

# The Intellectual & Technical Challenge of Quantum Computing

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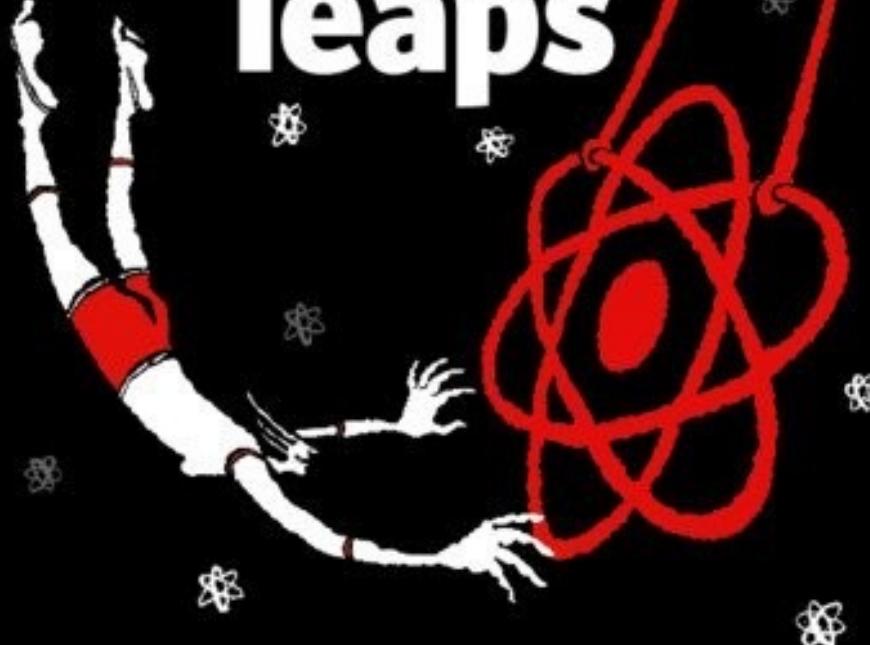
*AMCR & MSD  
Lawrence Berkeley  
National Laboratory*



MARCH 11TH-17TH 2017

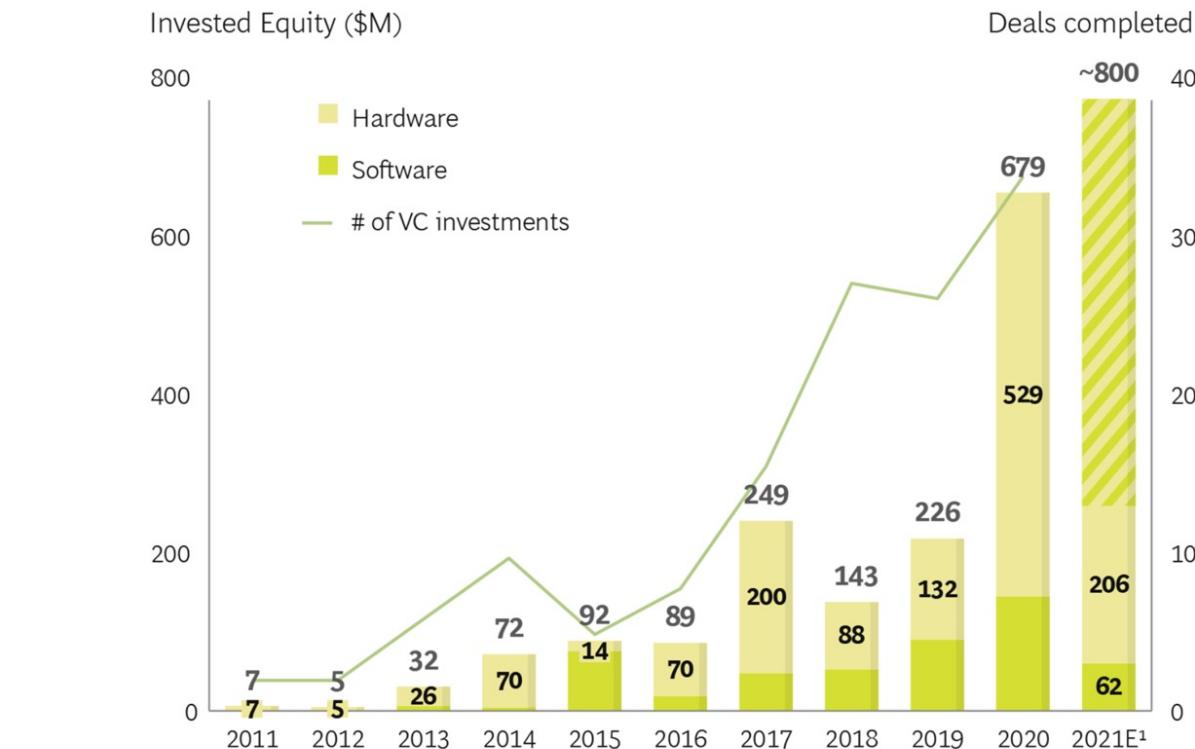
Ryancare attacked from left and right  
IS up against the wall in Mosul  
Taiwan and the one-China fiction  
Is there a bubble in the markets?

# Quantum leaps



A mind-bending technology goes mainstream

## What Happens When ‘If’ Turns to ‘When’ in Quantum Computing?



# BCG

THE BOSTON CONSULTING GROUP

JULY 21, 2021

By Jean-François Bobier, Matt Langione, Edward Tao, and Antoine Gourévitch

BCG estimates that quantum computing could create value of \$450 billion to \$850 billion in the next 15 to 30 years. Value of \$5 billion to \$10 billion could start accruing to users and providers as soon as the next three to five years.



### SOLVAY CONFERENCE 1927

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A. PICARD	E. HENRIOT	P. EHRENFEST	Ed. HERSEN	Th. DE DONDER	E. SCHRÖDINGER	E. VERSCHAFFELT	W. PAULI	W. HEISENBERG	R.H FOWLER	L. BRILLOUIN
P. DEBYE	M. KNUDSEN	W.L. BRAGG	H.A. KRAMERS	P.A.M. DIRAC	A.H. COMPTON	L. de BROGLIE	M. BORN	N. BOHR		
I. LANGMUIR	M. PLANCK	Mme CURIE	H.A. LORENTZ	A. EINSTEIN	P. LANGEVIN	Ch.E. GUYE	C.T.R. WILSON	O.W. RICHARDSON		

Absents : Sir W.H. BRAGG, H. DESLANDRES et E. VAN AUBEL



Einstein & Bohr in 1930  
(AIP Emilio Segré)

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MANJIT KUMAR

# QUANTUM

EINSTEIN, BOHR,  
AND THE GREAT DEBATE ABOUT  
THE NATURE OF REALITY

"One of the best guides yet  
to the central conundrums of modern  
physics." —John Banville

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Our *observations* of the world around reflect only some aspects of a much more complex, hidden reality!

We *need* this underlying structure to explain basic observations, even though we cannot directly measure it

We are now entering an era where we can finally use the quantum nature of matter as an engineering resource

**1** Quantum-advantaged mathematical function

## Sparse matrix math

**4** Computational problem types

**100+** High-value industry use cases  
\*Sizing at tech maturity



Pharma: Drug discovery  
\$40-80B

Aerospace: Computational fluid dynamics  
\$10-20B

Chemistry: Catalyst design  
\$20-50B

Energy: Solar conversion  
\$10-30B

Finance: Market simulation  
(e.g. derivative pricing)  
\$20-35B

Finance: Portfolio optimization  
\$20-50B

Insurance: Risk management  
\$10-20B

Logistics: Network optimization  
\$50-100B

Aerospace: Route optimization  
\$20-50B

Machine Learning

Automotive: Automated vehicles, AI algorithms  
\$0-10B

Finance: Anti-fraud, anti-money laundering  
\$20-30B

Tech: Search/ads optimization  
\$50-100B

Cryptography

Government: Encryption and decryption  
\$20-40B

Corporate: Encryption and decryption  
\$20-40B

Machine learning applications to impact most, if not all, industries

# Using Quantum for the Heavy Lifting

## Pharma Now

- \$2.5 Billion / new drug
  - Pre-clinical research selects 0.1% of small molecules for clinical trial
  - 10% of clinical trials are successful
- *Problem is that quantum effects in molecules evade classical simulation*

### Computation of Molecular Spectra on a Quantum Processor with an Error-Resilient Algorithm

J. I. Colless, V. V. Ramasesh, D. Dahmen, M. S. Blok, and M. E. Kimchi-Schwartz<sup>‡</sup>

Quantum Nanoelectronics Laboratory, Department of Physics,  
University of California, Berkeley, California 94720, USA;  
and Center for Quantum Coherent Science, University of California,  
Berkeley, California 94720, USA

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Computational Research Division, Lawrence Berkeley National Laboratory,  
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and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

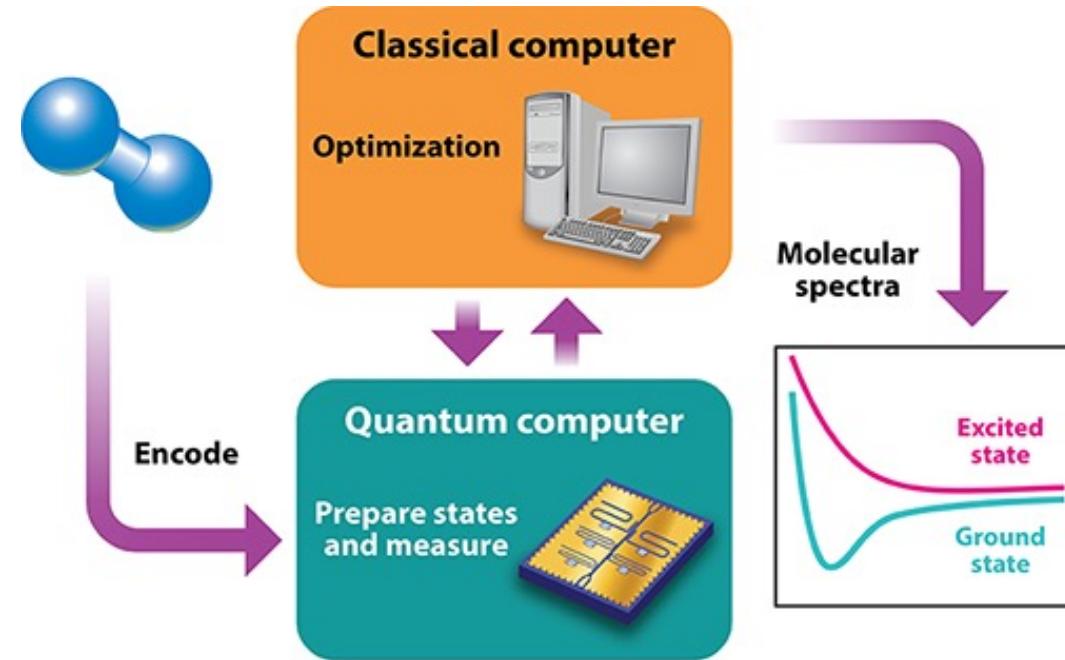
(Received 7 August 2017; published 12 February 2018)

## Physics

### VIEWPOINT

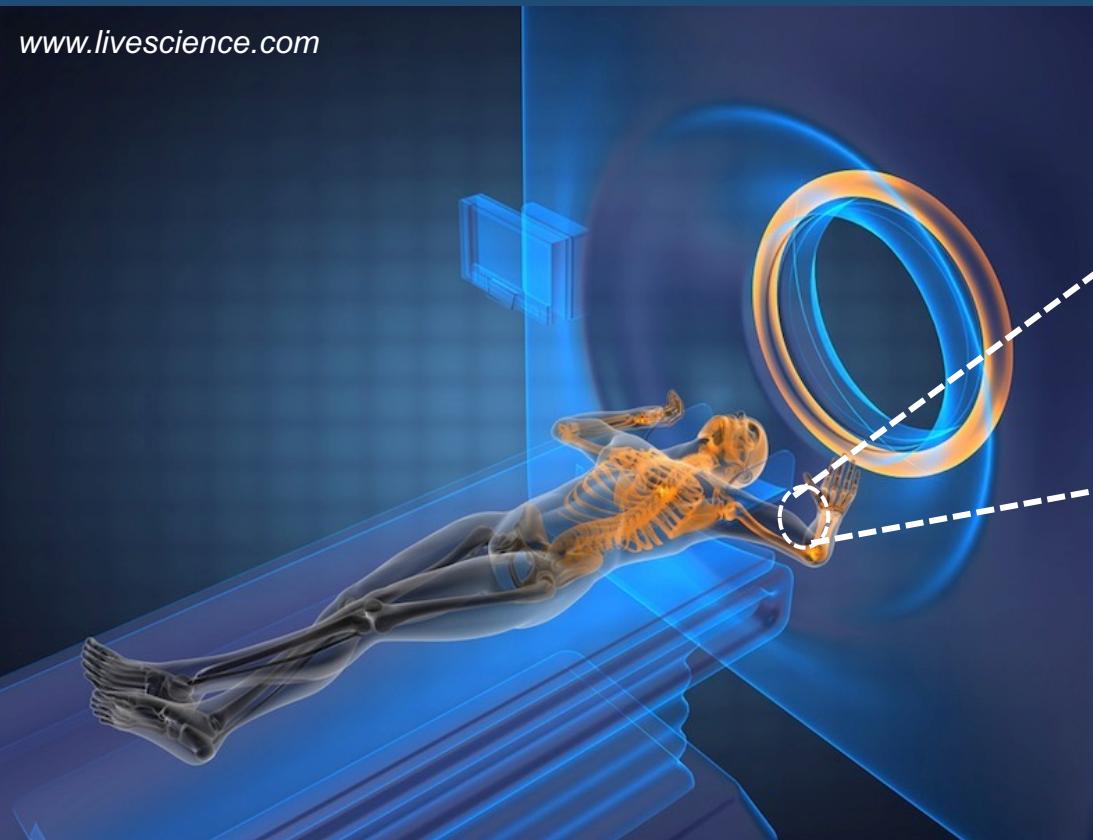
## Quantum Computer Simulates Excited States of Molecule

Excited-state energies of the hydrogen molecule have been calculated using a two-qubit quantum computer.

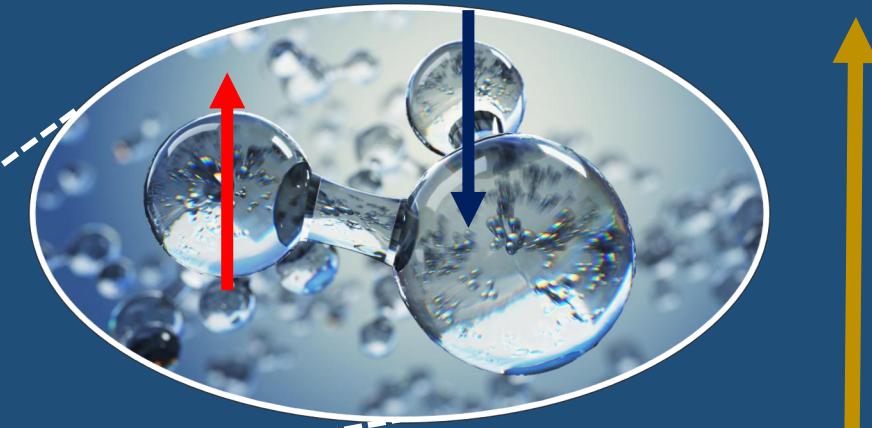


# The Quantum World Around Us

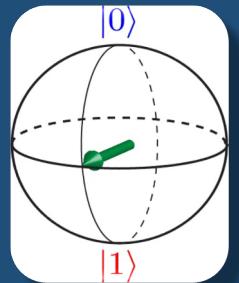
A MRI Scan Relies on Quantum Mechanics!



Water molecules have two hydrogens which have nuclear spin (up or down)



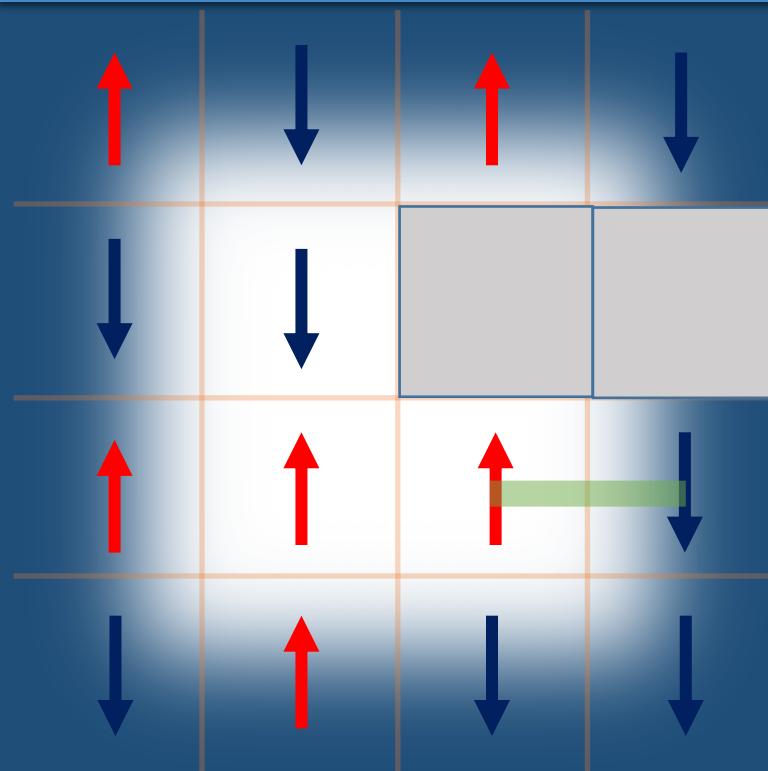
- Always observe or
- Prepare superposition: = +
- Would measure: 50% , 50%



**QUANTUM SYSTEMS CAN EXIST IN MANY DIFFERENT CONFIGURATIONS, EVEN IF WE CAN'T OBSERVE ALL OF THEM!**

# The Power of Entanglement

- Let's build a computer one spin (quantum bit) at a time !
- Unlike MRI which measures average properties of a group of spins, we need to address each spin individually



Entangled State

$2^N \gg 2N$ : NEED MORE NUMBERS THAN PARTICLES IN THE UNIVERSE TO DESCRIBE ~ 300 ENTANGLED QUBITS

- Measurement reveals state to be  $a \cdot \uparrow + b \cdot \downarrow$
- If we don't observe, state is  $(a \cdot \uparrow + b \cdot \downarrow)$  and described by 2 numbers  $\{a,b\}$
- Adjacent bit is  $(c \cdot \uparrow + d \cdot \downarrow)$  and described by 2 numbers  $\{c,d\}$
- Couple these two bits and consider product:  $(a \cdot \uparrow + b \cdot \downarrow) \times (c \cdot \uparrow + d \cdot \downarrow)$

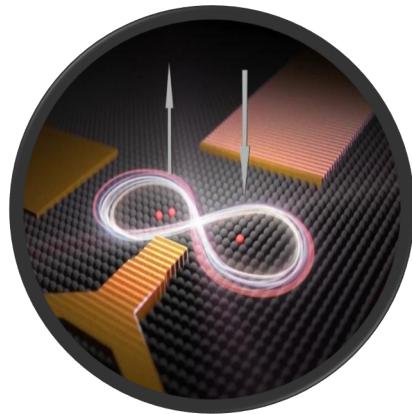
$$ac \cdot \uparrow\uparrow + ad \cdot \uparrow\downarrow + bc \cdot \downarrow\uparrow + bd \cdot \downarrow\downarrow$$

cannot describe

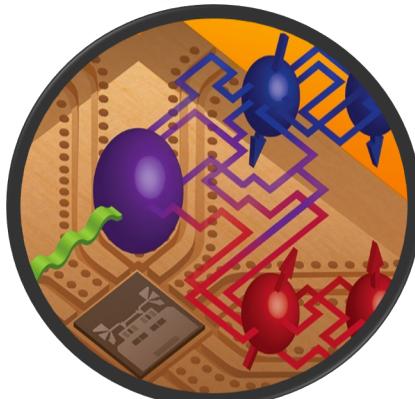
$$\uparrow\uparrow + \downarrow\downarrow$$

If  $a = 0$ , lose  $ac \cdot \uparrow\uparrow$   
If  $d = 0$ , lose  $bd \cdot \downarrow\downarrow$

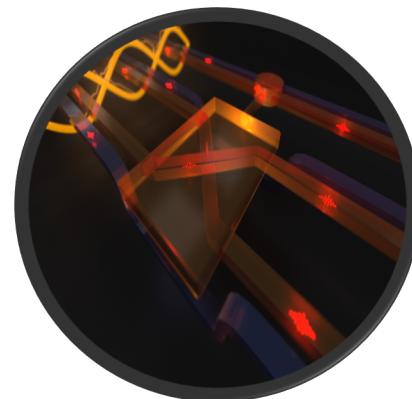
# Types of Quantum Bits & Progress



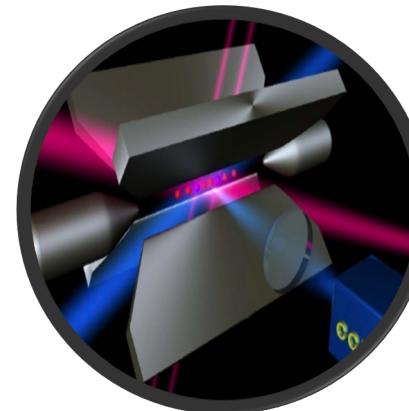
**Dopants in  
Silicon / Diamond**  
[www.sciencedaily.com](http://www.sciencedaily.com)



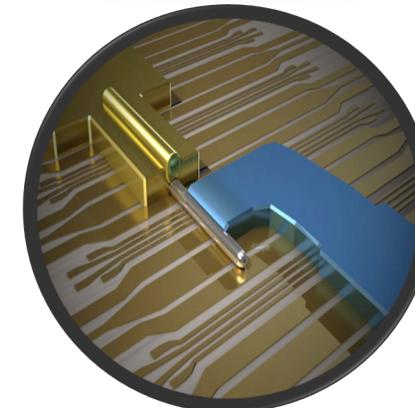
**Superconducting  
Circuits**  
[www.qnl.berkeley.edu](http://www.qnl.berkeley.edu)



**Photonic  
Circuits**  
[www.phys.org](http://www.phys.org)



**Trapped  
Ions**  
[www.quantumoptics.at](http://www.quantumoptics.at)



**Topological  
Wires**  
[www.microsoft.com](http://www.microsoft.com)

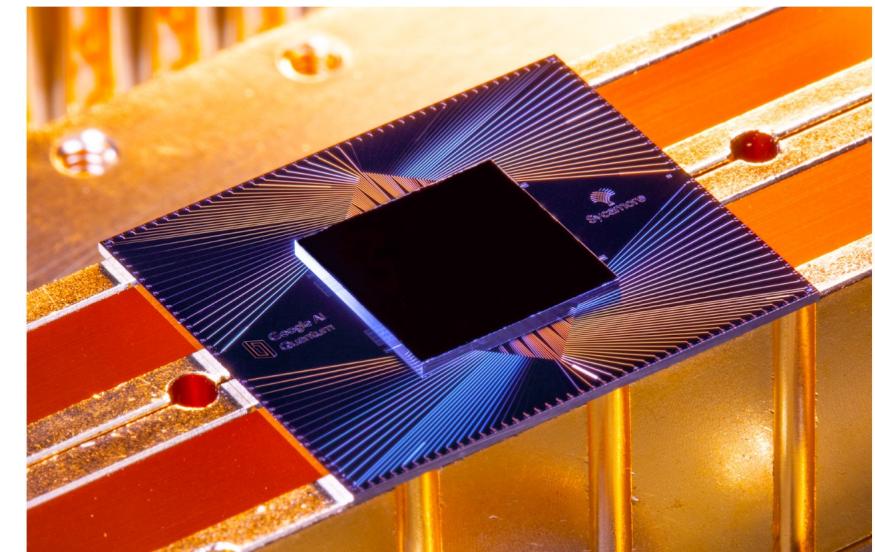
The New York Times

## Why Google's Quantum Supremacy Milestone Matters

The company says its quantum computer can complete a calculation much faster than a supercomputer. What does that mean?

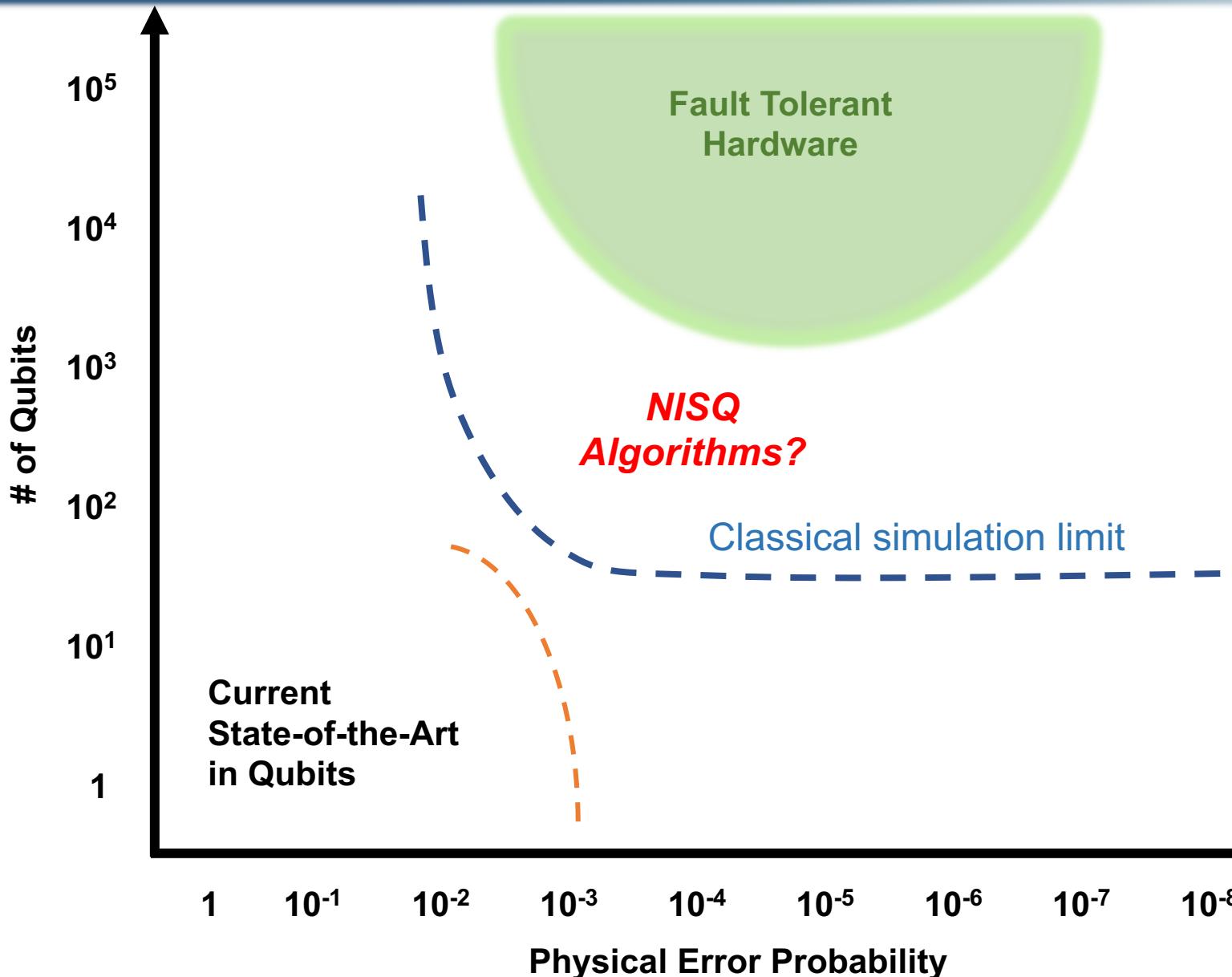
By Scott Aaronson

Dr. Aaronson is the founding director of the Quantum Information Center at the University of Texas at Austin.



Google A.I. Quantum's Sycamore processor. Erik Lucero/Google

# Surpassing the Classical Limit



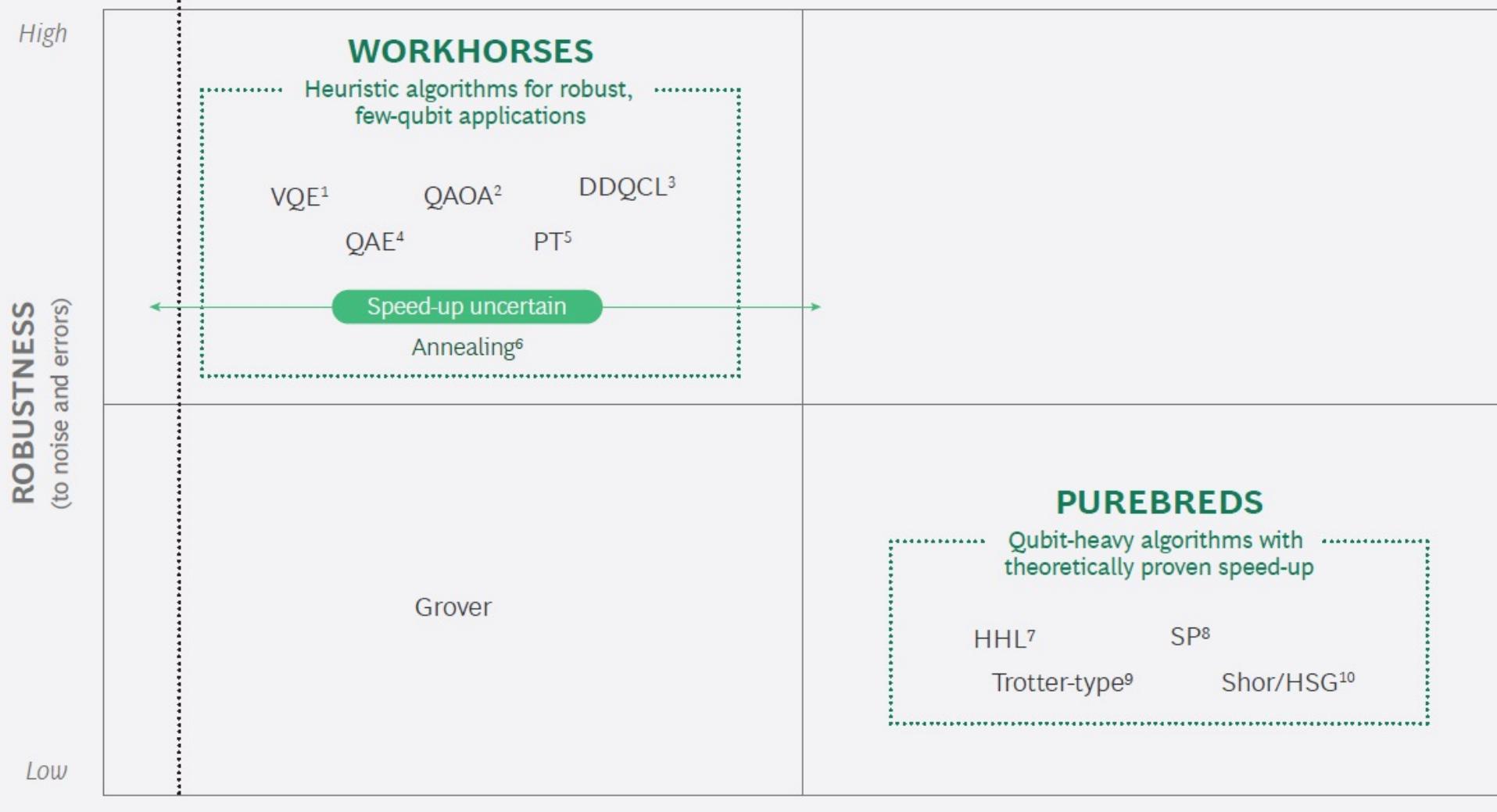
## NOISY, INTERMEDIATE SCALE QUANTUM (NISQ) ERA

- 10-100 physical qubits
- Minimal error correction
- Purely quantum & hybrid algorithms
- < 100 Logical gate operations

***Today, we will talk about...***

- Building better superconducting qubits (materials & architecture)
- Characterizing noise using quantum circuits (algorithms)
- Tailoring noise to improve performance

## → Realm of Quantum Advantage

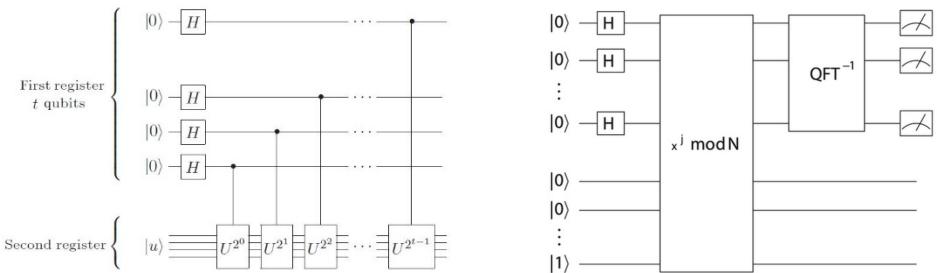


Sources: BCG analysis; expert interviews.

# PURE QUANTUM ROUTINES

## Shor Factoring Algorithm:

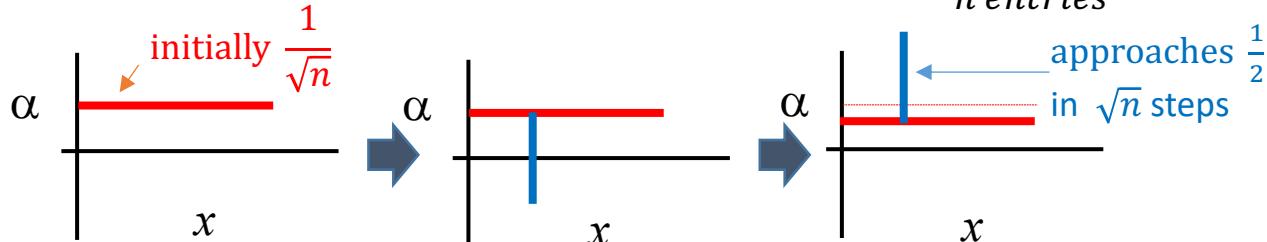
- Exponential speed up over best known classical algorithms
- Modular arithmetic and period finding (QFT)



## Grover Search Algorithm:

- Polynomial speed up over best known classical algorithms  $\sqrt{n}$  versus  $n$
- Relies on phase inversion and mean subtraction

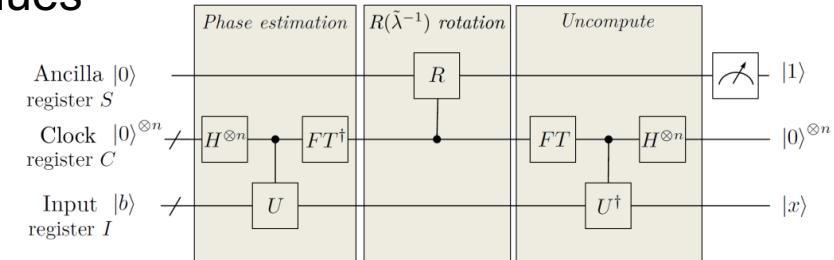
$$f(x) = 1 \text{ for } x = x^* \text{ else } f(x) = 0 \quad |\Psi\rangle = \sum_{n \text{ entries}} \alpha_n |x\rangle$$



## HHL Linear Equation Algorithm:

- Exponential speed up over best known classical algorithms
- Use phase estimation to approximate eigenvalues

$$\begin{array}{c} A\vec{x} = \vec{b} \\ \downarrow \\ A|x\rangle = |b\rangle \end{array}$$



arXiv:1802.08227v1

## Some Challenges..

- deep quantum circuits (many gates)
- fault tolerance, error correction
- Q-RAM
- often have fine print...

*Quantum Algorithms Make use of Entanglement, Superposition, Interference, Projection,..*

- need to understand resource allocation
- influence classical algorithms!

# QUANTUM INSPIRED CLASSICAL ROUTINES

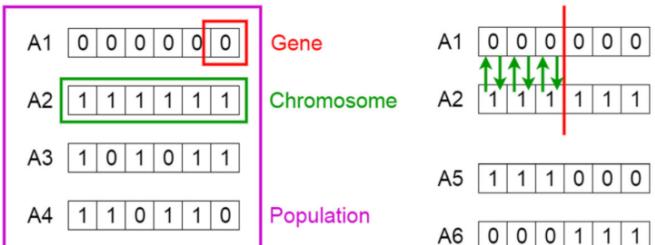
## Matrix Completion Problem

(see also the Netflix problem):

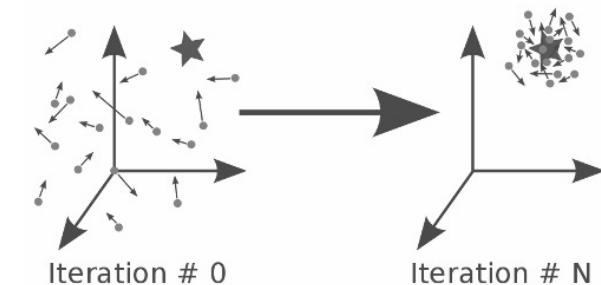
- i) Sample preference matrix  $T_{ij}$  for users (i) and products (j)
- ii) Low rank approximation
- iii) Generate suggestions for users

$T$  ( $n \times m$  matrix):  $O[\text{poly}(k)\text{poly}(mn)]$   
Reduced rank  $k$

## Genetic Algorithms



## Social Behavior Routines



## Quantum Recommendation System

Iordanis Kerenidis<sup>\*1</sup> and Anupam Prakash<sup>†2</sup>

- <sup>1</sup> CNRS, IRIF, Université Paris Diderot, Paris, France and Centre for Quantum Technologies, National University of Singapore, Singapore  
jkeren@liafa.univ-paris-diderot.fr
- <sup>2</sup> Centre for Quantum Technologies and School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore  
aprakash@ntu.edu.sg

$T$  ( $n \times m$  matrix):  $O[\text{poly}(k)\text{polylog}(mn)]$   
Reduced rank  $k$

## QUANTUM COMPUTING

Major Quantum Computing Advance Made Obsolete by Teenager

- $\ell^2$  - norm sampling

## Quantum-inspired genetic algorithms

Ajit Narayanan and Mark Moore  
Department of Computer Science  
University of Exeter  
Exeter, United Kingdom, EX4 4PT  
ajit@dcs.exeter.ac.uk

- Interfere different “universes” in parallel

### Genetic Quantum Algorithm and its Application to Combinatorial Optimization Problem

Kuk-Hyun Han  
Dept. of Electrical Engineering, KAIST,  
373-1, Kusong-dong Yusong-gu  
Taejon, 305-701, Republic of Korea  
khhan@vivaldi.kaist.ac.kr

Jong-Hwan Kim  
Dept. of Electrical Engineering, KAIST,  
373-1, Kusong-dong Yusong-gu  
Taejon, 305-701, Republic of Korea  
johkim@vivaldi.kaist.ac.kr

- Each gene is a classical superposition
- Use rotating gates for diversity

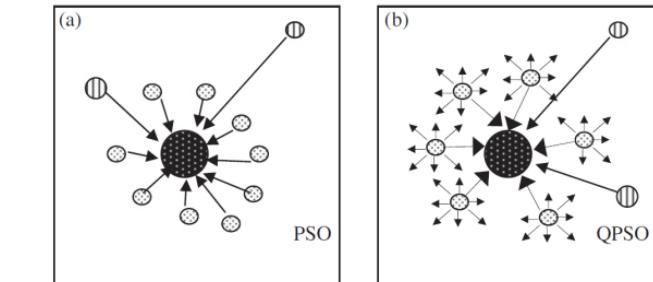
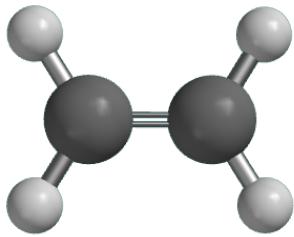


Fig. 1. The movements of particles in PSO and QPSO; (a) PSO (b) QPSO.

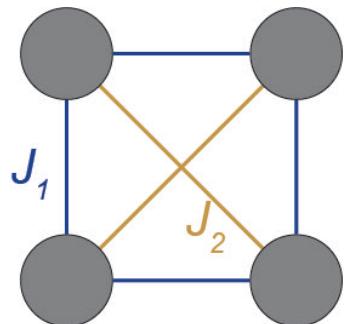
# VARIATIONAL QUANTUM EIGENSOLVER (VQE)

**Goal:** Minimize cost function  $H$

$H$  encodes problem of interest, such as:



molecular structure



Highly correlated materials

## Applications

- Drug design
- Better N<sub>2</sub>-fixation for fertilizer production
- Understanding High-T<sub>c</sub> superconductivity

**Procedure:**

Map  $H$  to qubit Hamiltonian  $H$

VQE optimization cycle

Quantum Processor

2. Prepare  $|\psi(\vec{\theta})\rangle$

3. Measure

$\langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle$

Classical Processor

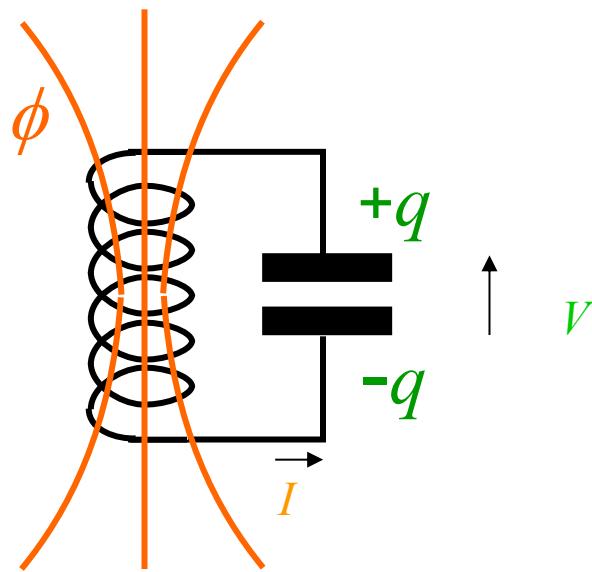
1. Select  $\vec{\theta}$

4. Choose new  $\vec{\theta}$   
w/ optimizer (e.g. SPSA)

Repeat 2-4 until convergence

# *Superconducting Quantum Hardware*

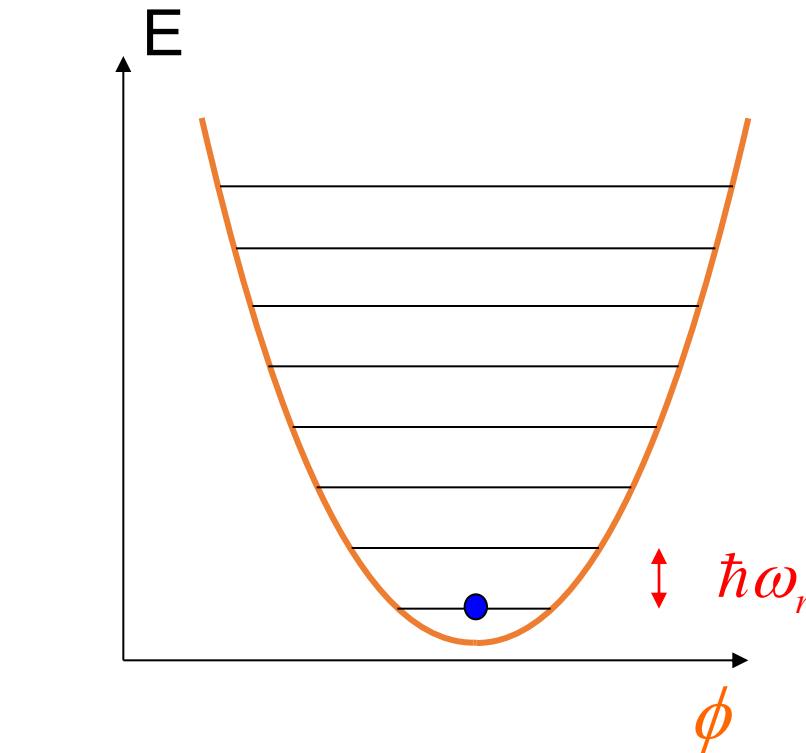
# LC OSCILLATOR AS A QUANTUM CIRCUIT



$$[\phi, q] = i\hbar$$

$$\phi = LI$$

$$q = CV$$

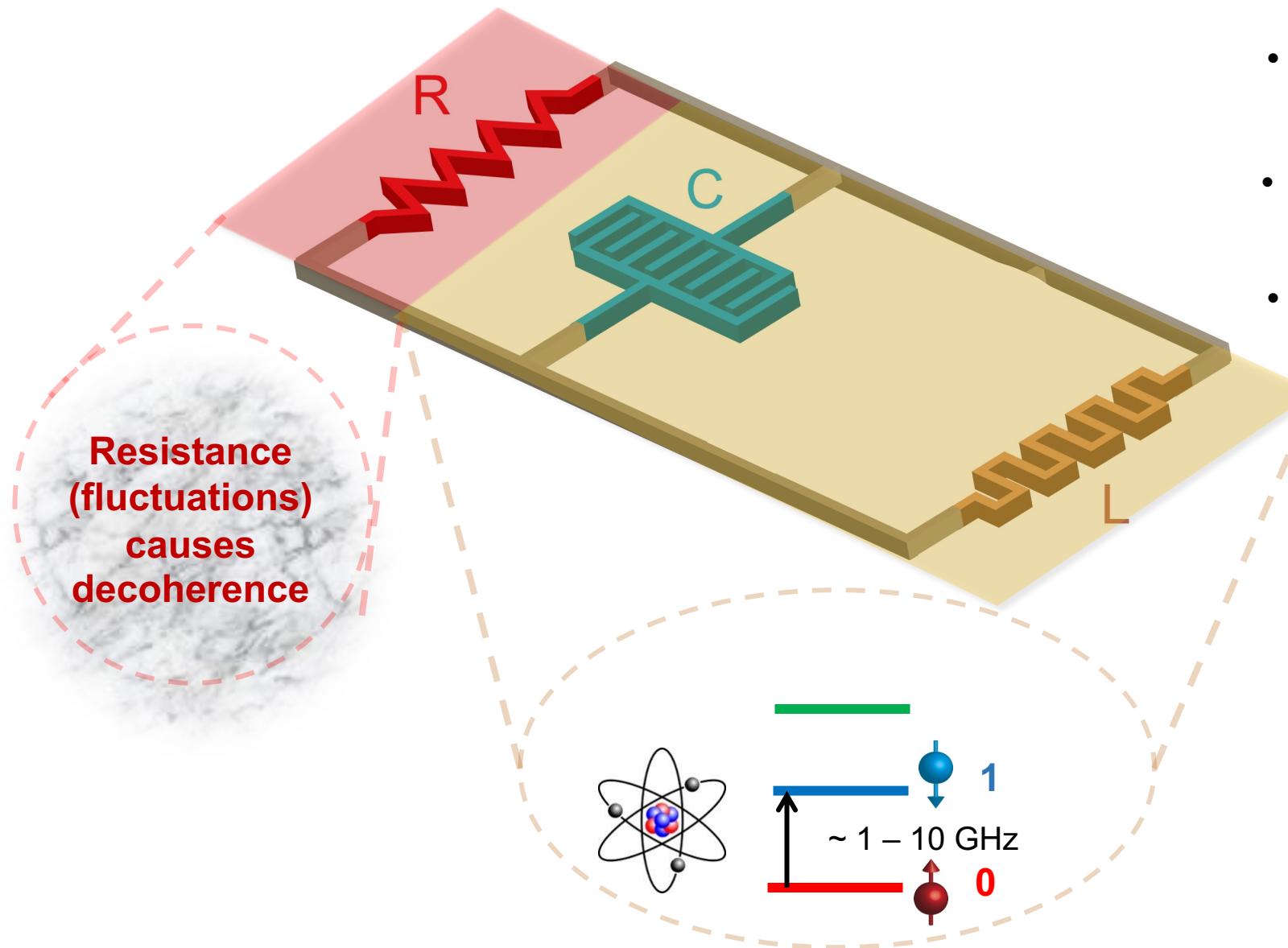


$\hbar\omega_r > k_B T$

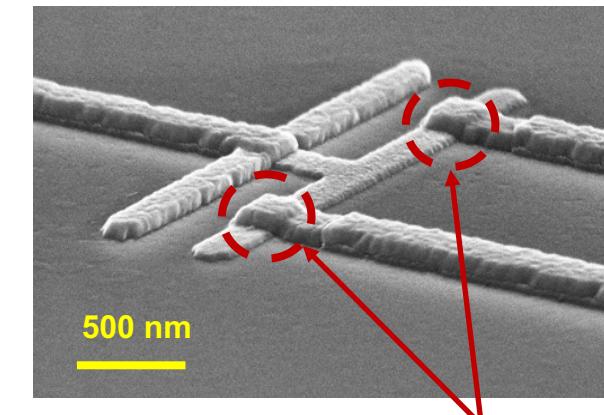
1GHz  
(~ 50 mK)

10mK

# A Qubit is just a Nonlinear Oscillator



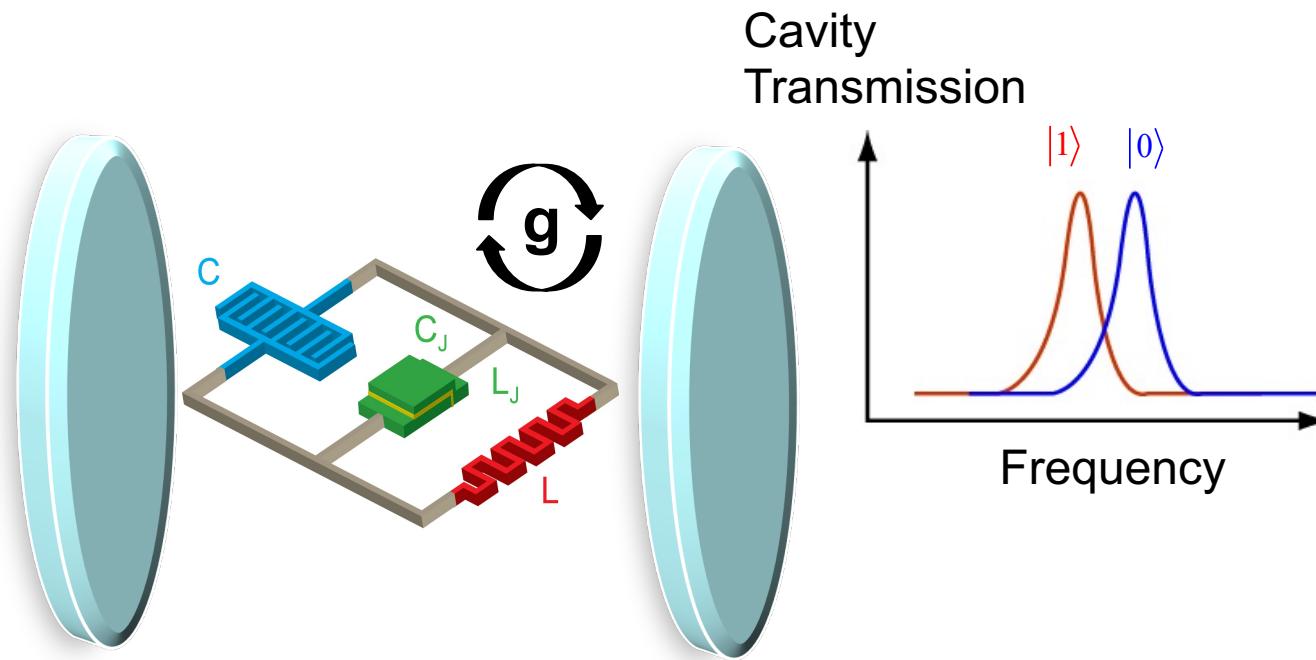
- Classical harmonic oscillator: all energies (currents) are allowed
- Quantum harmonic oscillator: only certain energies (currents) are allowed
- Tunnel junction  $\rightarrow$  Nonlinear, isolate **0, 1**



Al/AlOx/Al Josephson tunnel junctions

# MEASUREMENT : COUPLE TO E-M FIELD OF CAVITY

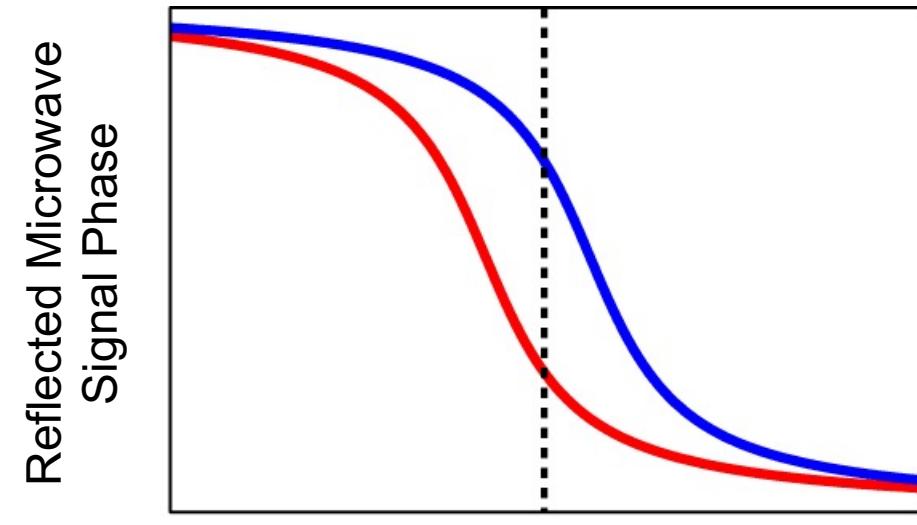
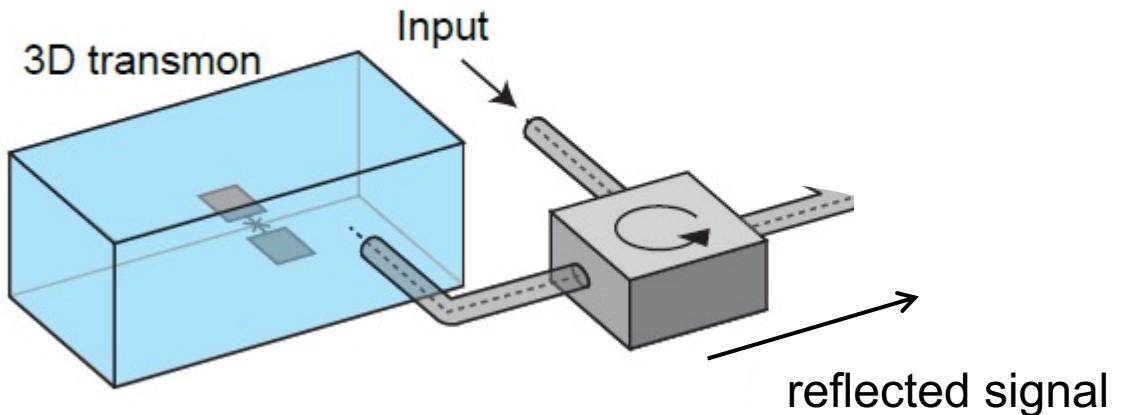
(Jaynes-Cummings)



$$H = \frac{1}{2}\hbar\omega_q\sigma_z + \hbar\omega_r(a^\dagger a + \frac{1}{2}) + \hbar g(a^\dagger\sigma_- + a\sigma_+)$$

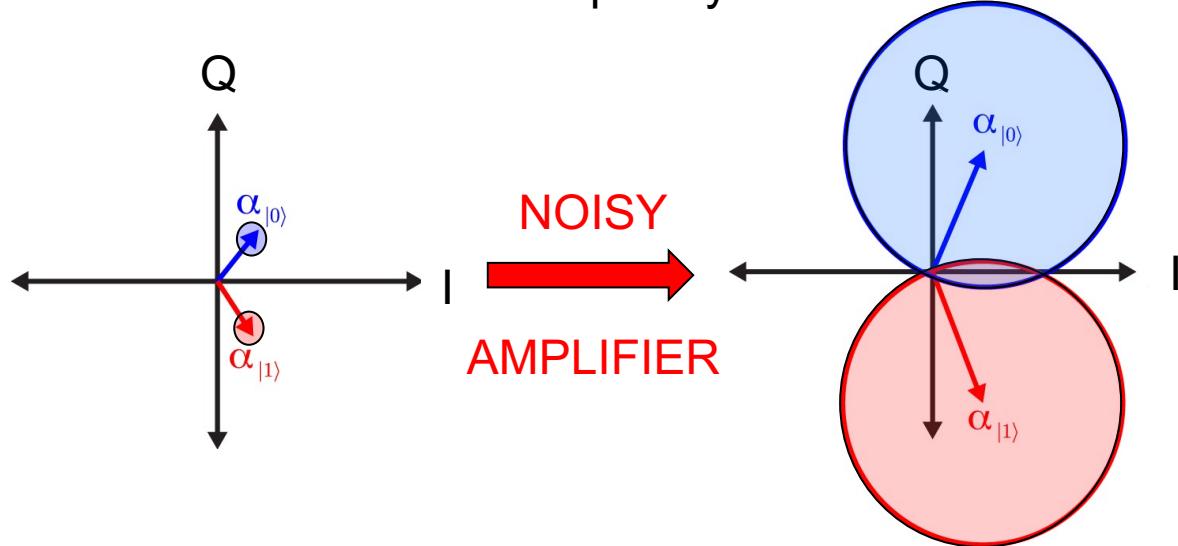
$$H_{disp} = \frac{1}{2}\hbar\omega_q\sigma_z + \hbar(\omega_r + \boxed{\chi\sigma_z})(a^\dagger a + \frac{1}{2})$$

# MEASURING QUBIT STATES: MICROWAVE REFLECTOMETRY



$$\begin{aligned} A \sin(\omega t + \phi) &= A \sin(\omega t) \cos(\phi) + A \cos(\omega t) \sin(\phi) \\ &= \underbrace{[A \cos(\phi)]}_{\text{I}} \sin(\omega t) + \underbrace{[A \sin(\phi)]}_{\text{Q}} \cos(\omega t) \end{aligned}$$

- Measure Single Quadrature
- Homodyne Measurement: Voltage (Phase 'Q')



# HYBRID ALGORITHMS & CHEMISTRY

PHYSICAL REVIEW X 8, 011021 (2018)

Featured in Physics

## Computation of Molecular Spectra on a Quantum Processor with an Error-Resilient Algorithm

J. I. Colless, V. V. Ramasesh, D. Dahlen, M. S. Blok, and M. E. Kimchi-Schwartz<sup>‡</sup>

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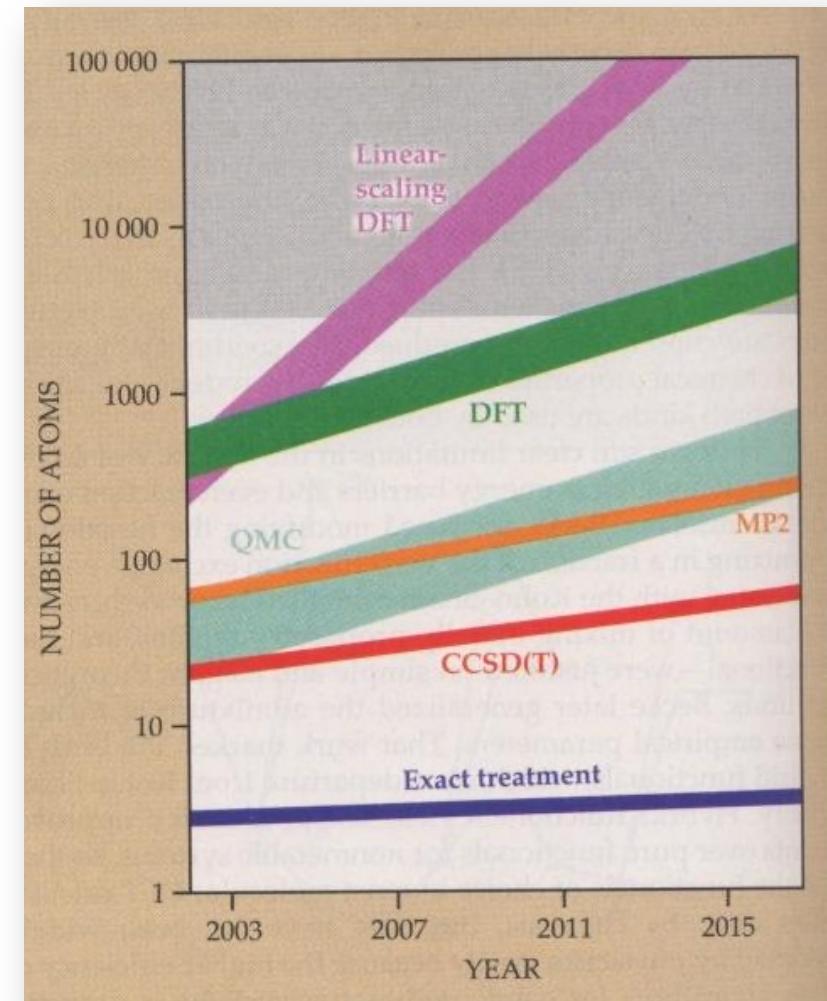
I. Siddiqi<sup>\*</sup>

Quantum Nanoelectronics Laboratory, Department of Physics,  
University of California, Berkeley, California 94720, USA;  
Center for Quantum Coherent Science, University of California, Berkeley, California 94720, USA;  
and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

**Memory Requirements for Exact (Full Configuration Interaction)**

System	Memory (PB)	Max Qubits
TACC Stampede	0.192	43
Titan	0.71	45
K Computer	1.4	46
APEX2020	4-10	48-49

M. Head-Gordon, M. Artacho,  
*Physics Today* 4 (2008)

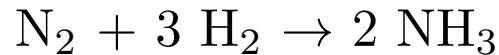


# GRAND SOLUTIONS FROM A GRAND DEVICE

## Humans: Haber Process

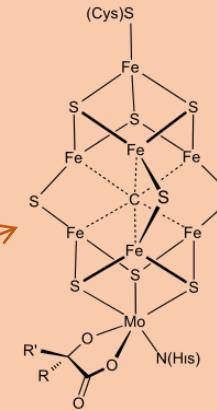
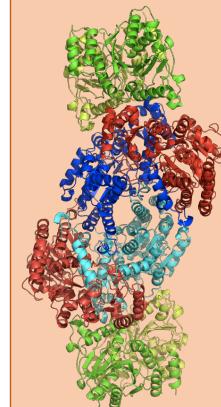
400 C & 200 atm

1-2% of ALL energy on earth,  
used on Haber process



## Nature: Nitrogenase

25 C & 1 atm



“FeMoco”

Beyond all current classical methods

Both electronic structure and substrate attachment almost totally unknown

**Classically** – No clear path to accurate solution  
**Quantum Mechanically** – 150-200 logical qubits for solution

# VARIATIONAL QUANTUM EIGENsolver (VQE)

Variational Formulation:

$$\text{Minimize } \langle \Psi | H | \Psi \rangle$$

Decompose as:

$$\mathcal{H} = h_{\alpha}^i \sigma_{\alpha}^i + h_{\alpha\beta}^{ij} \sigma_{\alpha}^i \sigma_{\beta}^j + h_{\alpha\beta\gamma}^{ijk} \sigma_{\alpha}^i \sigma_{\beta}^j \sigma_{\gamma}^k + \dots$$

By Linearity:  $\langle \psi | \mathcal{H} | \psi \rangle \equiv \langle \mathcal{H} \rangle = \mathcal{H} = h_{\alpha}^i \langle \sigma_{\alpha}^i \rangle + h_{\alpha\beta}^{ij} \langle \sigma_{\alpha}^i \sigma_{\beta}^j \rangle + h_{\alpha\beta\gamma}^{ijk} \langle \sigma_{\alpha}^i \sigma_{\beta}^j \sigma_{\gamma}^k \rangle + \dots$

---

Easy for a Quantum Computer:

$$\langle \sigma_{\alpha}^i \sigma_{\beta}^j \sigma_{\gamma}^k \dots \rangle$$



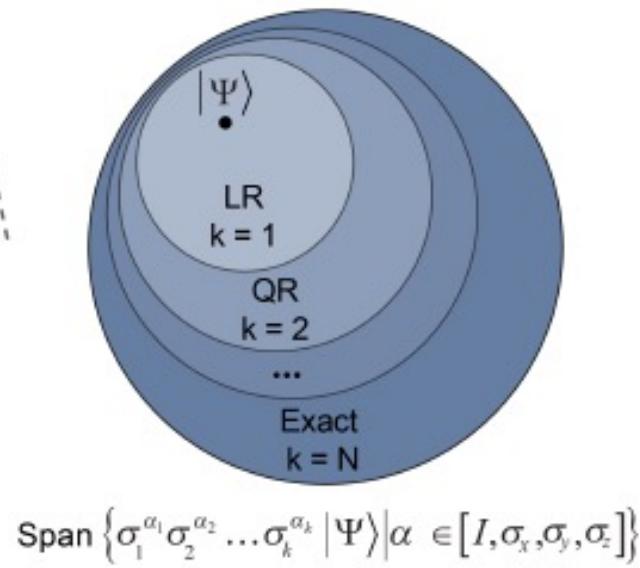
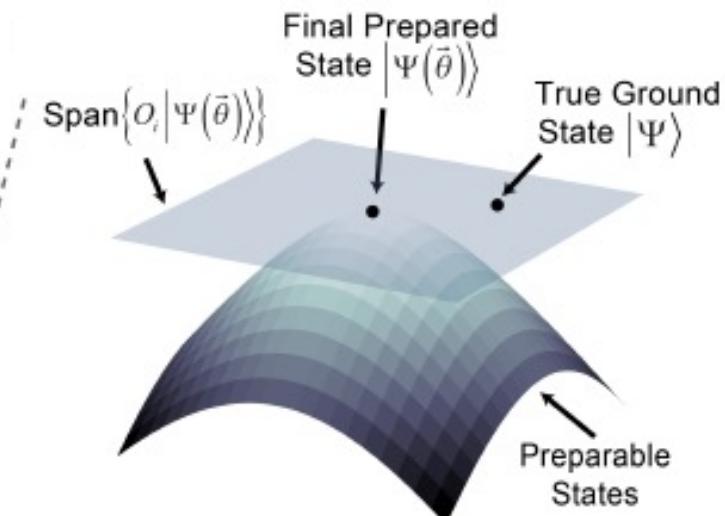
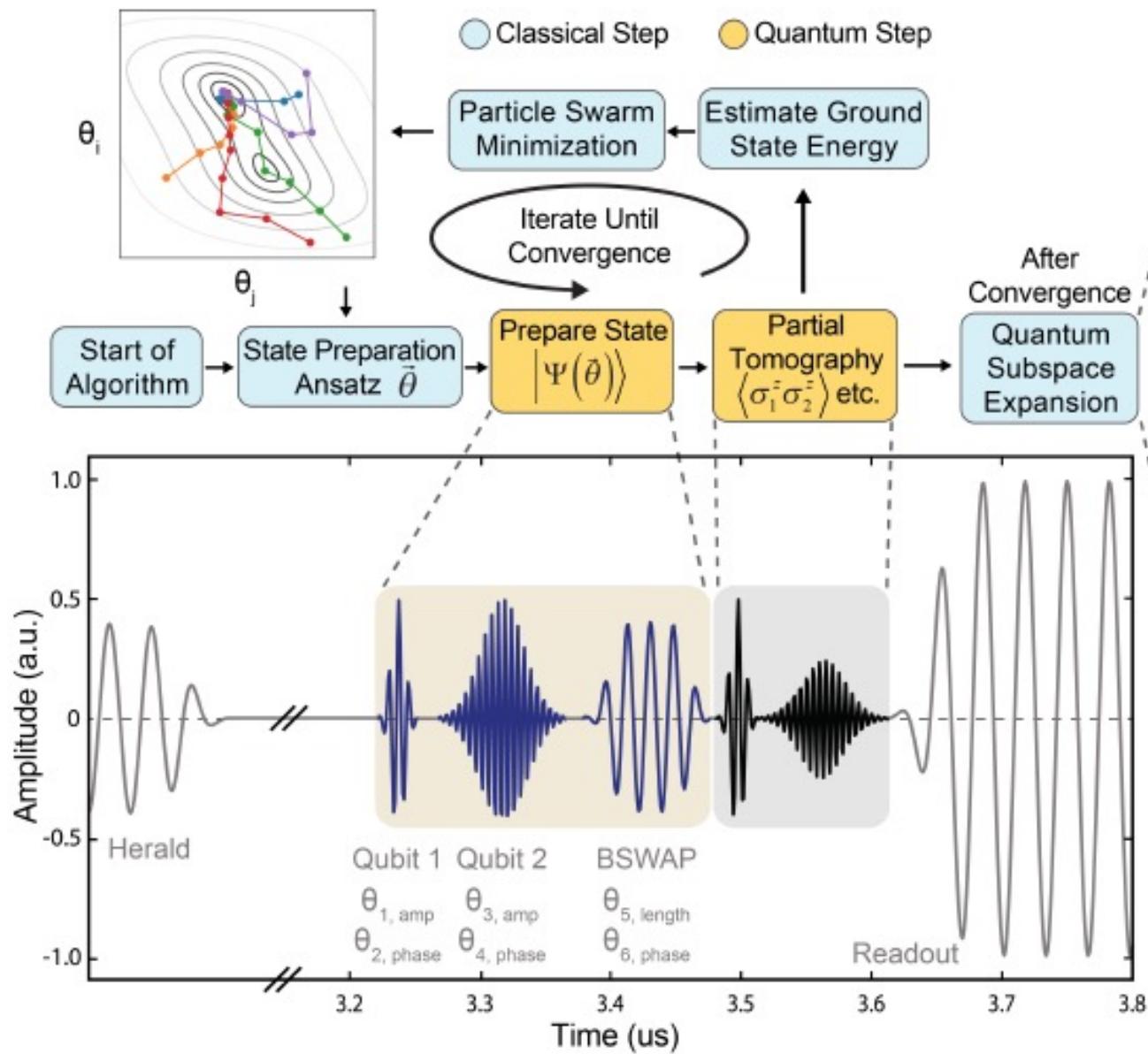
Easy for a Classical Computer:

$$+, \times \rightarrow \langle H \rangle$$

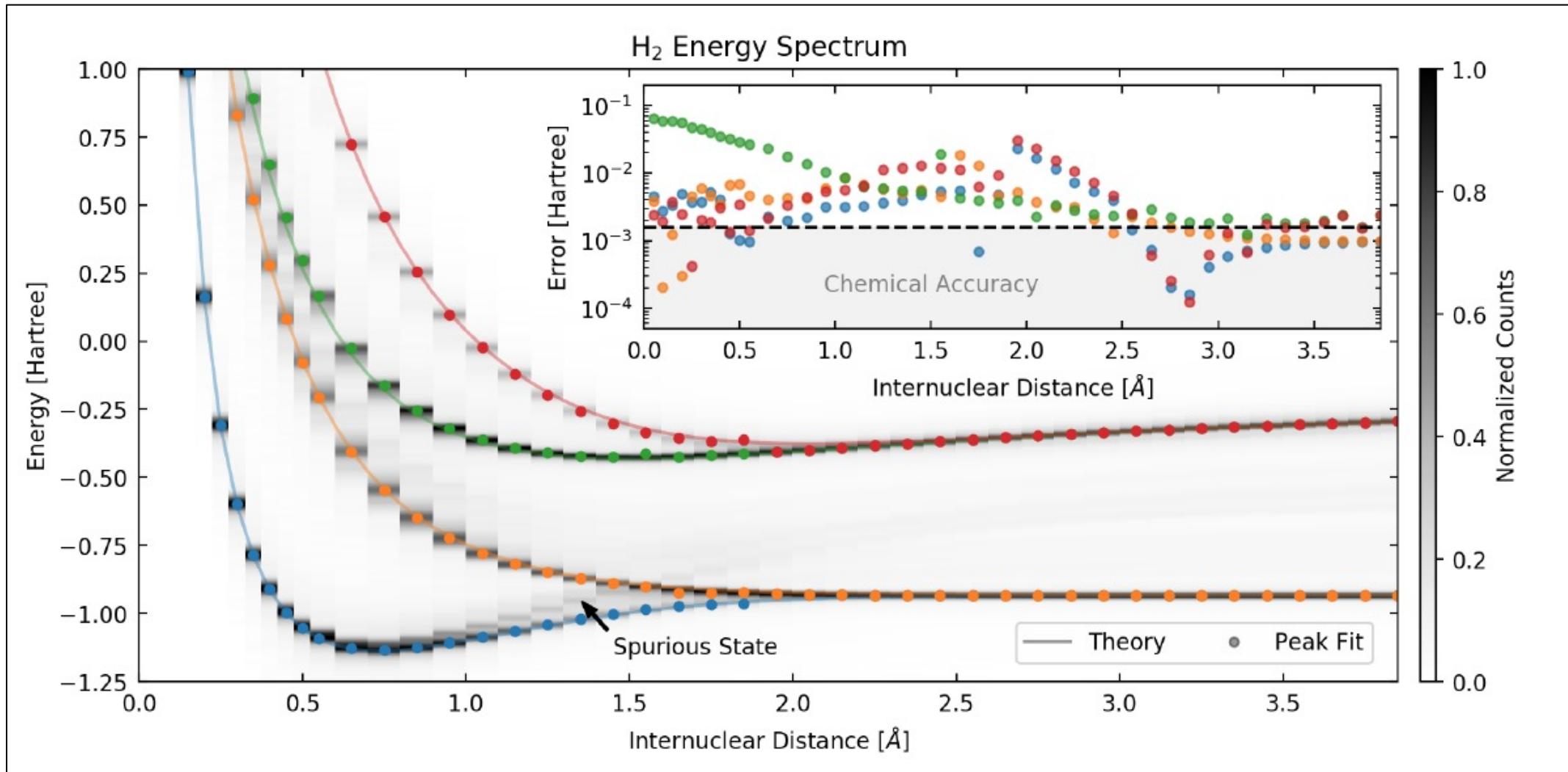
## Hybrid Scheme:

- Parameterize quantum state with classical experimental parameters
- Compute averages using quantum computer
- Update state using classical minimization algorithm (e.g. particle swarm)

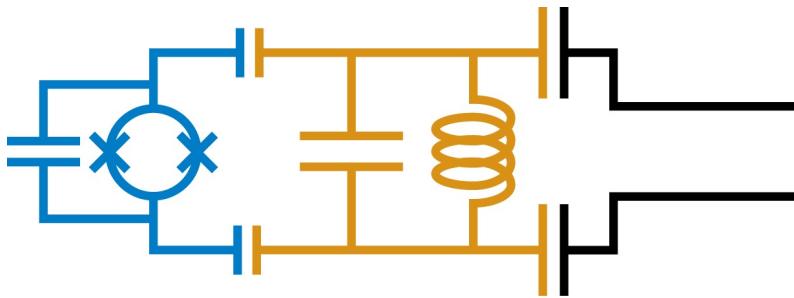
# VQE ALGORITHM



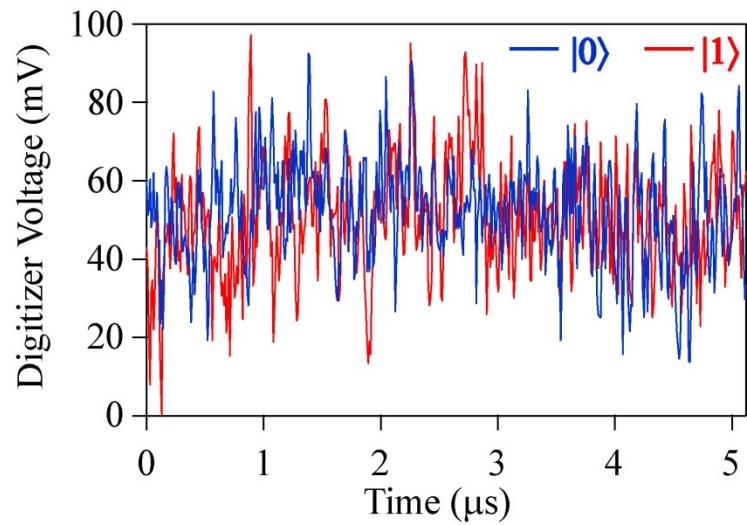
# $H_2$ REVISITED



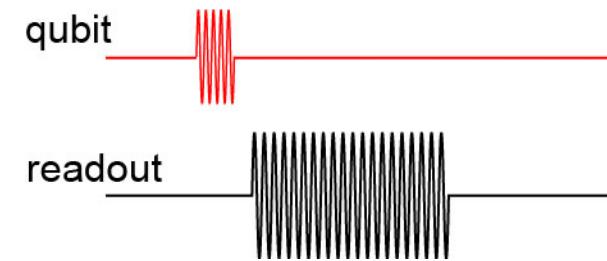
# SINGLE SHOT MEASUREMENTS



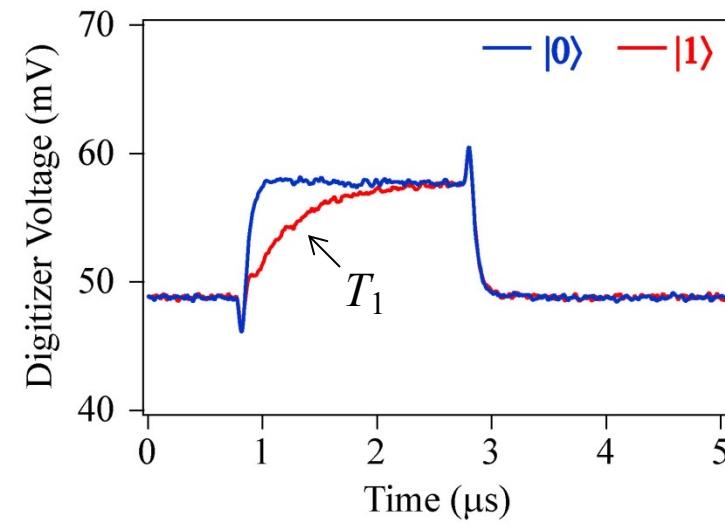
Single measurement trace



$10^4$   
Averages

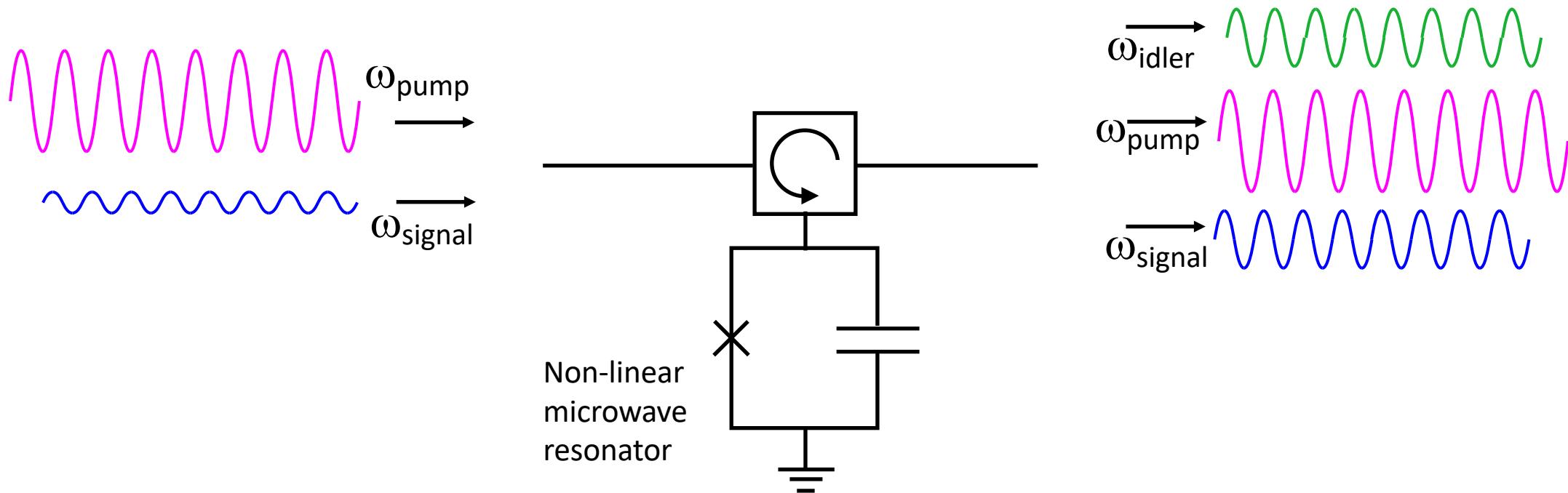


Averaged measurement trace

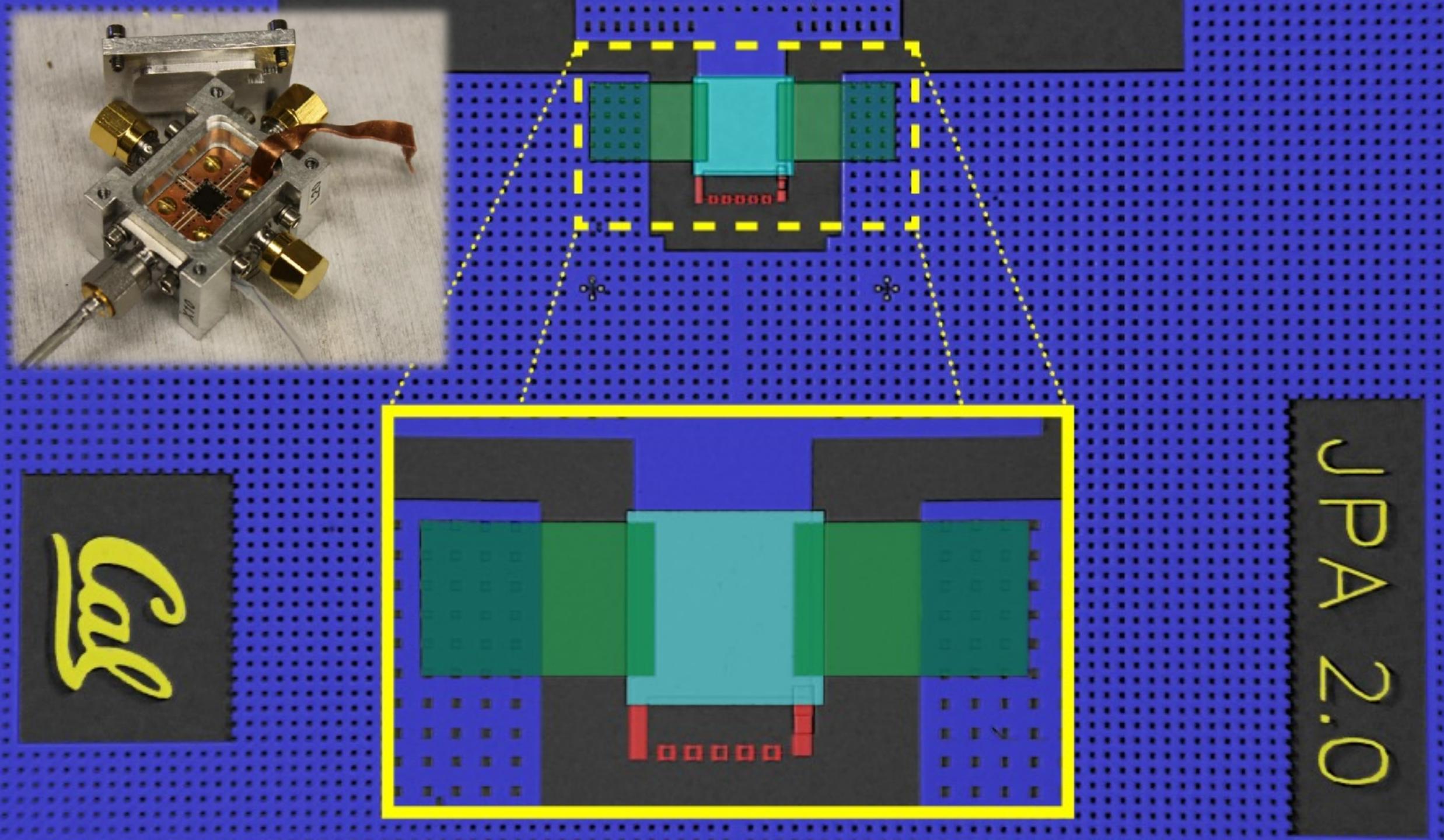


Amplifier ( $T_{\text{SYS}} = 7\text{K}$ ) noise masks qubit state information

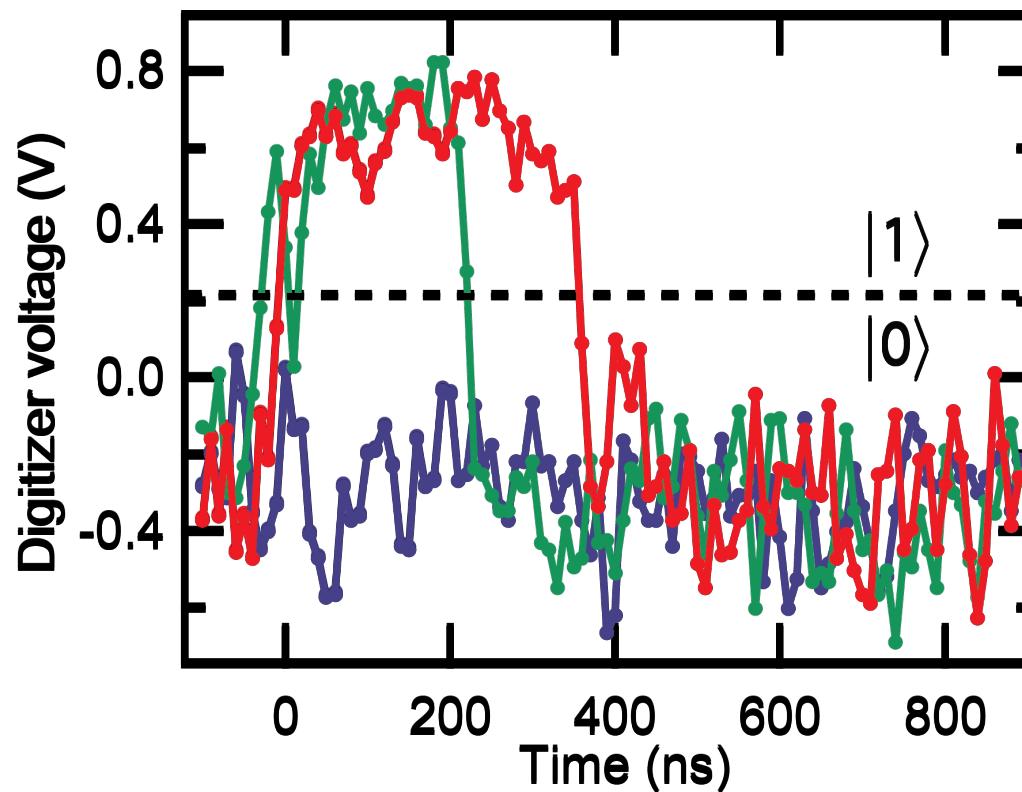
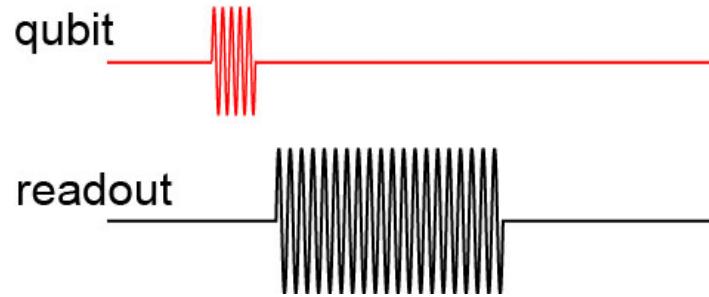
# SUPERCONDUCTING PARAMETRIC AMPLIFIERS (RESONANT CAVITY BASED)



$$\begin{aligned} G &= 20 \text{ dB} \\ f_0 &= 4-8 \text{ GHz} \\ f_{-3\text{dB}} &= 10-50 \text{ MHz} \\ T_N &\sim 1.2 T_Q \end{aligned}$$



# SINGLE SHOT MEASUREMENTS



PRL 106, 110502 (2011)

PHYSICAL REVIEW LETTERS

week ending  
18 MARCH 2011

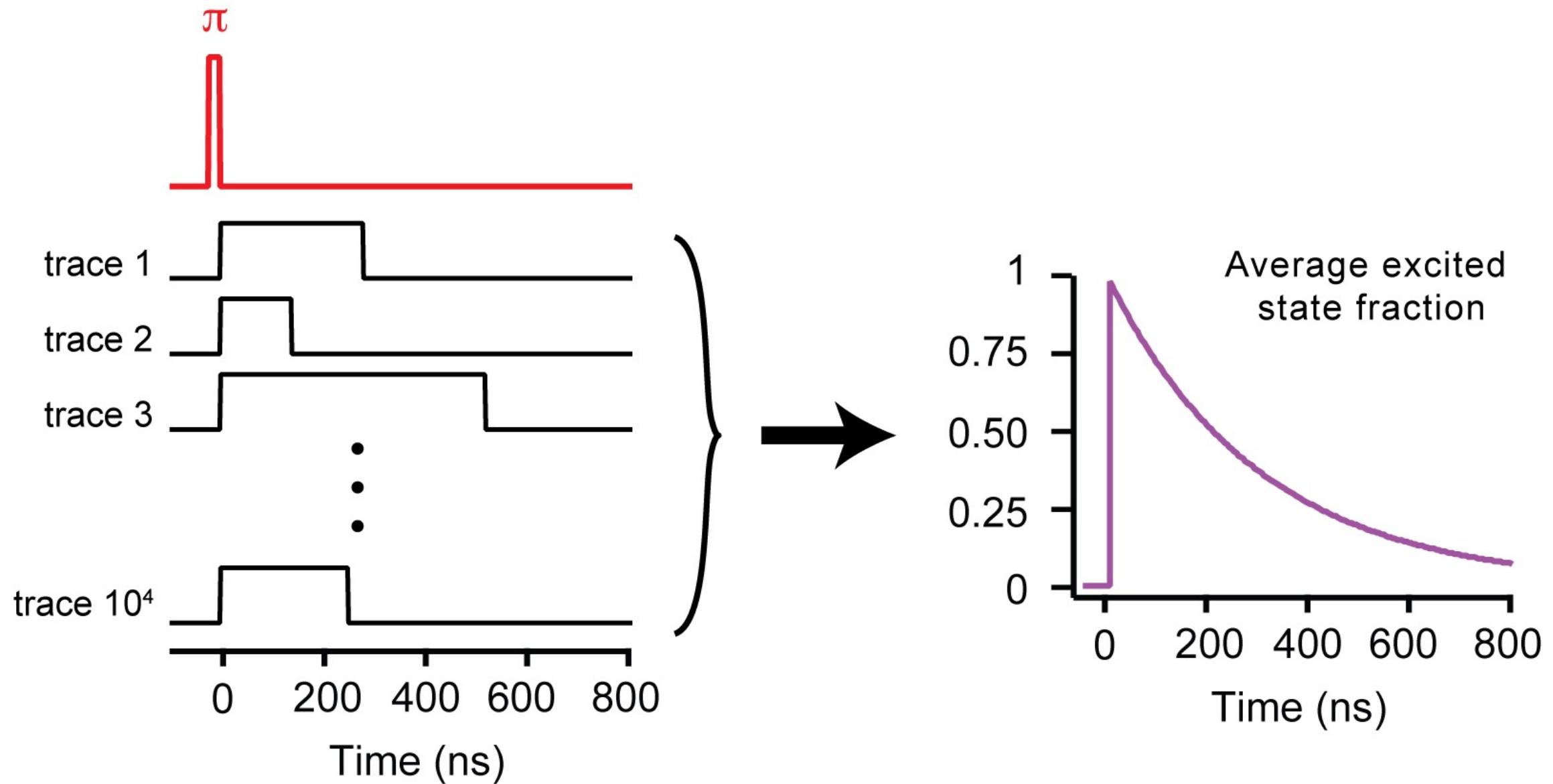
## Observation of Quantum Jumps in a Superconducting Artificial Atom

R. Vijay, D. H. Slichter, and I. Siddiqi

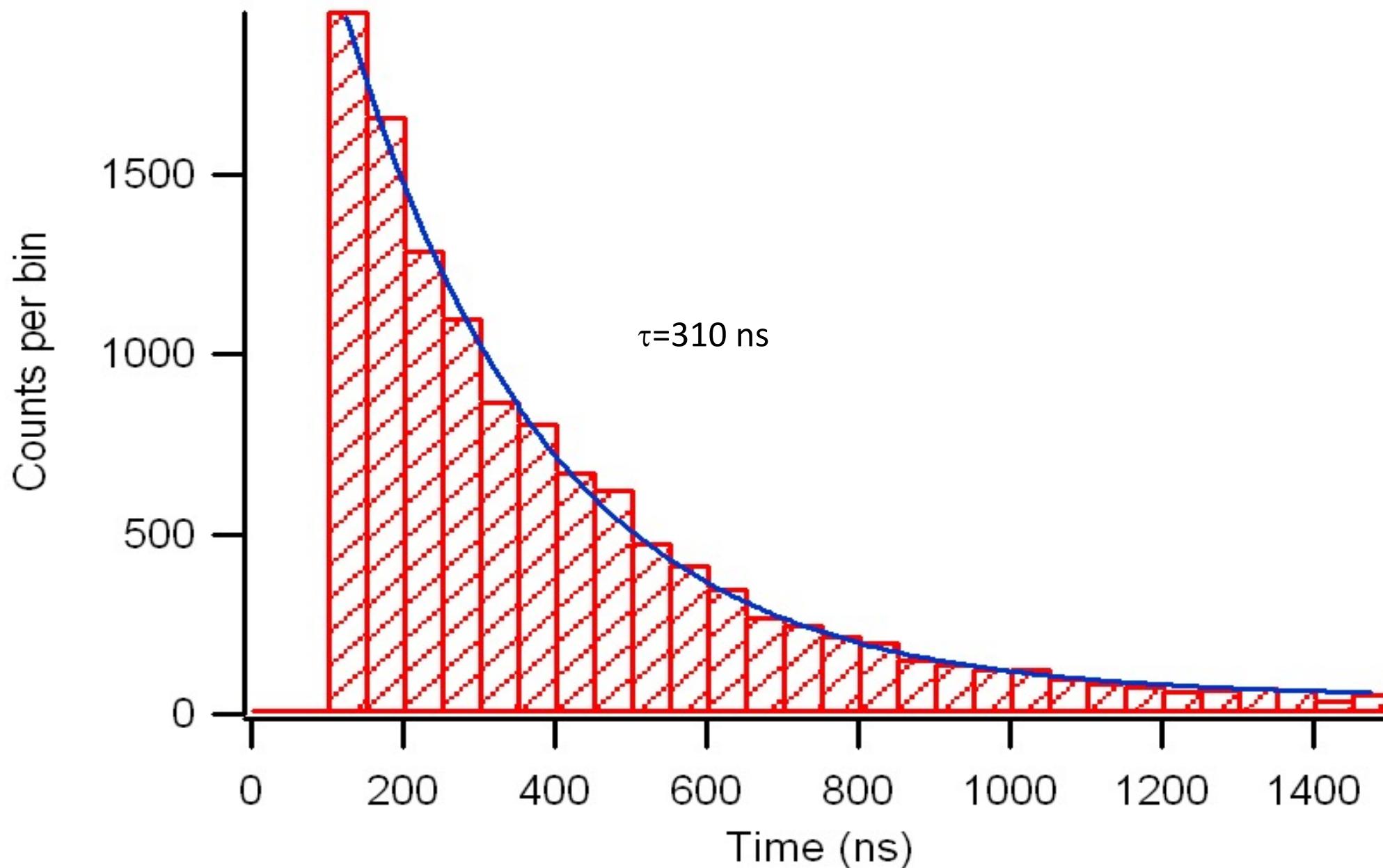
Quantum Nanoelectronics Laboratory, Department of Physics, University of California, Berkeley, California 94720, USA

# *Unraveling the Ensemble*

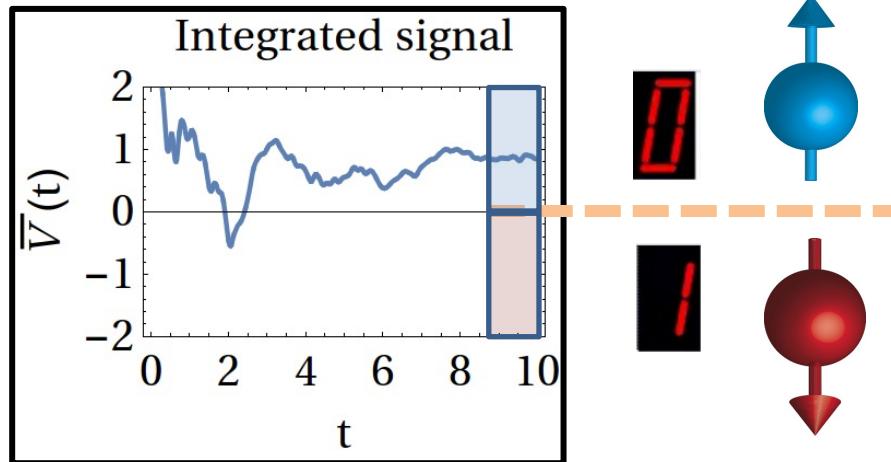
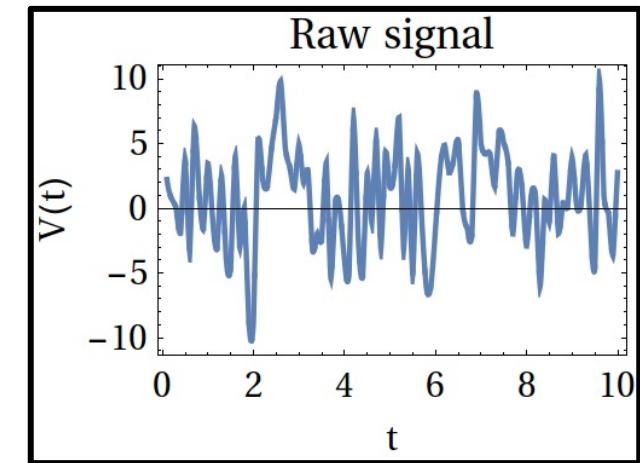
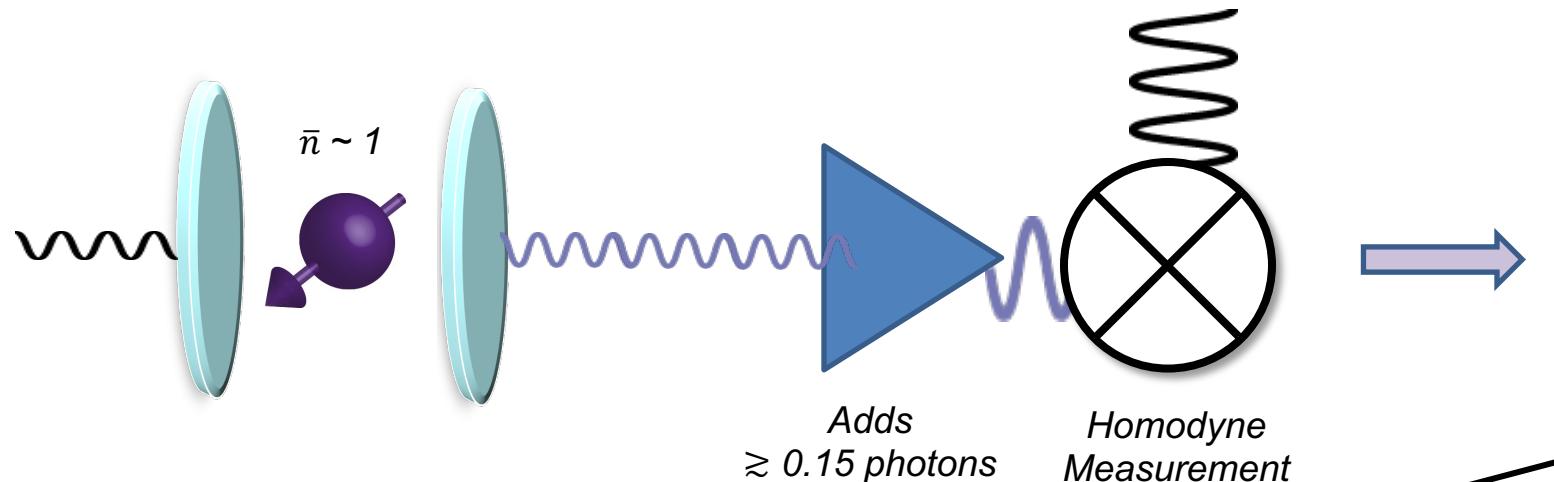
# STOCHASTIC QUANTUM JUMPS



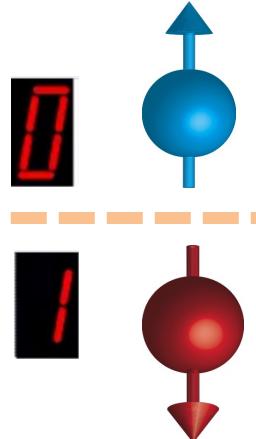
# JUMP STATISTICS



# HOMODYNE DETECTION



(Strong Measurement)

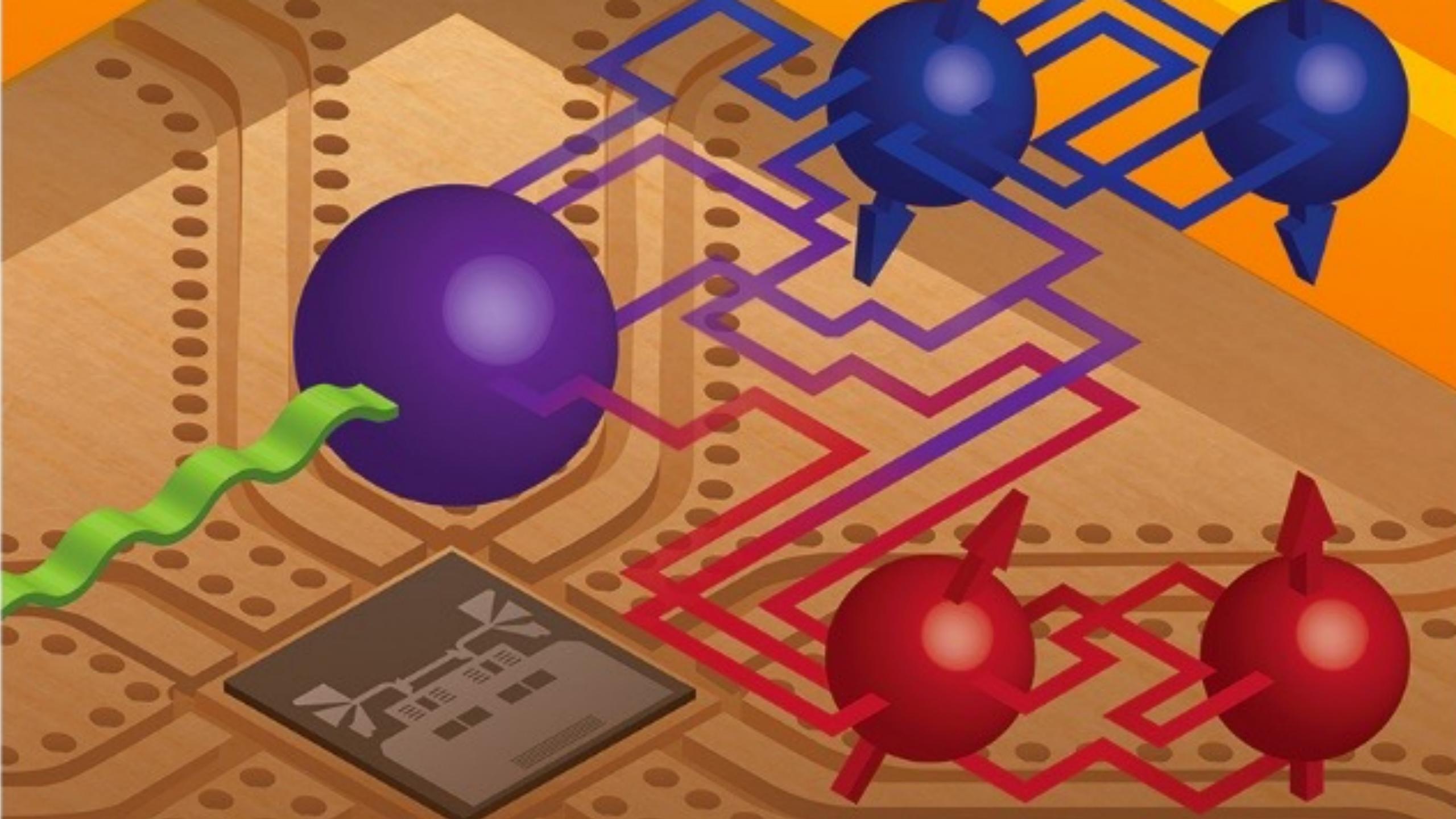


(Weak Measurement)

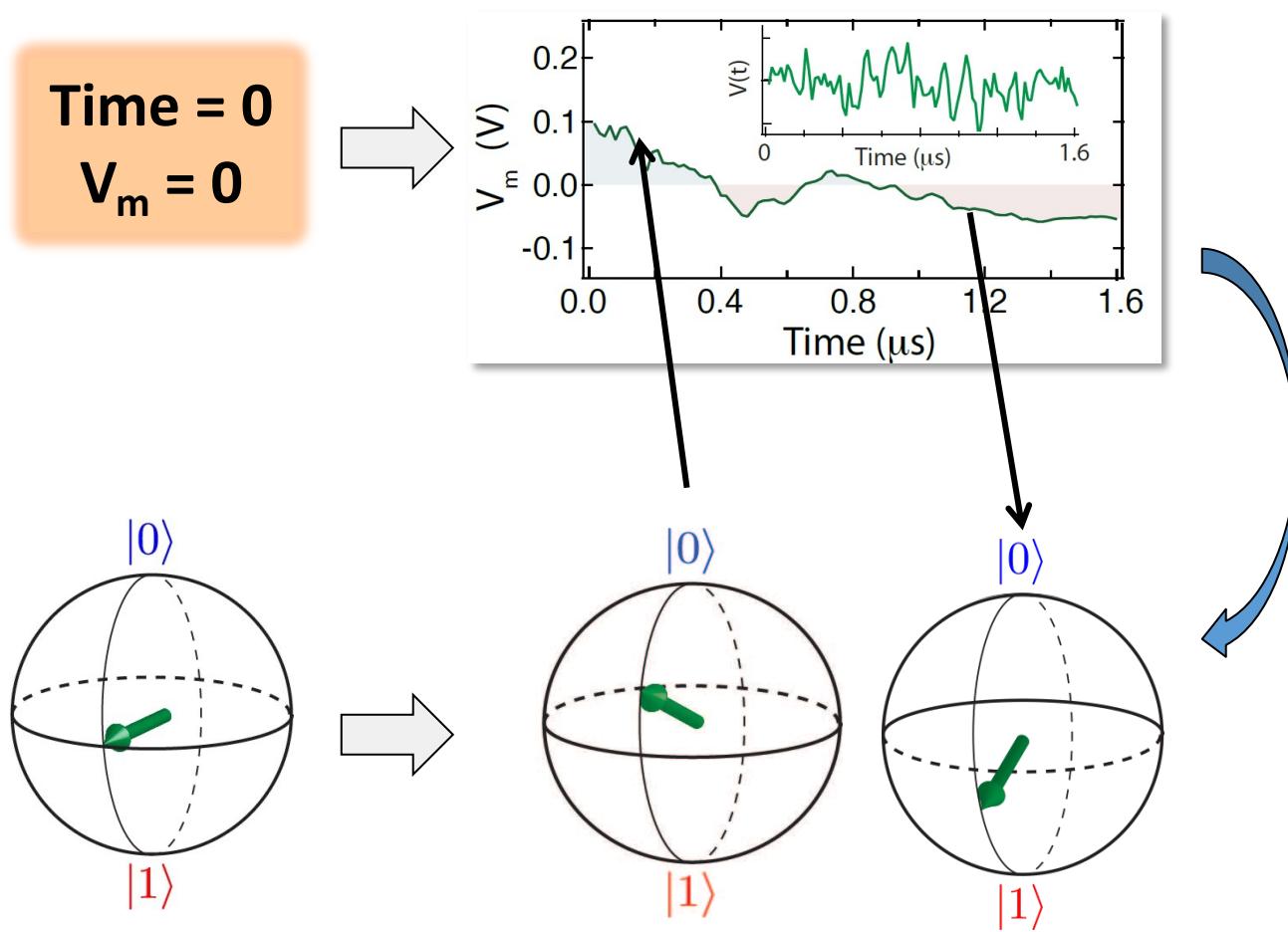


THE NATIVE ANALOG INFORMATION  
CAN BE USED FOR...

- Trajectory Reconstruction
- Entanglement Generation
- Quantum Feedback
- Validate Measurements



# RECONSTRUCTING THE QUBIT STATE

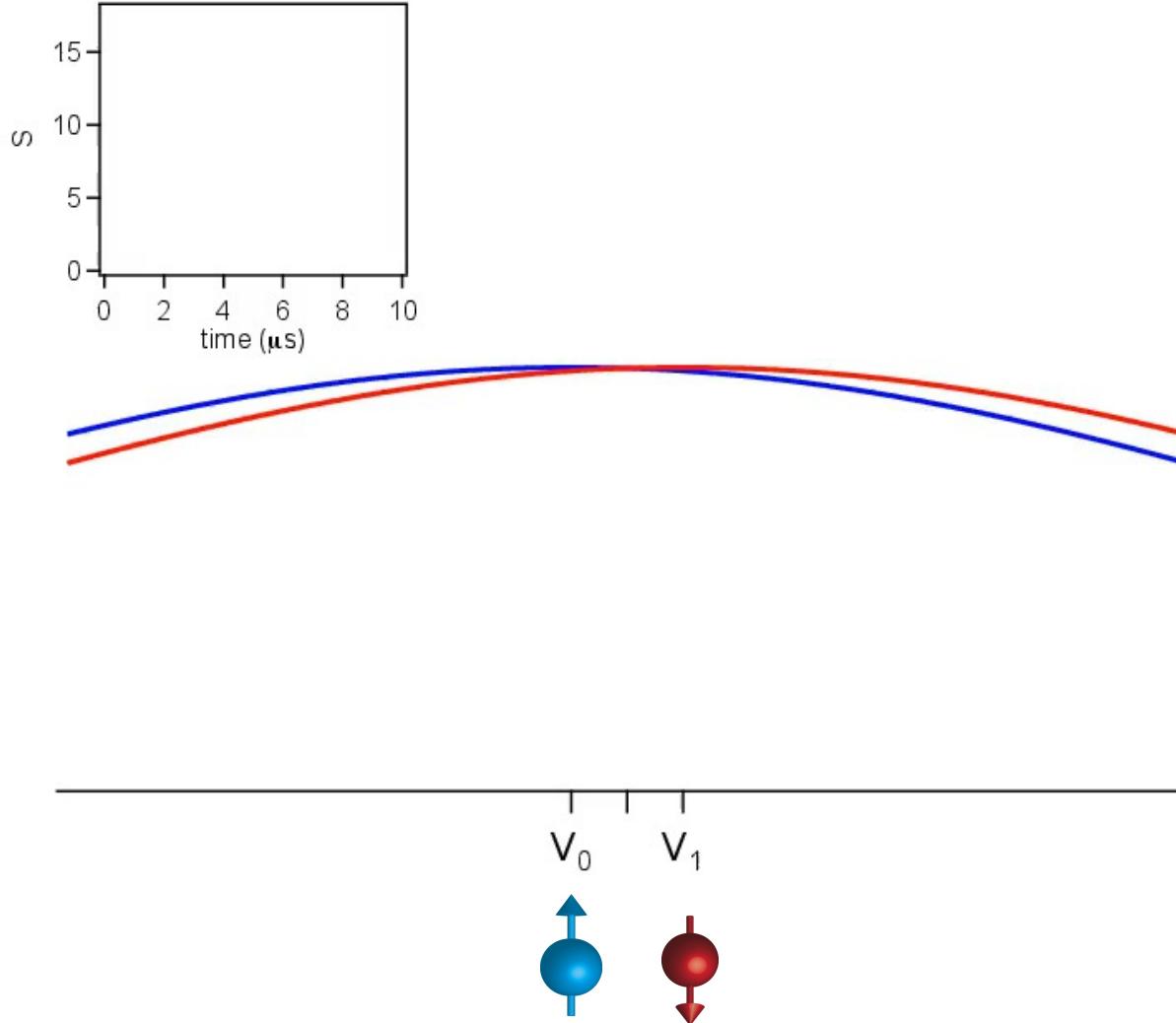


Thomas Bayes  
1701-1761

## BAYES RULE

- Update guess based on new information
- Update qubit state based on  $V_m(t)$
- Widely used in economics, math, engineering, law,...

# MEASURING SPIN UP & SPIN DOWN



$$S = \frac{\Delta V^2}{\sigma^2}$$

histogram separation  
histogram width

$$S = \frac{64\tau\chi^2\bar{n}\eta}{\kappa}$$

$\tau$ : measurement time

$\chi$ : dispersive shift

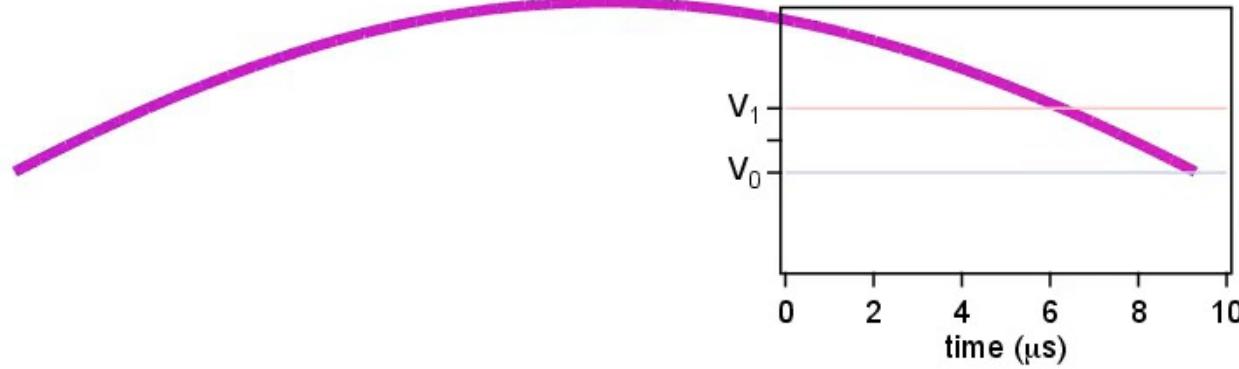
$\bar{n}$ : photon number

$\kappa$ : cavity decay rate

$\eta$ : detector efficiency

$$\eta = 0.49$$

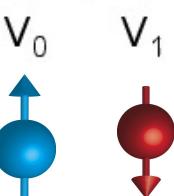
# INTEGRATED VOLTAGE: TRAJECTORY



$$V_m(\tau) = \frac{1}{\tau} \int_0^\tau V(t) dt$$

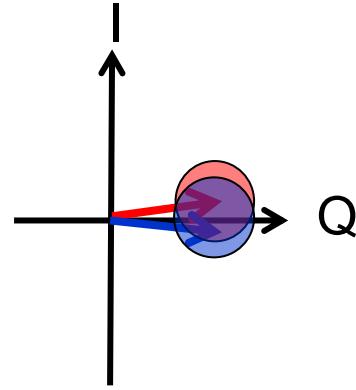


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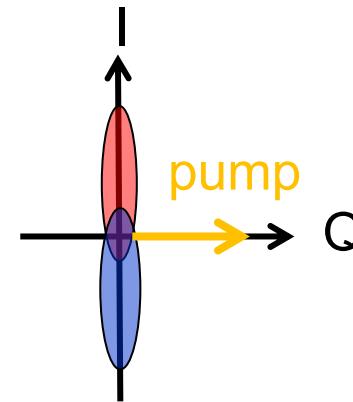


# BACKACTION OF SINGLE QUADRATURE MEASUREMENT

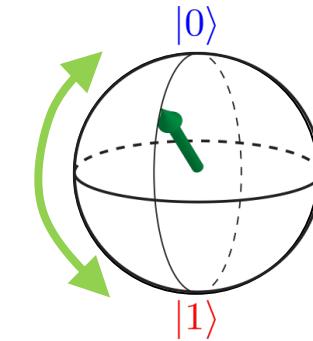
Cavity Output  $\theta=0$



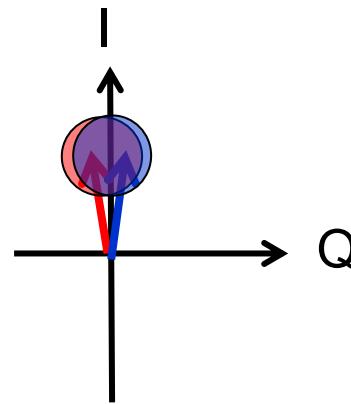
After Amplification  $\theta=0$



- Obtain qubit state information
- Tip Bloch vector

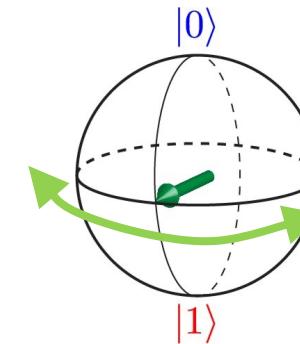


Cavity Output  $\theta=\pi/2$

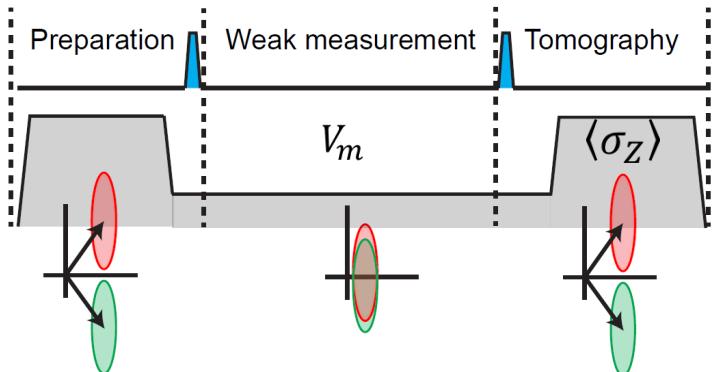


After Amplification  $\theta=\pi/2$

- Obtain cavity photon number information
- Rotate Bloch vector



# VERIFYING BAYESIAN UPDATING



- Initial state along +X
- Measure Z (phase quadrature)

**WANT**       $\langle \sigma_Z \rangle | V_m \stackrel{\text{def}}{=} Z^Z$

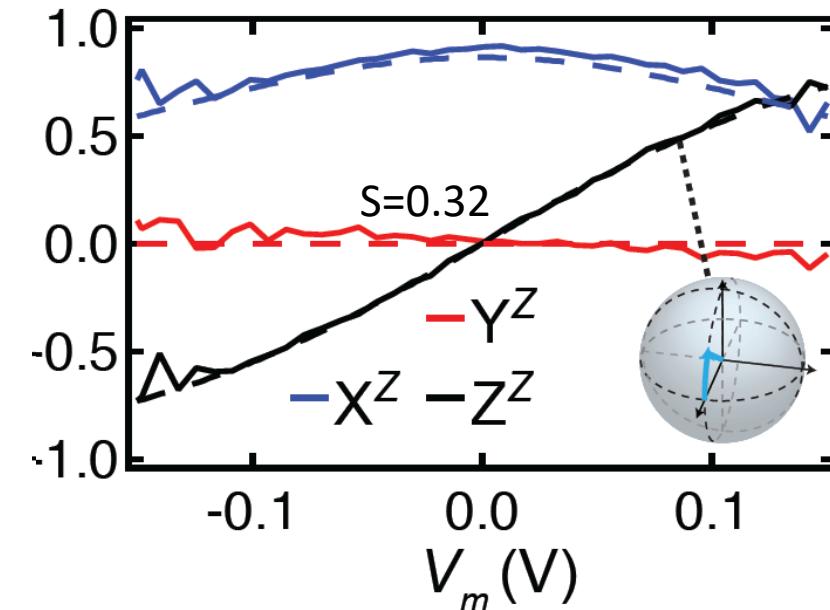
**TO**             $\langle \sigma_X \rangle | V_m \stackrel{\text{def}}{=} X^Z$

**EVALUATE:**     $\langle \sigma_Y \rangle | V_m \stackrel{\text{def}}{=} Y^Z$

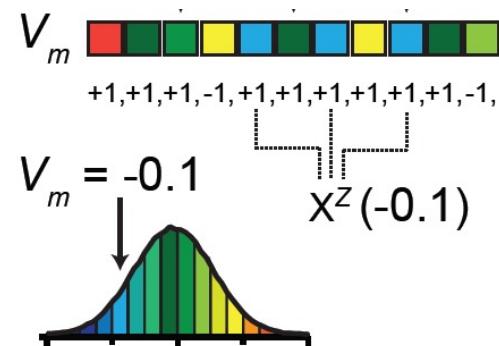
**BAYES  
RULE:**     $Z^Z = \tanh\left(\frac{V_m S}{2\Delta V}\right)$

$$X^Z = \sqrt{1 - \langle \sigma_Z \rangle^2} e^{-\gamma\tau}$$

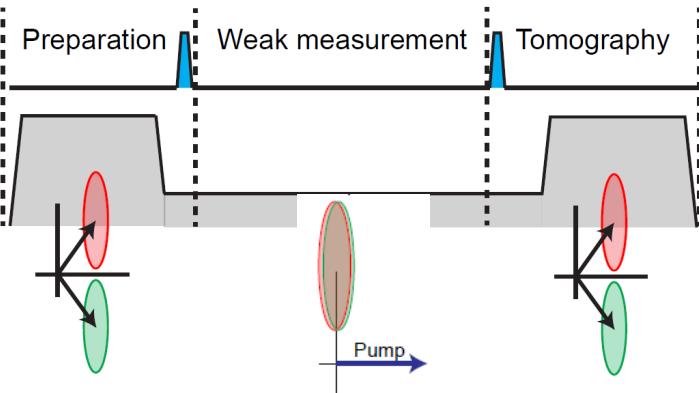
$$\gamma = 8\chi^2 \bar{n}(1 - \eta)/\kappa + 1/T_2^*$$



**TOMOGRAPHIC  
PROCEDURE:**



# WEAK MEASUREMENT OF THE PHOTON NUMBER



**WANT  
TO  
EVALUATE:**

$$\langle \sigma_z \rangle |V_m \rangle \stackrel{\text{def}}{=} Z^\phi$$

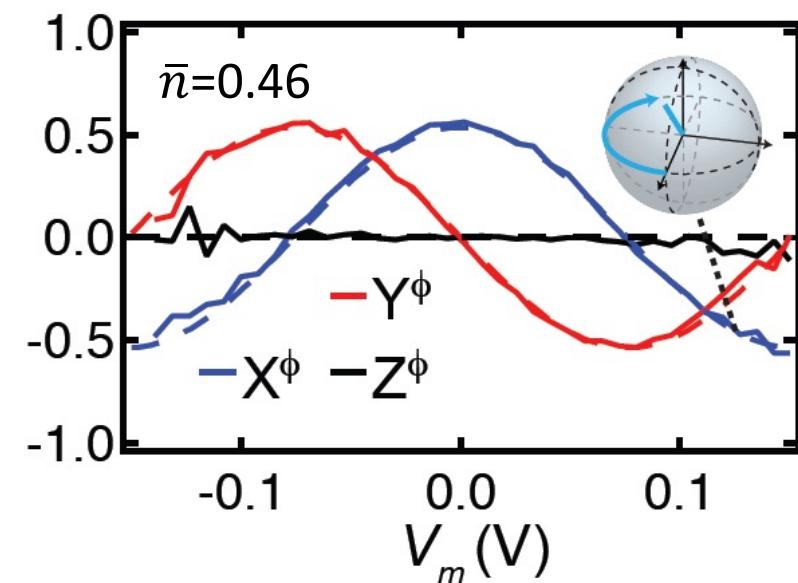
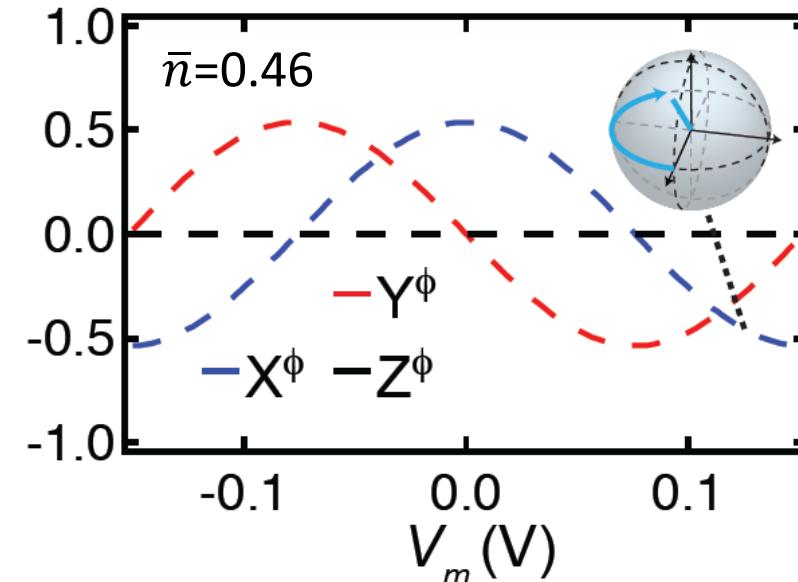
$$\langle \sigma_x \rangle |V_m \rangle \stackrel{\text{def}}{=} X^\phi$$

$$\langle \sigma_y \rangle |V_m \rangle \stackrel{\text{def}}{=} Y^\phi$$

**BAYES  
RULE:**

$$X^\phi = \cos\left(\frac{SV_m}{2\Delta V}\right)e^{-\gamma\tau}$$

$$Y^\phi = \sin\left(\frac{SV_m}{2\Delta V}\right)e^{-\gamma\tau}$$



# A SINGLE QUANTUM TRAJECTORY

