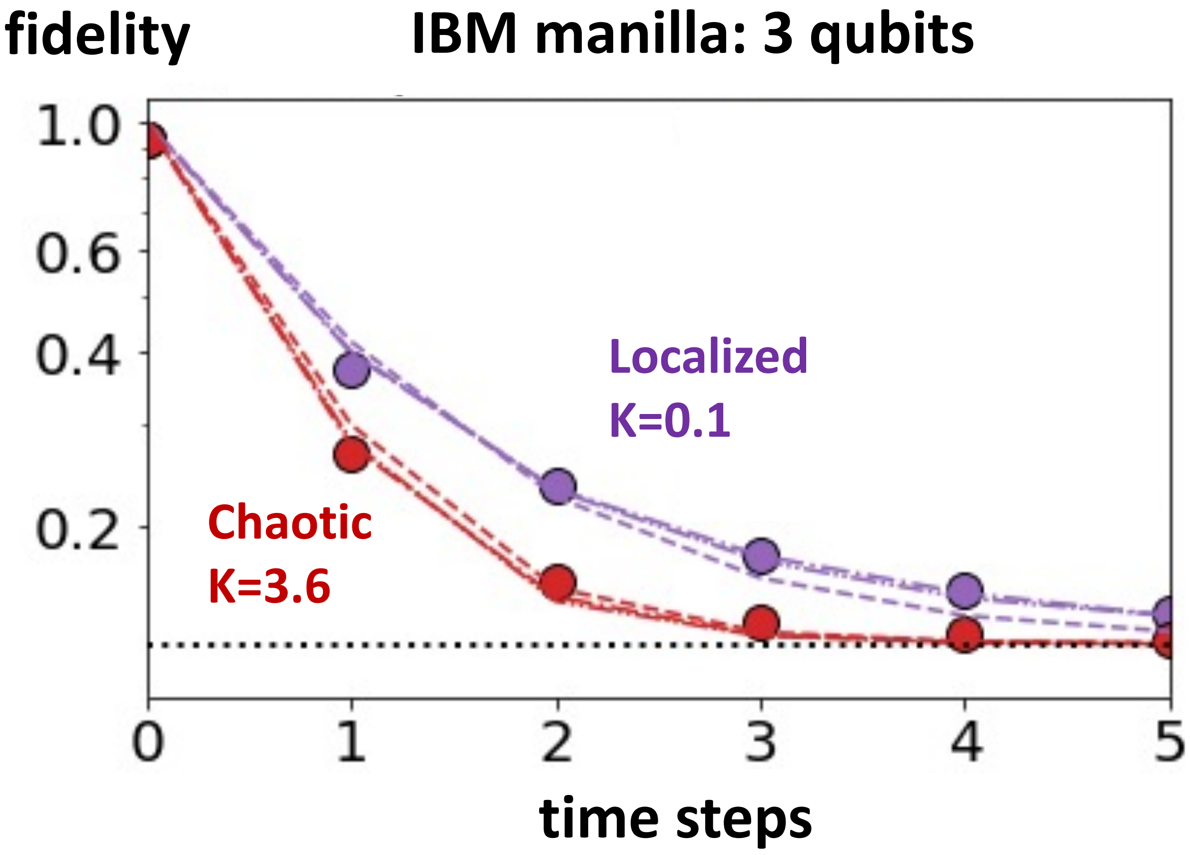
*M. D. Porter, I. Joseph, Quantum **6**, 799 (2022)

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

- **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 $1/T_2^*$



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

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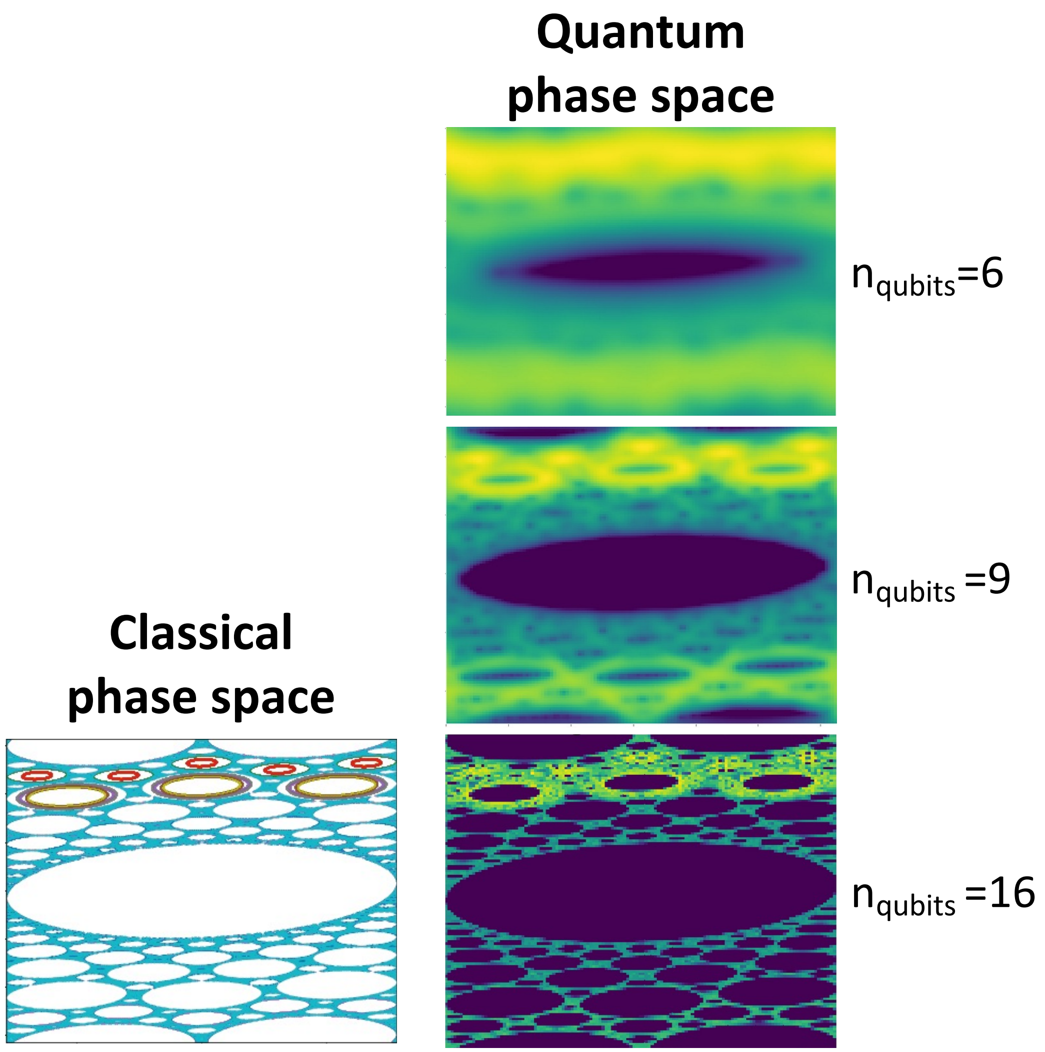
- **Conclusions & Outlook**



Conclusions & Outlook

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

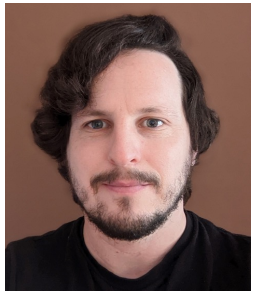
- **Quantum computing holds great promise for accelerating scientific discovery**
  - Efficient Fourier transforms, sparse linear solvers, sparse Hamiltonian simulation, variational eigensolvers, …
  - Chemistry, materials science, high-energy physics, nuclear physics, …, **fusion energy science!**

- **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
  - We've also explored passive and active error mitigation, e.g. quantum optimal control
  - Decoherence controls the **"information confinement time"**

Our team consists of experts in MFE, HEDS and QIS

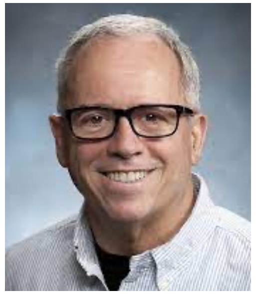
- **Core Team**
  - **MFE:** Ilon Joseph (PI), Vasily Geyko, *Jeff Parker (FY20)*
  - **HEDS:** Frank Graziani, Stephen Libby, Yuan Shi (U Colorado Boulder)
  - **QIS:** Jonathan DuBois (co-PI), Al Castelli, Max Porter (Sandia), Gabriel Woolls (Caltech/Berkeley)


Al Castelli


Jonathan DuBois

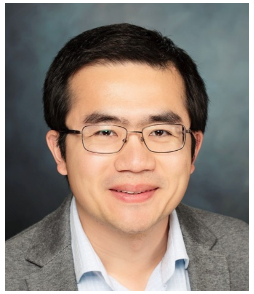

Vasily Geyko


Ilon Joseph


Frank Graziani


Steve Libby


Max Porter


Yuan Shi

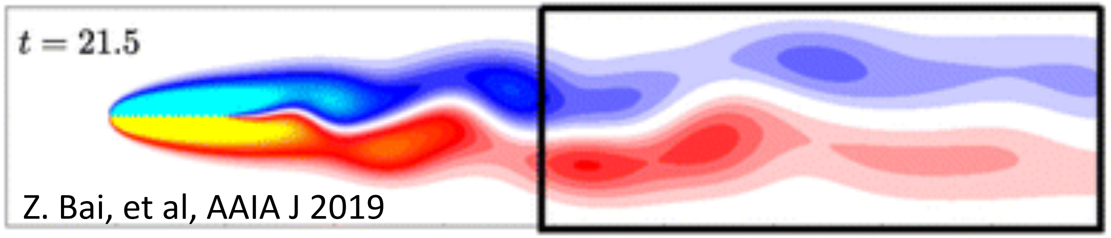

Gabriel Woolls

- **LLNL Collaborators**
  - **Quantum Coherent Device Physics Group:** Kristi Beck (formerly IonQ), Yaniv Rosen, Xian Wu (now at Rigetti)
  - **NACS:** Roger Minich, Kyle Wendt; **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)

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

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



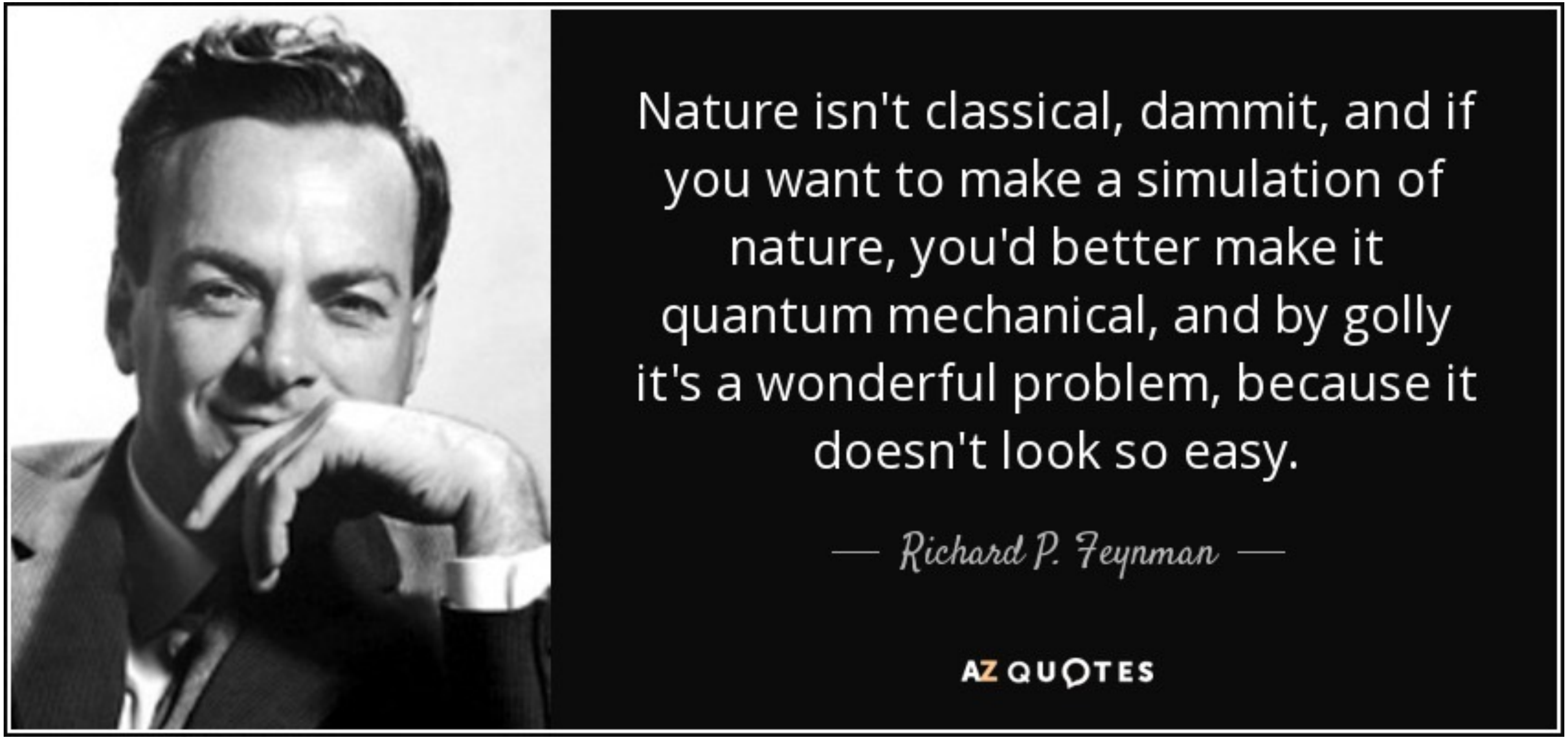
Z. Bai, et al, AAIA J 2019

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

- **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]
  - Imagine a quantum dynamic mode decomposition: qDMD or quantum sparse identification of nonlinear dynamics qSINDy

[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

The key insight …



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- F. Gaitan, "Finding flows of a Navier–Stokes fluid through quantum computing." *npj Quantum Information* **6.1** (2020): 1-6
- S. Lloyd, G. De Palma, C. Gokler, B. Klani, Zi-Wen Liu, M. Marvian, F. Tennie, T. Palmer, “Quantum algorithm for nonlinear differential equations,” arXiv:2011.06571 (2020)
- I. Y. Dodin, E. A. Startsev, “On applications of quantum computing to plasma simulations,” arXiv:2005.14369, *Physics of Plasmas* **28**, 092101 (2021)
- I. Y. Dodin, E. A. Startsev, “Quantum computation of nonlinear maps,” arXiv:2105.07317 (2021)
- A. Engel, G. Smith, S. E. Parker, “Linear embedding of nonlinear dynamical systems and prospects for efficient quantum algorithms,” *Physics of Plasmas* **28:6** (2021) 062305.
- Jin-Peng Liu, H.Ø. Kolden, H.K. Krovi, N.F. Loureiro, K. Trivisa, and A.M. Childs, “Efficient quantum algorithm for dissipative nonlinear differential equations,” *Proceedings of the National Academy of Sciences* **118:35** (2021) e2026805118
- D. Giannakis, A. Ourmazc, P. Pfeffer, J. Schumacher, J. Slawinska, arXiv:2012.06097; Phys. Rev. A **105** (2022) 052404

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

- **Quantum Sensing:** improves measurement sensitivity
  - Heisenberg limit for noise/signal ratio scales as 1/N instead of 1/sqrt(N)
- **Quantum Communications:** secure information transfer
  - Intrinsically parallel data transfer / data compression
- **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-Enhanced Advanced LIGO Detectors in the Era of Gravitational-Wave Astronomy

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

China Demonstrates Quantum Encryption By Hosting a Video Call

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

Quantum supremacy using a programmable superconducting processor

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

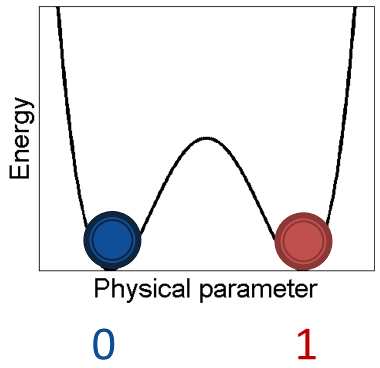
Strong Quantum Computational Advantage Using a Superconducting Quantum Processor

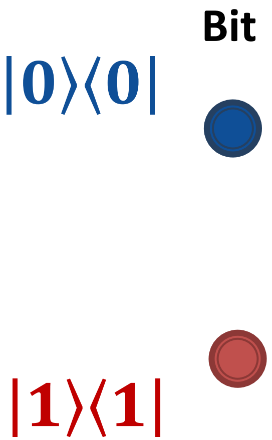
Yulin Wu, *et al.* Phys. Rev. Lett. 127, 180501 (2021)

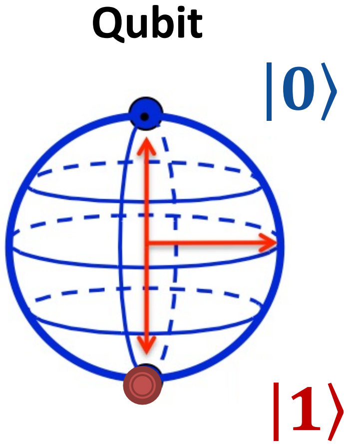
Han-Sen Zhong, *et al.* Phys. Rev. Lett. 127, 180502 (2021)

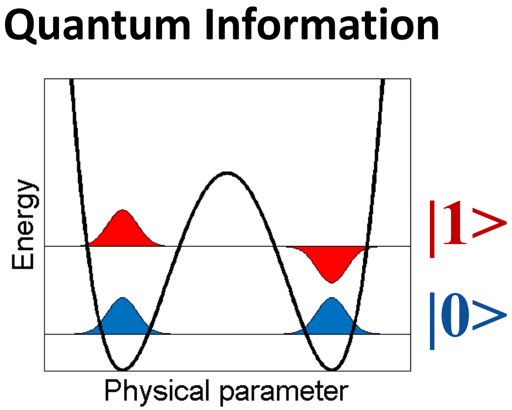
Phase-Programmable Gaussian Boson Sampling Using Stimulated Squeezed Light

The qubit is the simplest complex Hilbert space









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

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

- **Probabilistic mixture of pure states described by the density matrix $\boldsymbol{\rho} = \boldsymbol{\rho}^\dagger \in \mathbf{H}_4 \sim \mathbb{R}^4$**

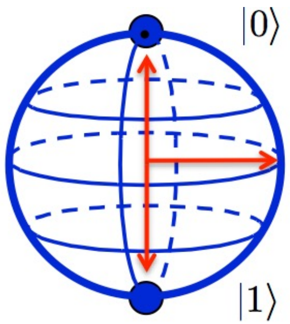
$$\boldsymbol{\rho} = \rho_{00}|0\rangle\langle 0| + \rho_{01}|0\rangle\langle 1| + \rho_{10}|1\rangle\langle 0| + \rho_{11}|1\rangle\langle 1|$$

- **Probability distribution function (PDF) $\boldsymbol{f} \in \mathbb{R}^2$**

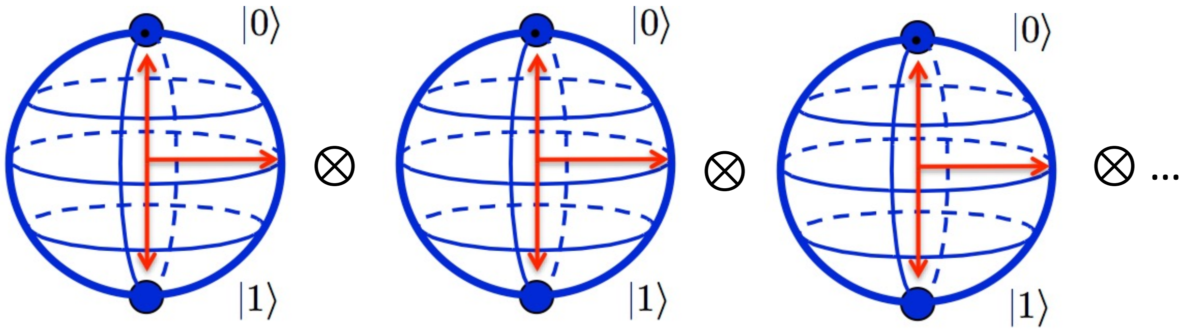
$$\boldsymbol{f} = \mathrm{Diag}(\boldsymbol{\rho}) = \rho_{00}|0\rangle\langle 0| + \rho_{11}|1\rangle\langle 1|$$

Quantum memory registers are "exponentially large"

Qubit: Dimension 2



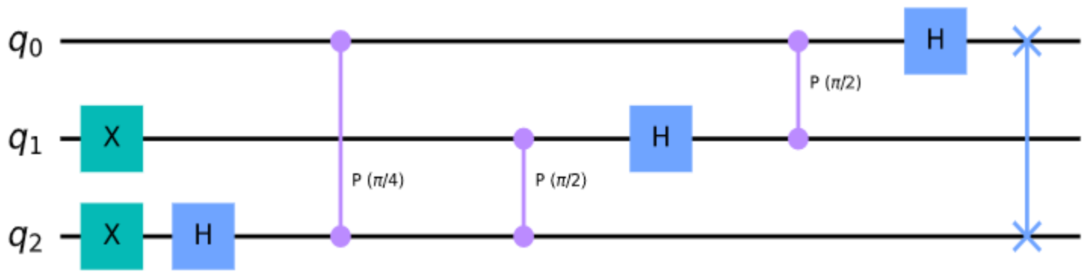
n Qubits → Hilbert Space Dimension: N = 2^n



- **Direct quantum simulation is extremely difficult due to exponentially large Hilbert space**
- **Why not use a "quantum machine" to simulate quantum physics?**
  - **Early-1980's:** Think of 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
- **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!**
  - Key resources are **superposition and interference,** often called **quantum parallelism** ☺
  - Any reversible classical computation can also be performed, but typically without a speedup ☹
- **Key Limitation: 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



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

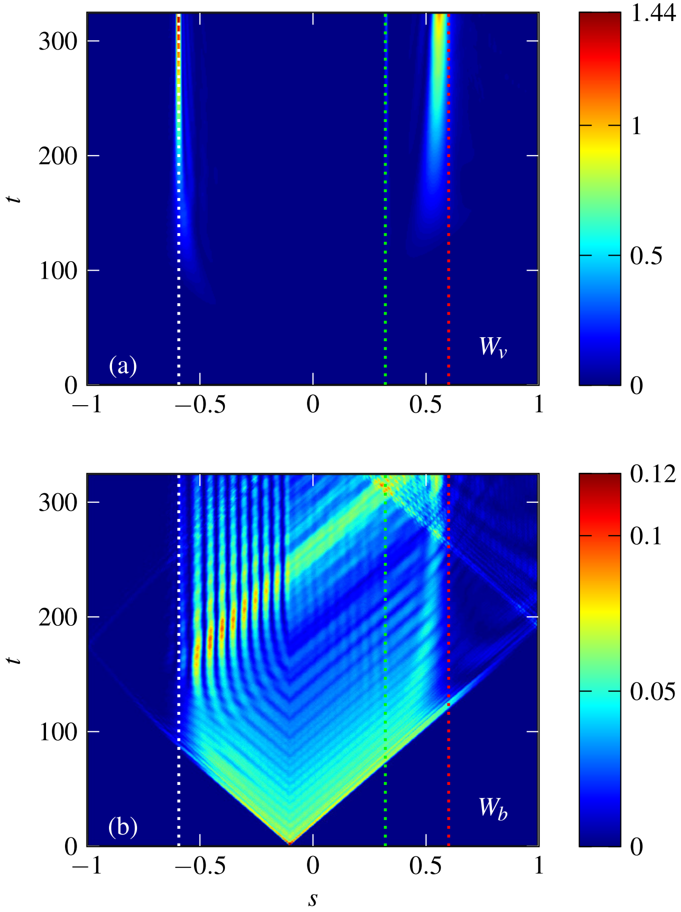
Hamiltonian simulation can achieve super-polynomial to exponential speedup by exploiting special structure and/or sparsity

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

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

- **Black box methods work well for sparse Hamiltonians**
  - “Efficiently row-computable sparse”
  - 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!



Novikau, Startsev, Dodin
Phys. Rev. A 2022

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

Quantum algorithms for ODEs and PDEs 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
- **Continuous Variable Model for classical and quantum field theory (CFT / QFT)**
  - 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

Solving for wavefunction is efficient for sparse linear evolution

- **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

$$\psi(z,t) = \sum_n \psi^n(t)\phi_n(z)$$

$$i\hbar\frac{d}{dt}\psi^n = \sum_m \psi^m H_m^n$$

- **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)

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)

Variational algorithms have a few key steps … and some 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

NASA Earth Observatory: Himalayas

Optimization landscape may have intrinsic difficulties such as …

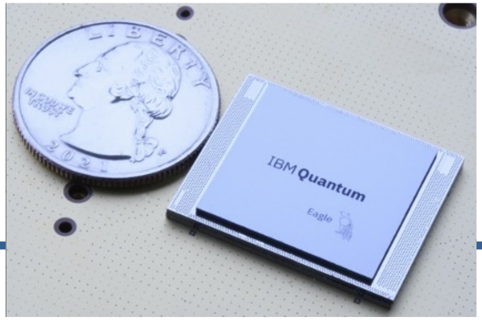
- Many local maxima and minima
- Barren plateaus with little information on the gradient of the cost function

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

To date, we’ve used superconducting hardware platforms & have begun to use ion traps

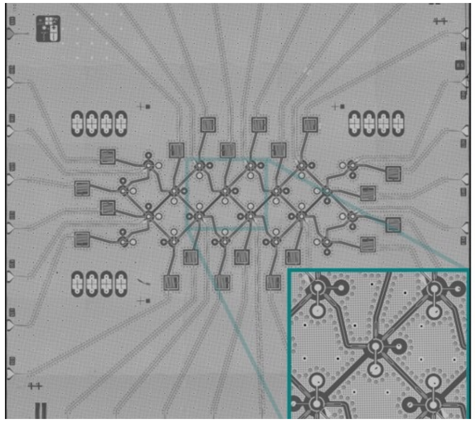
IBM-Q
Eagle
127 qubits



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

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

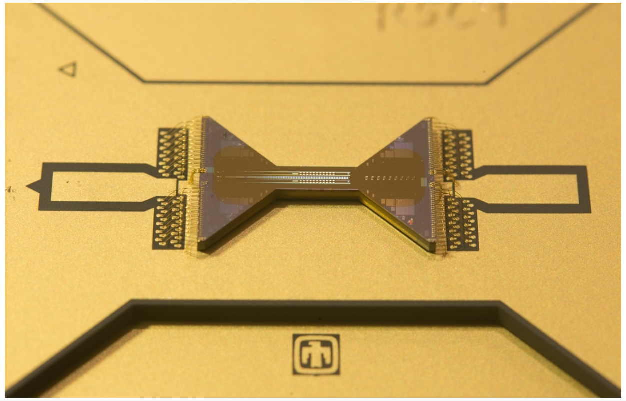
Rigetti
20 qubit device
(Aspen-M3 has 79 qubits)

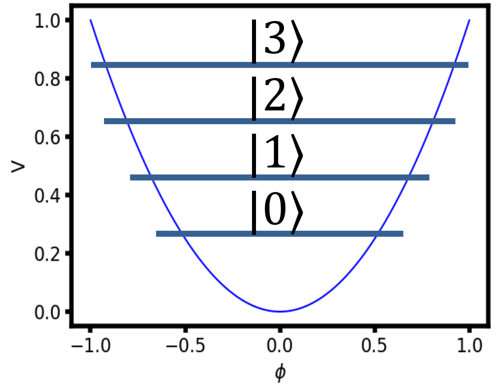


- **LLNL Quantum Design and Integration Testbed (QuDIT)**
  — Open access to 3-level and 4-level qudits rather than 2-level qubits

- **Sandia QSCOUT ion trap**

Sandia
Peregrine
6 qubits



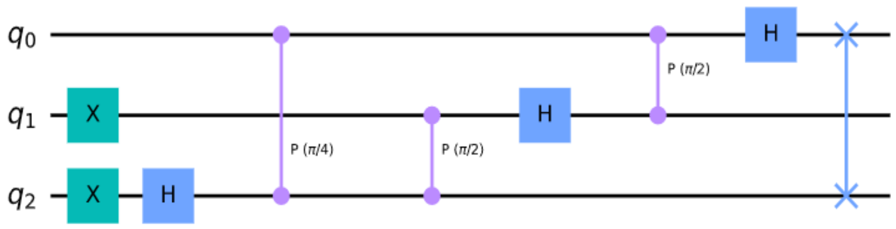


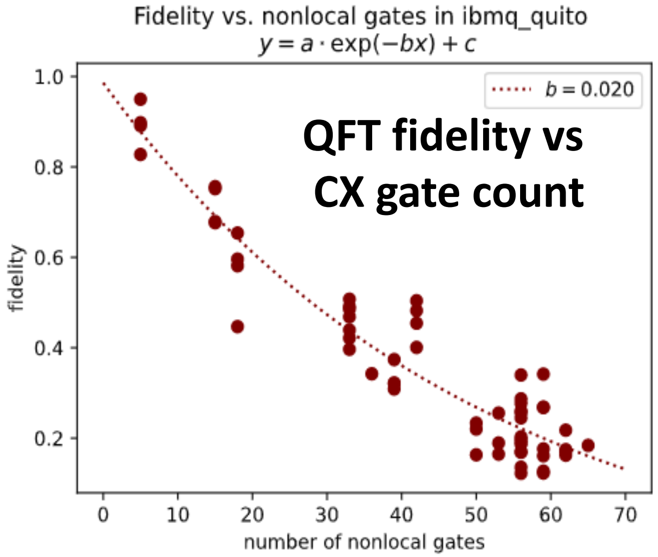
LLNL
Quantum Design & Integration Testbed (QuDIT)
~ 6 qubits

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

- **"Fidelity" is the figure of merit:** $F = \left|\langle\psi_{\mathbf{expected}}|\psi_{\mathbf{actual}}\rangle\right|^2$
  - 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



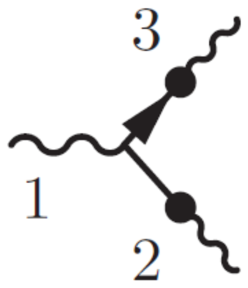


- **Infidelity for realistic calculations is ~2-5x worse than expected**
  - Fidelity does not always decay at an exponential rate
  - Coherent gate errors are important and need to be corrected for
  - Coherent errors can be much more damaging to intended calculations

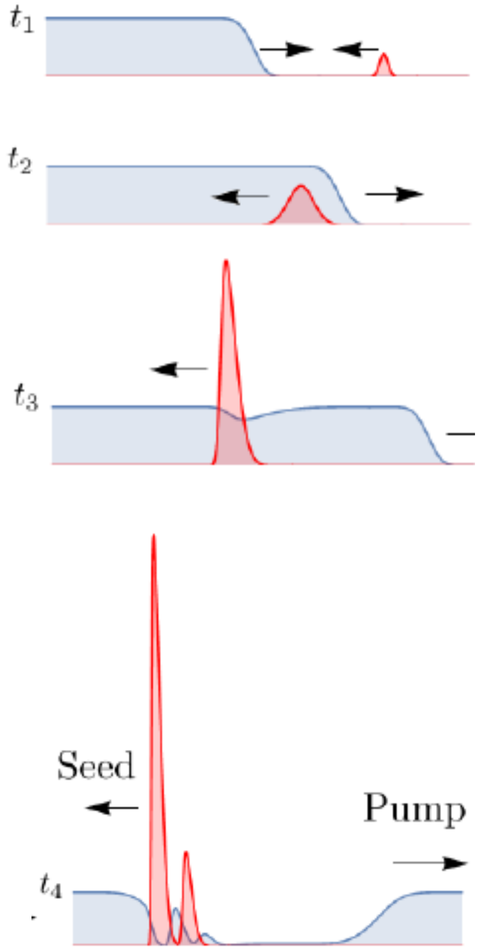
First plasma application: simulating three-wave interactions [1]

- **Cubic couplings are ubiquitous in plasmas, fluids, & nonlinear media**
  - Examples: nonlinear optics, laser-plasma interactions, weak turbulence, gauge theory, lattice QED …
  - Interaction Hamiltonian $H_I = igA_1^\dagger A_2 A_3 - ig^* A_1 A_2^\dagger A_3^\dagger$
  - Envelope equations for resonant interactions

    $$d_t A_1 = g A_2 A_3, \quad d_t A_2 = -g^* A_1 A_3^\dagger, \quad d_t A_3 = -g^* A_1 A_2^\dagger$$
  - Quantized version $[A_j, A_l^\dagger] = \delta_{jl}$



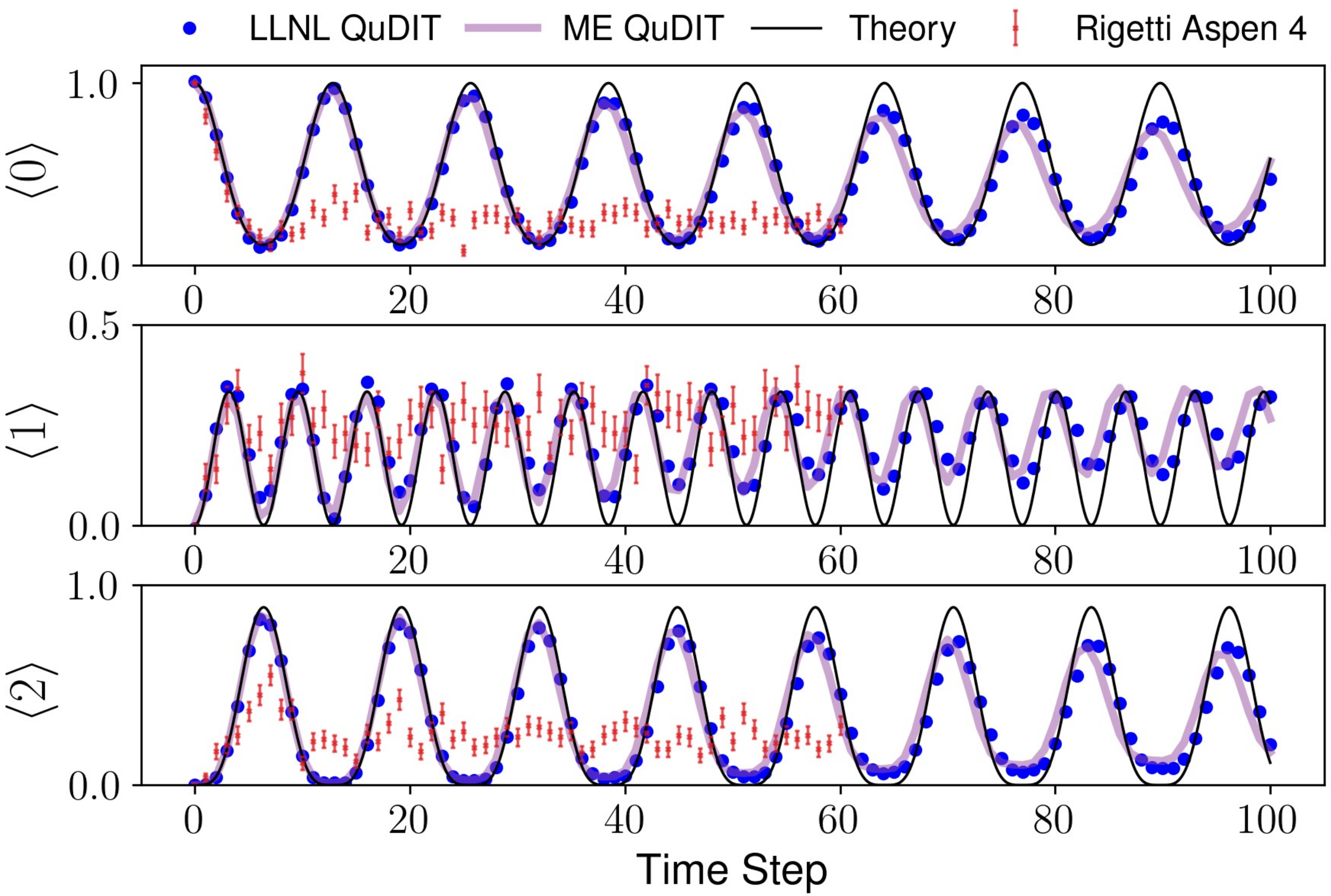
$$\omega_1 = \omega_2 + \omega_3$$
$$\mathbf{k}_1 = \mathbf{k}_2 + \mathbf{k}_3$$



- **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]

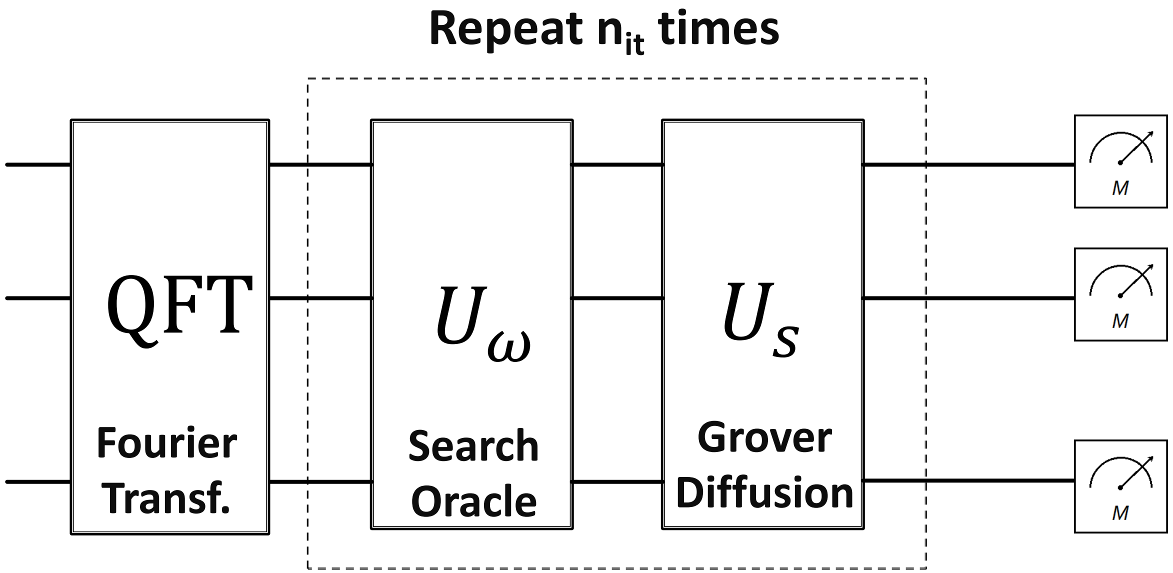


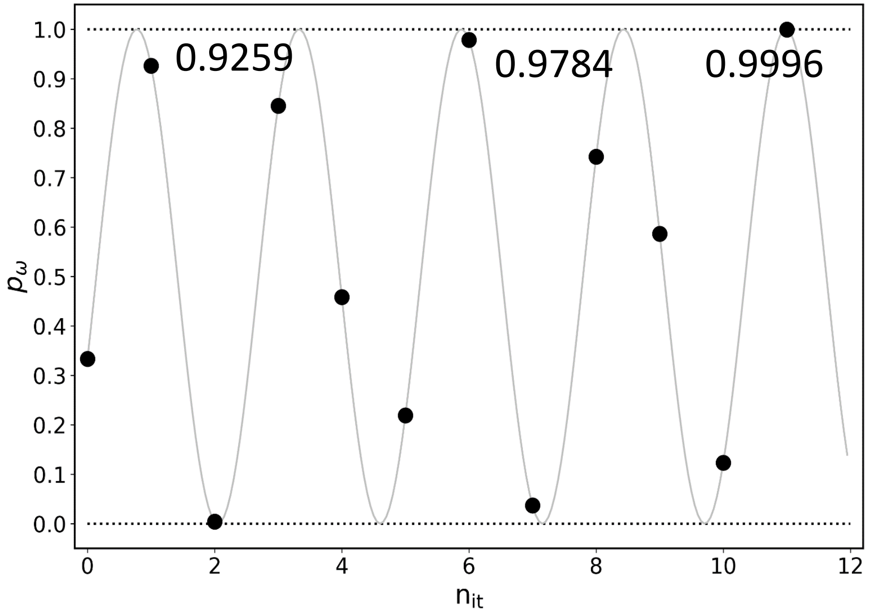
- Results of **LLNL QuDIT** (**blue**) are close to **analytic solution** (**black**) & match **Lindblad Master Equation (ME)** simulation (**purple**)
- Results of **Rigetti Aspen-4 platform** (**red**) perform well for first ~9 time-steps, but use **17x as many gates per step**
- On both platforms, 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)

Grover's search for 3-level qudits developed & improved using optimal control [1]

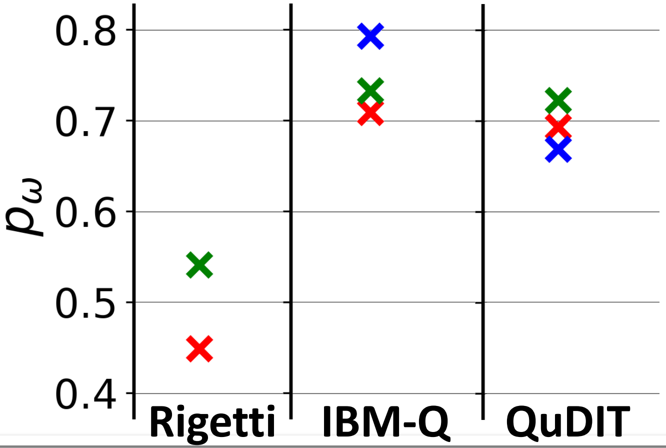
- **We developed a modified Grover's search algorithm for LLNL QuDIT**
  - Search on 3 items has a 92.6% success probability on the first iteration
  - Compare to 2-qubit case: search on 4 items has 100% success on 1st iteration





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

Expt. fidelity after 11 iterations



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

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**
  - Quantized classical systems recover classical limit at small $\hbar$, but requires 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

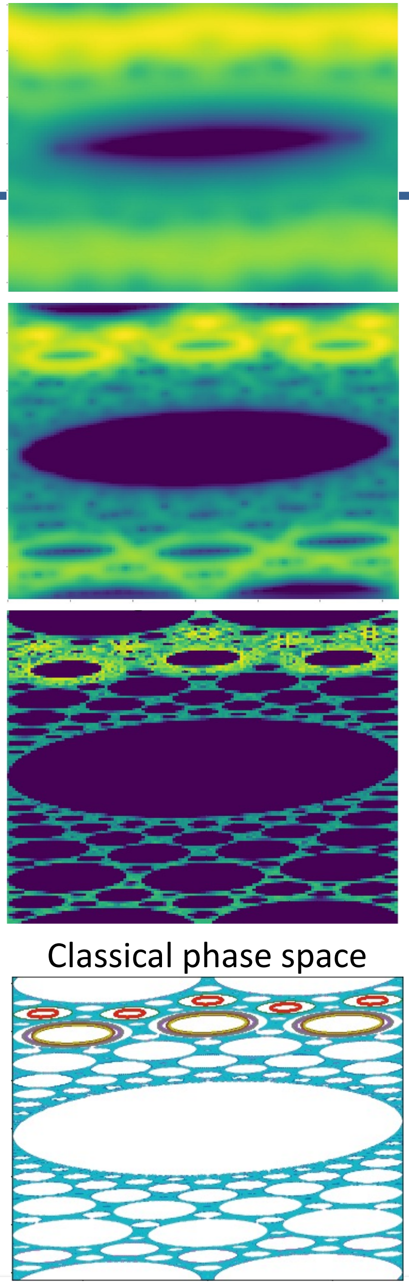
Quasiprobability (Husimi Q)

$n_{qubits}=6$

$n_{qubits}=9$

$n_{qubits}=16$

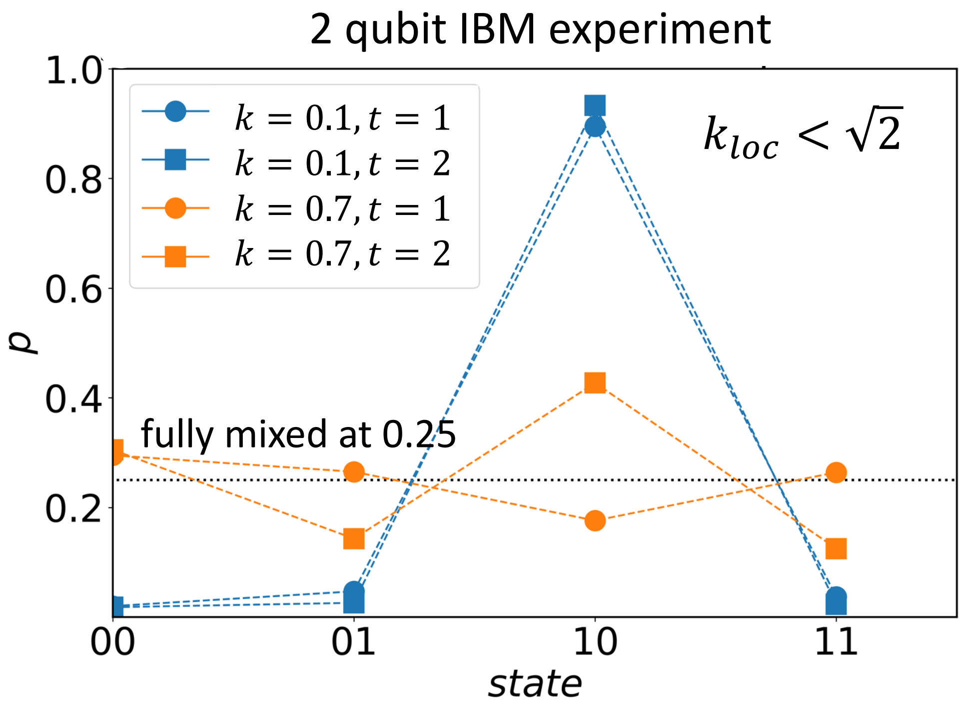
Classical phase space

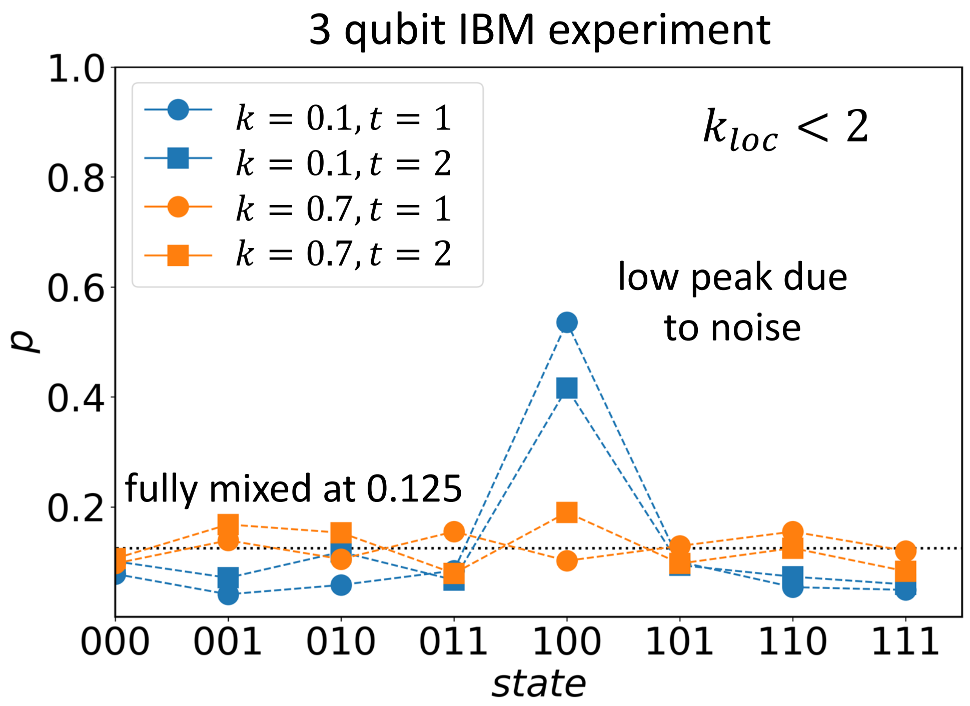


[1]A. Peres, *PRA* 30.4 (1984) 1610
[2]Ph. Jacquod et al., *Advances in Physics* 58.2, 67-196 (2009)
[3]R. A. Jalabert, H. M. Pastawski, *PRL* 86.12, 2490 (2001)
[4]G. Benenti et al., *PRL* 87.22, 227901 (2001)

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

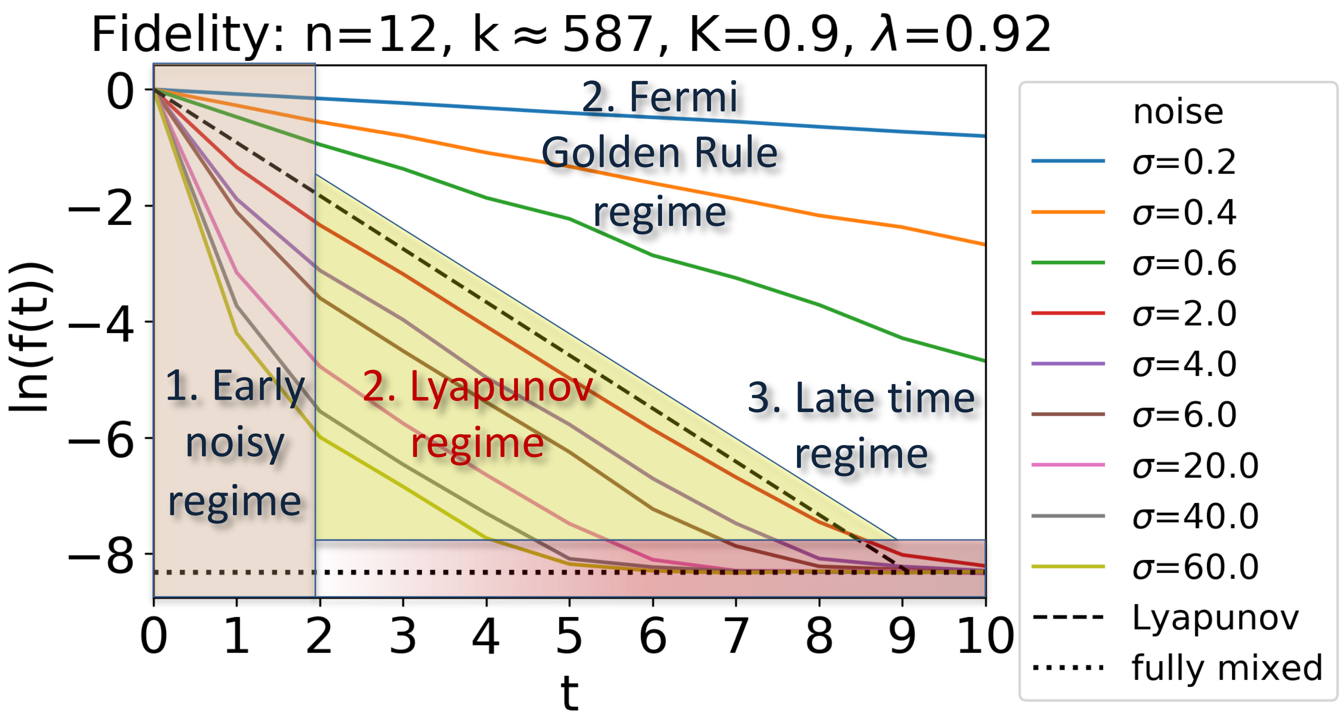
- **We see localization and diffusion for both 2 and 3 qubits**
  - Noise causes localization length decay

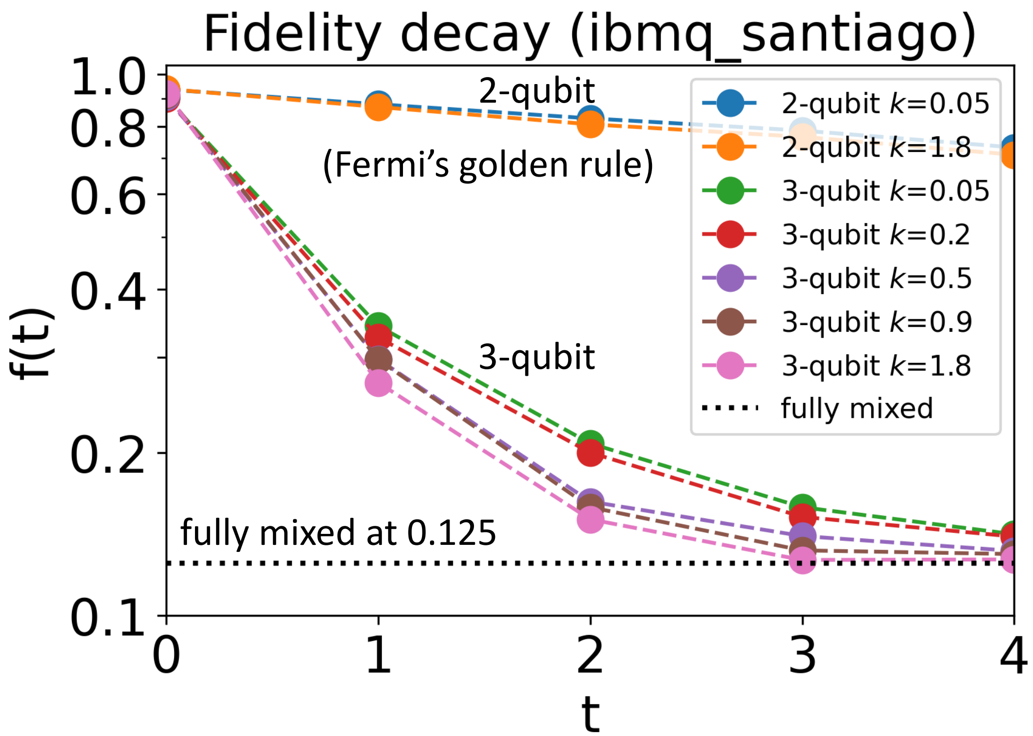




Statistical error $= 1/\sqrt{8{,}192}$ ~ 0.01

Theoretical and experimental studies have shown that the fidelity does in fact depend on the chaotic/diffusive nature of the dynamics





- **Lyapunov regime can be observed with enough qubits if the noise processes are small enough [1]**
  - Semiclassical regime requires at least 6 qubits
  - Experimental noise must be reduced by 2.5-13x
- **Experiments with 3 qubits on IBM-Q observe an effect that matches the expected trend [2]**
  - Diffusive decay is more rapid than localized
  - Effective noise is larger by 2x

[1] M. D. Porter, I. Joseph, arXiv:2110.07767, Quantum **6**, 799 (2022) [2] M. D. Porter, I. Joseph, arXiv:2206.04829

What about Generalized Eigenvalue Problems?

- **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

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

- 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

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

Quantum phase estimation can be applied to ideal MHD stability

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

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