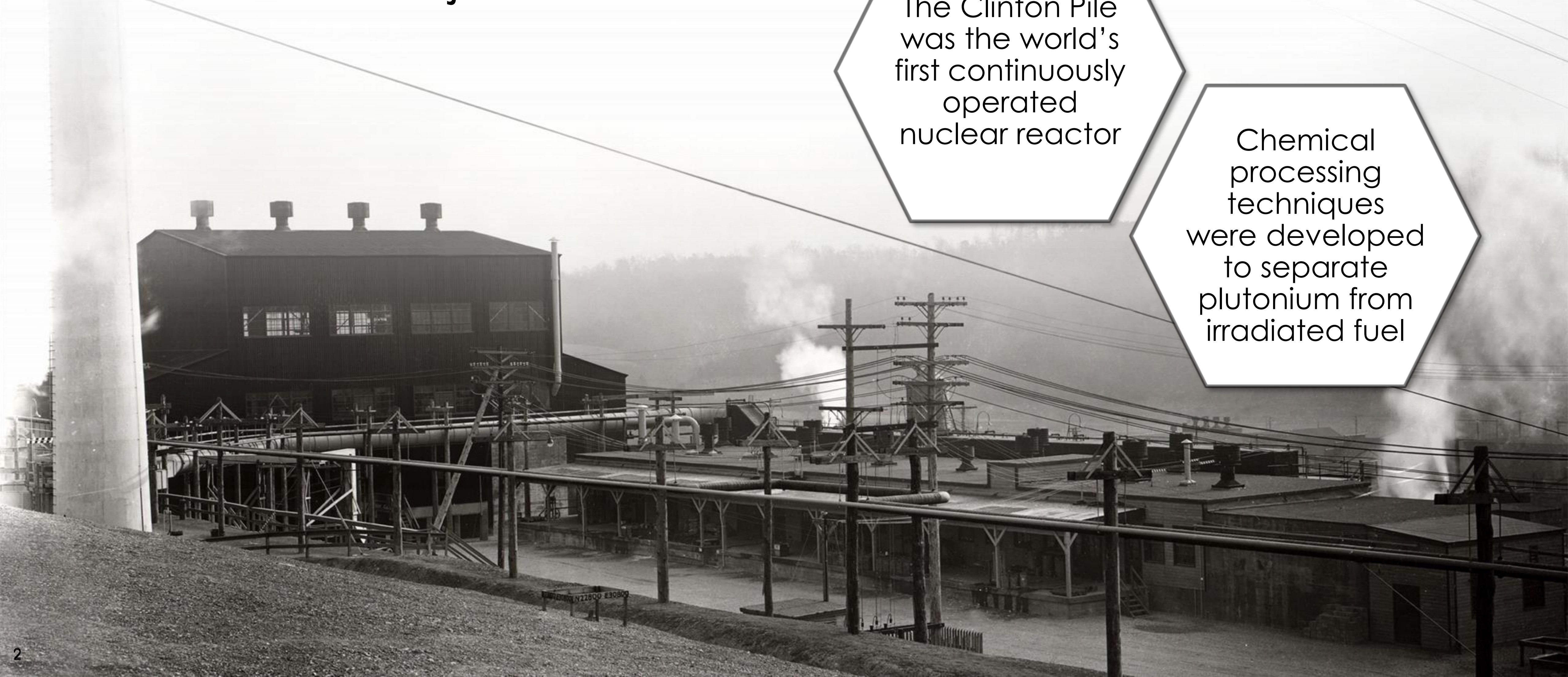
Quantum Computing on Modern Architecture

Raphael Pooser, Oak Ridge National Laboratory

Oak Ridge National Laboratory evolved from the Manhattan Project



The Clinton Pile was the world's first continuously operated nuclear reactor

Chemical processing techniques were developed to separate plutonium from irradiated fuel

ORNL is DOE's largest science laboratory

Oak Ridge National Laboratory

$1.9B
FY19 expenditures

4,900
employees

$750M
modernization investment

Nation's most diverse energy portfolio

3,200
research guests annually

Nation's largest materials research portfolio

Forefront scientific computing facilities

World's most intense neutron source

World-class research reactor

2,356
journal articles published in CY18

Managing major DOE projects: US ITER, exascale computing

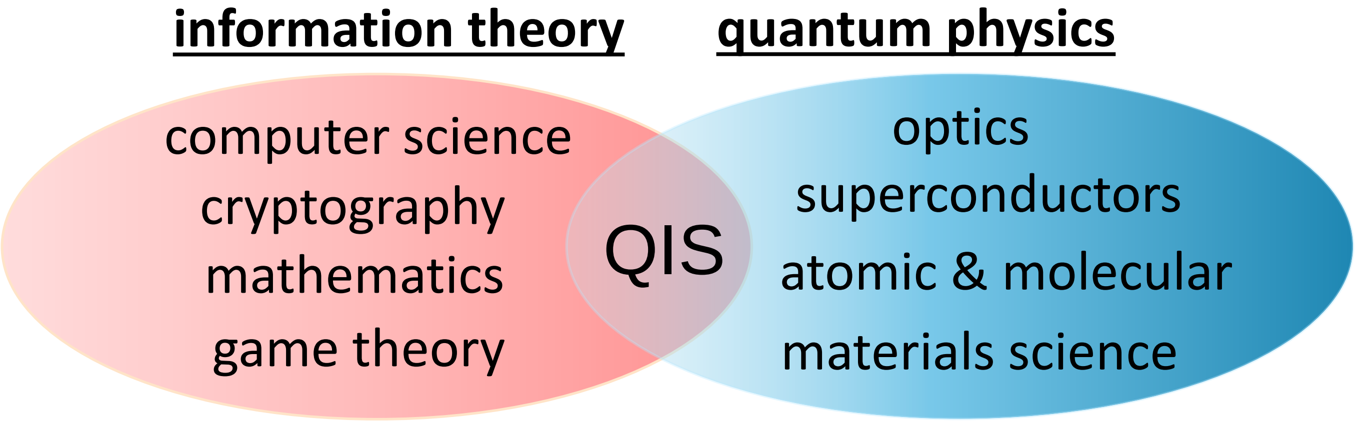
241
invention disclosures in FY19

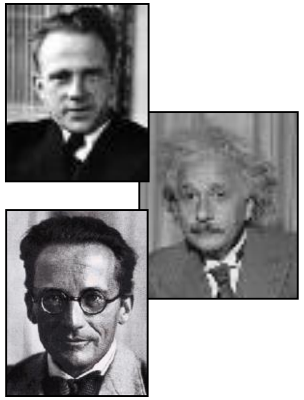
72
patents issued in FY19

What is Quantum Information Science?

- Information is physical
- The Laws of Physics determine what information *is* and what you can do with it
- The rules of quantum physics are *weird*
  - superposition, entanglement, uncertainty

Quantum information science (QIS) is the science of exploiting quantum weirdness to yield revolutionary new capabilities in sensing, communication, and computing.





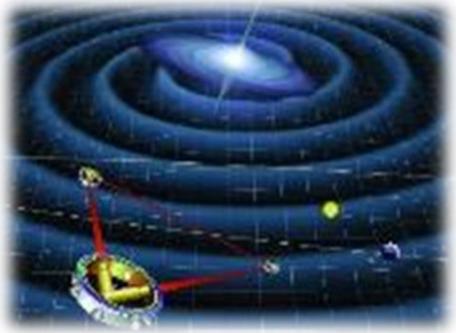
Differences between quantum and classical info

	Classical	Quantum
state space	real-valued	complex-valued
log(# states)	linear(# particles)	exp(# particles)
what a state tells us	value of every physical quantity	probability distribution for every quantity
physical encoding	in large objects (naturally robust)	in small objects (easily perturbed)
readability	reading is inert	reading degrades it
what information is	something known	something possessed
information sharing?	yes - can perfectly copy	no - cannot perfectly copy
where information resides	locally	can be non-local

- Quantum state space is **big** and has **rich structure**.
- Quantum information can show **unusual correlations** across time and space.
- Quantum information has **limited readability**.
- Quantum information is **fragile**.

The Potential of QIS

- Sensing
  - Imaging with greatly reduced noise
  - Ultrasensitive magnetometers and gravitometers

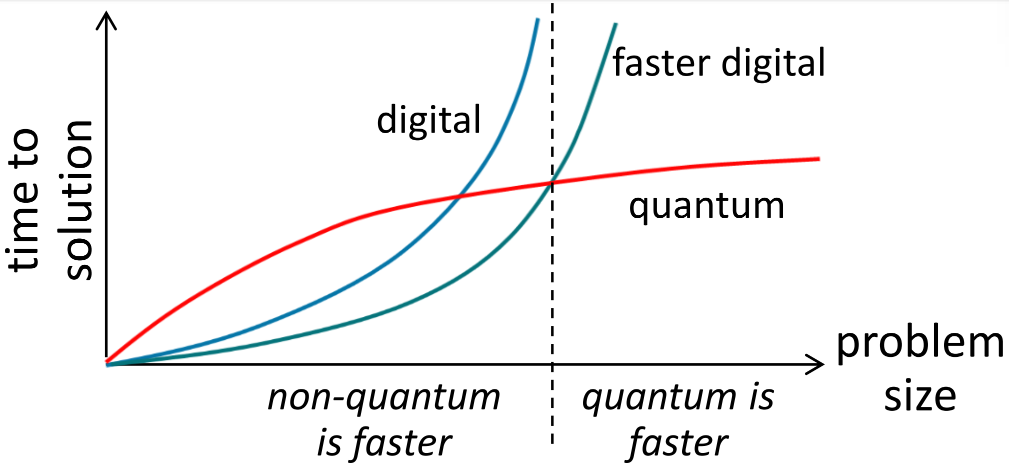


Gravitational waves

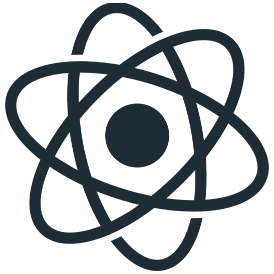
- Communication
  - Unbreakable encryption
  - Verifiably secret random numbers

All are examples of technologies which use QIS to enable new Quantum Technologies

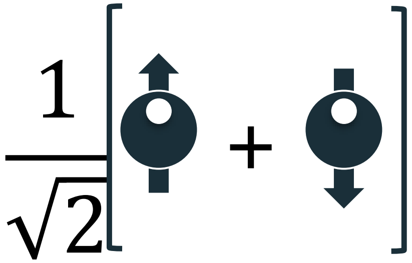
-
  - Combinatorial optimization
  - Constraint satisfaction
  - Function inversion
  - Finding subgroups
  - Linear algebra



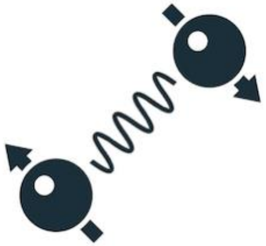
QIS Concepts



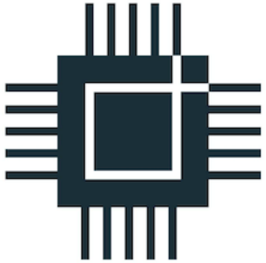
Qubit concepts



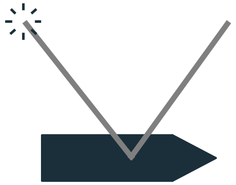
Superposition



Entanglement



Technologies



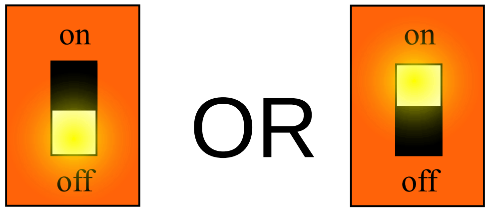
Sensors

communications

Computers

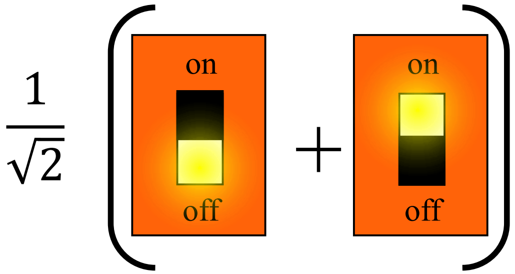
Bit versus qubit

bit



Either / or, not both

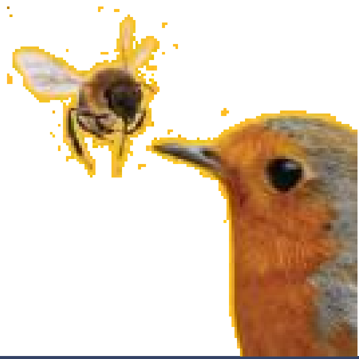
qubit



A qubit can be in a **superposition** of both on and off

Quantum Entanglement

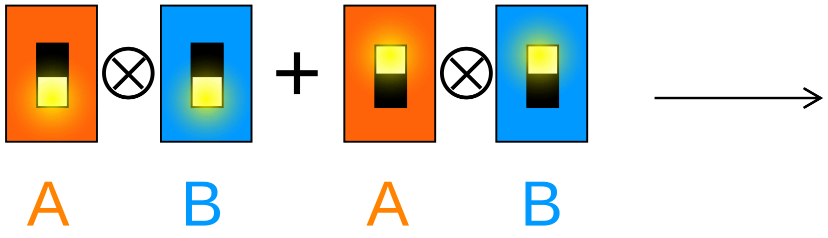
- One of the most important ingredients for Quantum Information and Quantum Computing is Quantum Entanglement
- Involved in all quantum algorithms (including Shor's) and quantum resources
- Used in quantum sensors to obtain enhanced signal to noise ratios
- Used to achieve unconditional security in quantum communication protocols



Quantum Entanglement

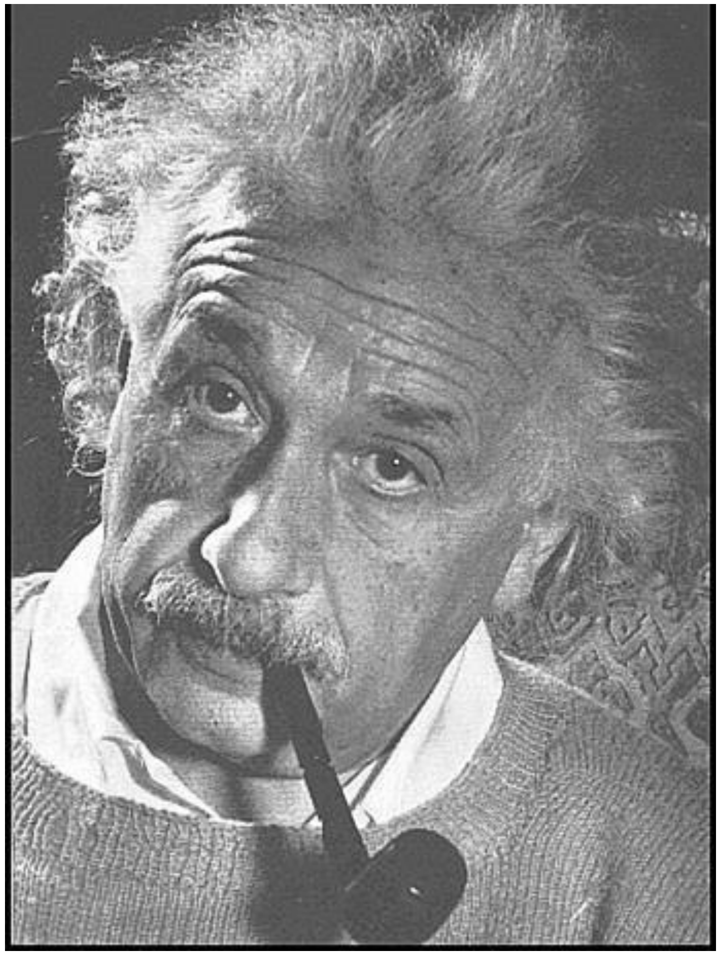
- Einstein, Podolsky, and Rosen, 1935: quantum mechanics predicts entanglement

- Variables like position and momentum can be entangled between two particles:



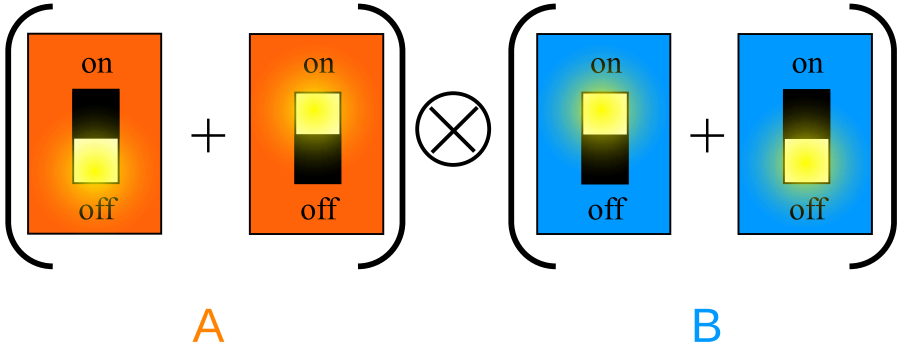
$$\int |\, x\rangle_A \,|\, x\rangle_B dx;$$

$$\int |\, p\rangle_A \,|\, -p\rangle_B dp$$



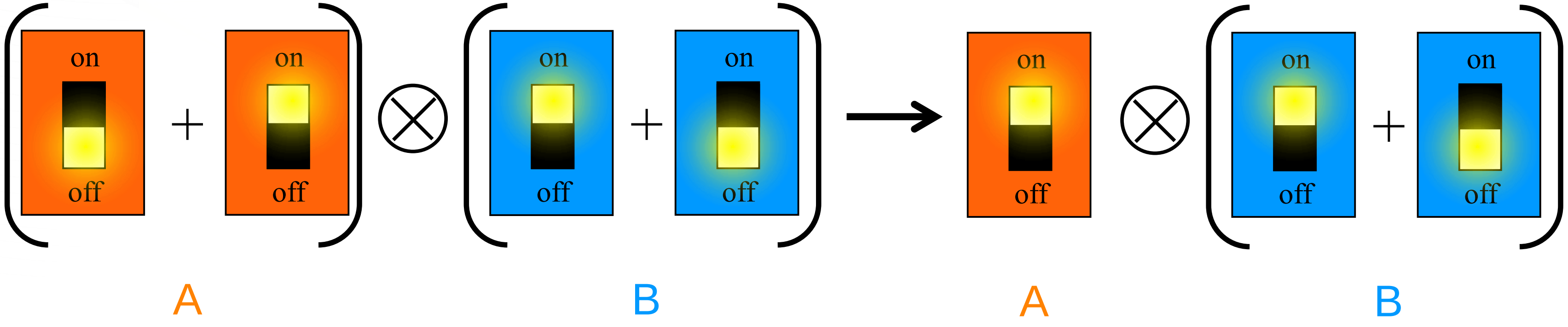
Quantum Entanglement

- The state of multiple qubits can be written mathematically as tensor products
- Factorisable superposition:



Quantum Entanglement

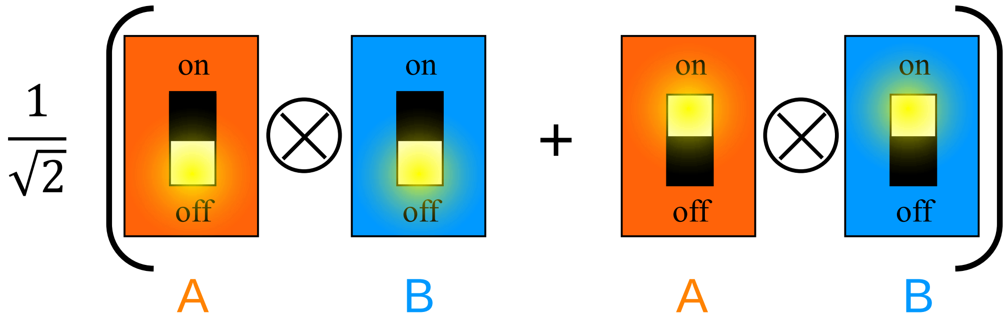
- Make a measurement on qubit A



The measurement causes the superposition for qubit A to **collapse** to one of the two possibilities, on or off. Qubit B is unaffected.

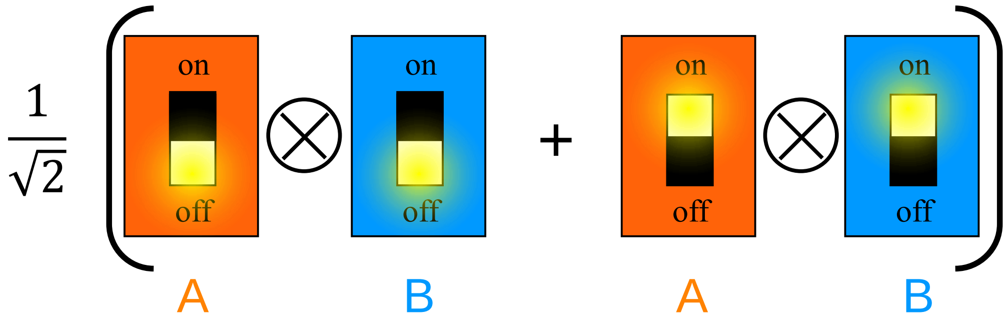
Quantum Entanglement

- A different type of superposition:



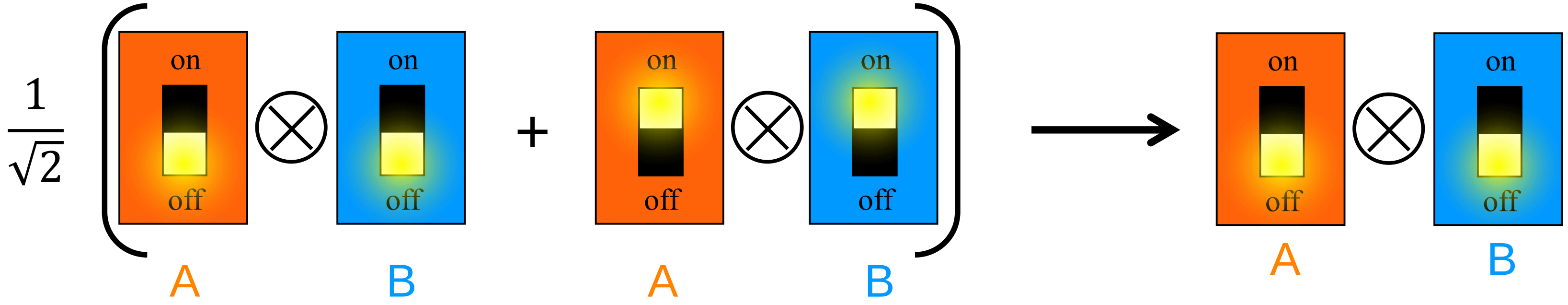
Quantum Entanglement

- What happens in this case if we make a measurement on qubit A?



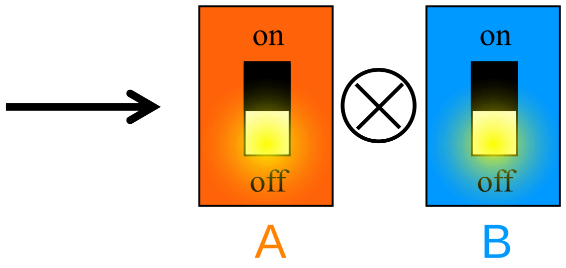
Quantum Entanglement

- The superposition collapses to a specific state, depending on the measurement result for A (Copenhagen Interpretation)



Quantum Entanglement

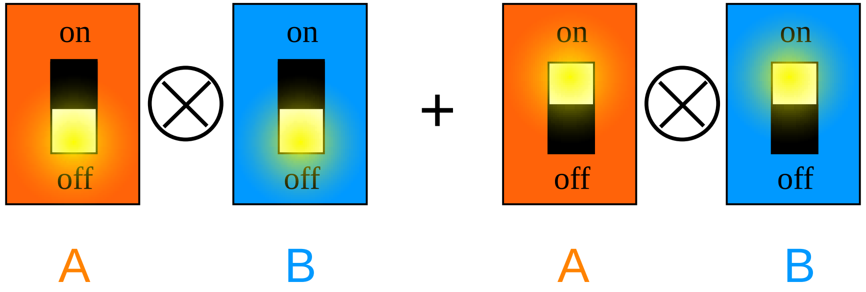
- The state of qubit B is also affected. We now know what position B is in without having touched it: **non local correlations**.



Definition: Quantum Entanglement is a non factorisable superposition between multiple quantum mechanical objects. Leads to non local correlations.

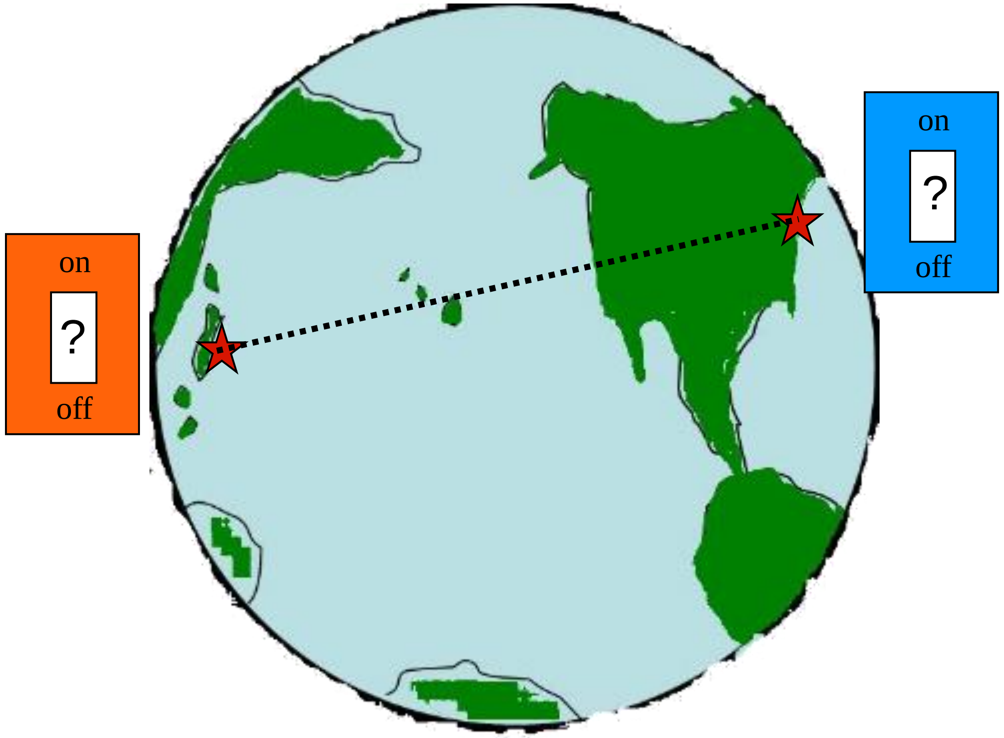
How non local?

- Example: Alice and Bob share two different switches that are entangled



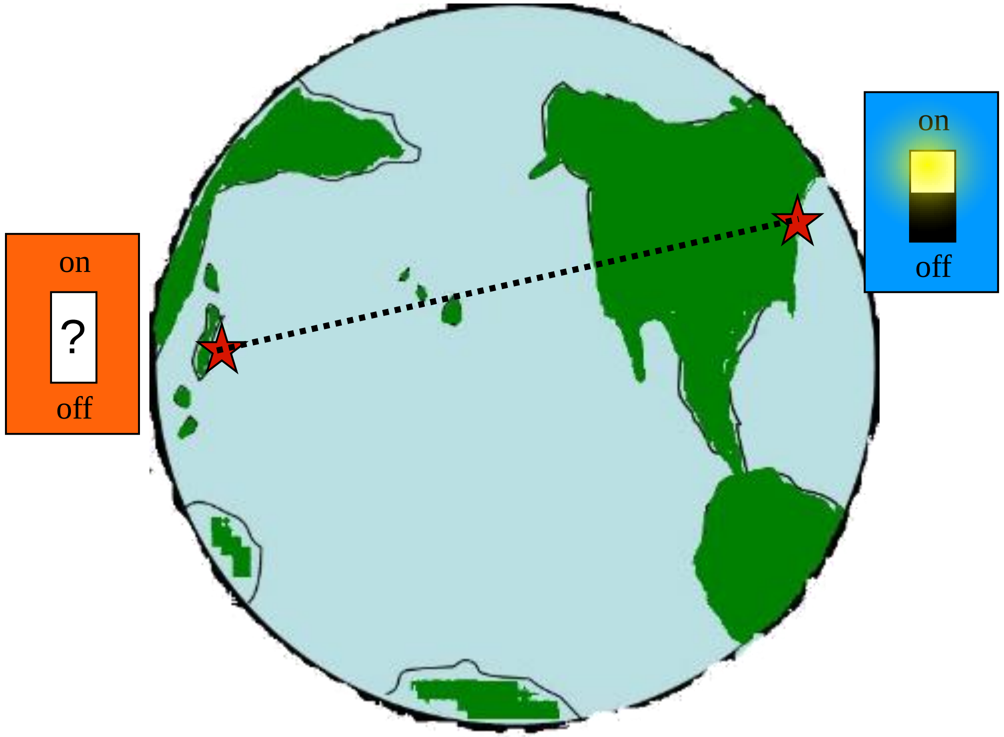
How non local?

- Bob is in New york and Alice is in Tokyo; both have access to their switches locally.



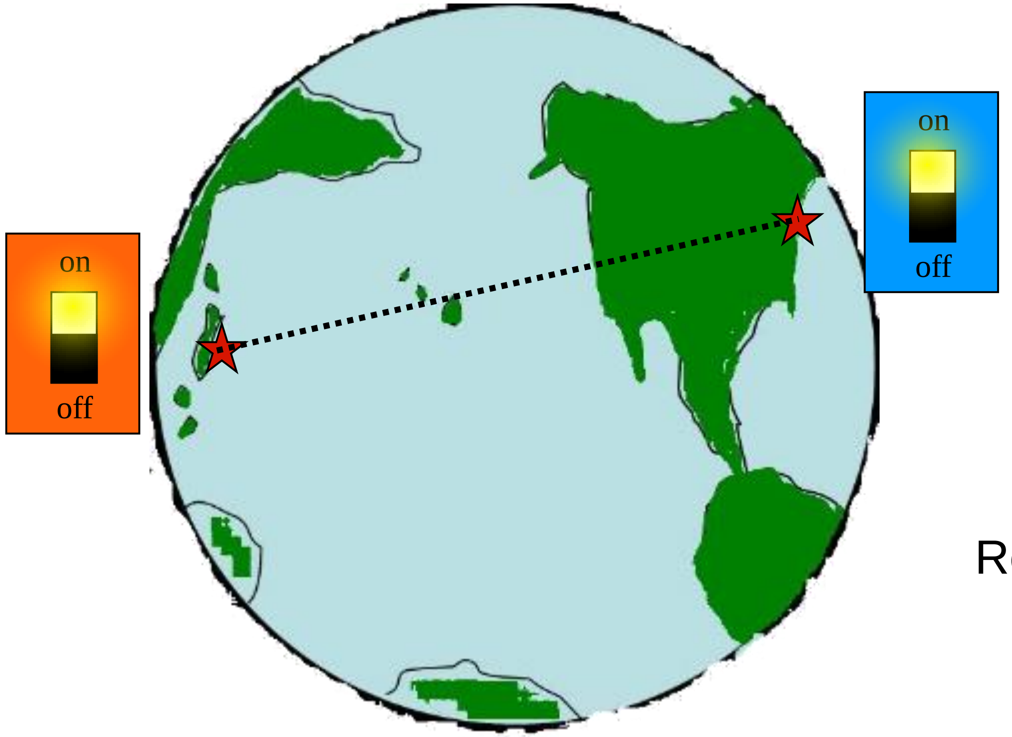
How non local?

- Bob measures his switch and finds it’s on.

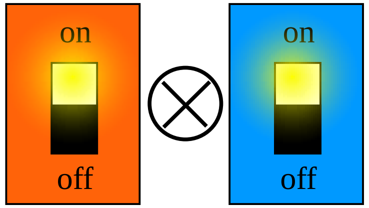


How non local?

- Bob will know the result of Alice’s measurement because he collapsed the superposition. The results still have to be communicated classically.



Resulting eigenstate:



Quantum Computing

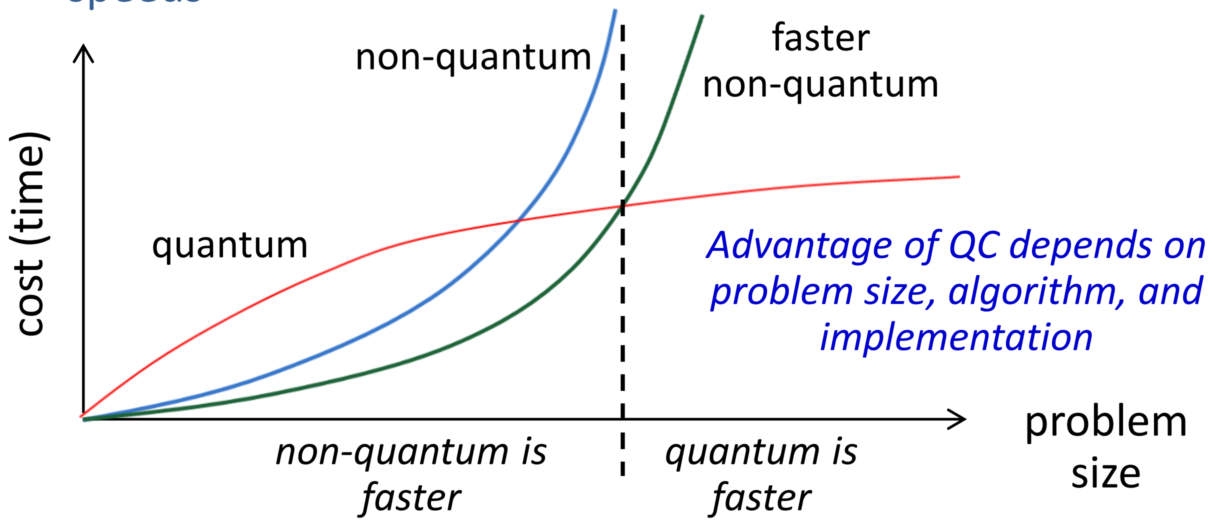
Oak Ridge National Laboratory

Motivation & Background

- A Quantum Computer would threaten the security of the public key infrastructure
- Development of a universal quantum computer requires the precise control of matter at the atomic scale

The Quantum Difference

- A Quantum Computer offers better scaling, not faster clock speeds



Applications

- Factoring (for code-breaking)
- Quantum machine learning
- Unstructured database search
- Large-scale simulation of physical systems
- Enhanced capabilities for computational science

The difference between quantum and classical

0
1

1 qubit

0
1

1 bit

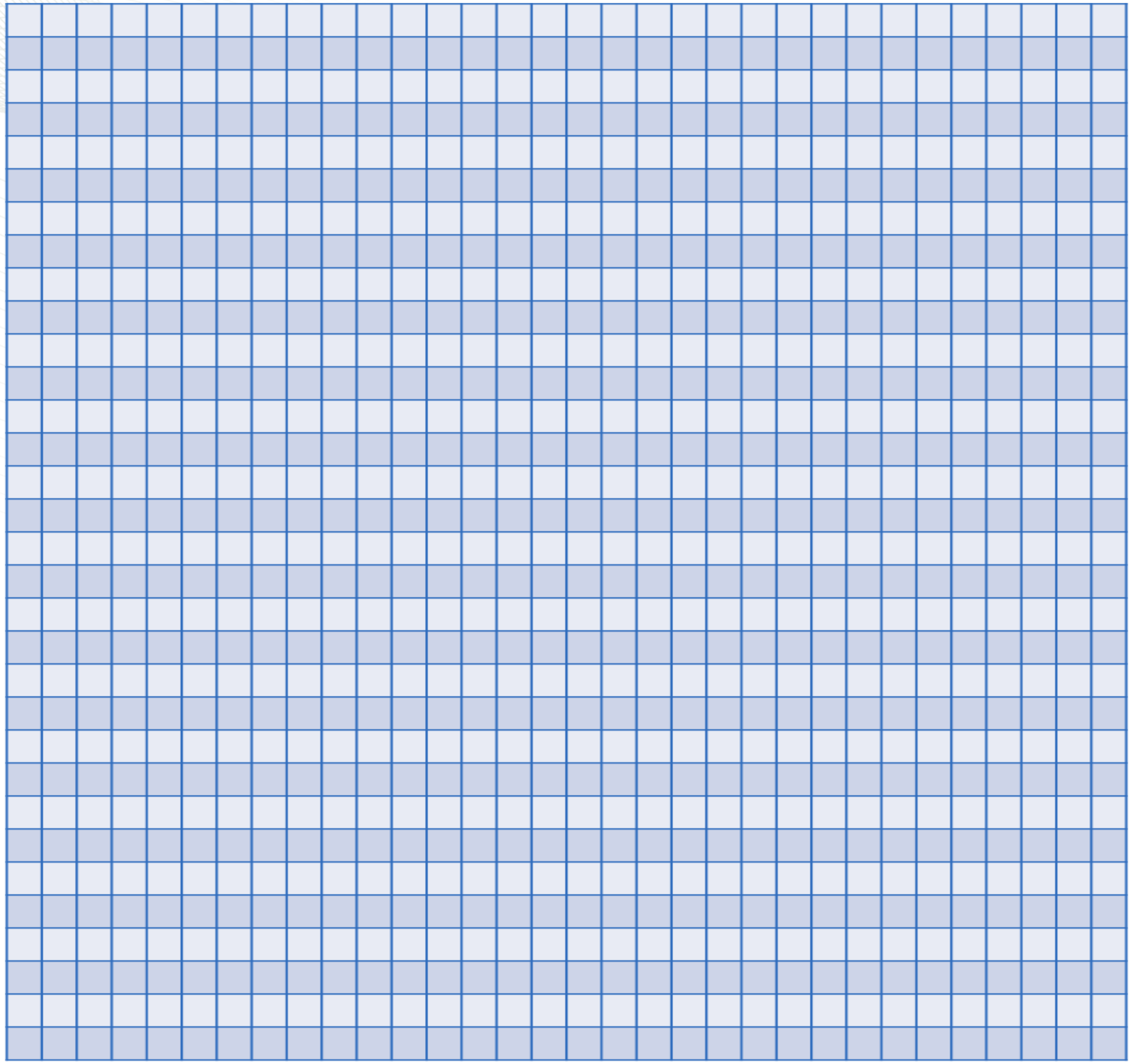
The difference between quantum and classical

3 qubits

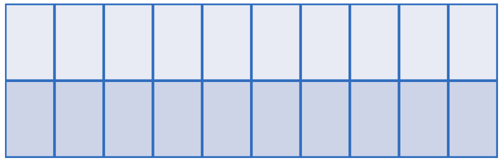
0		
1		

3 bits

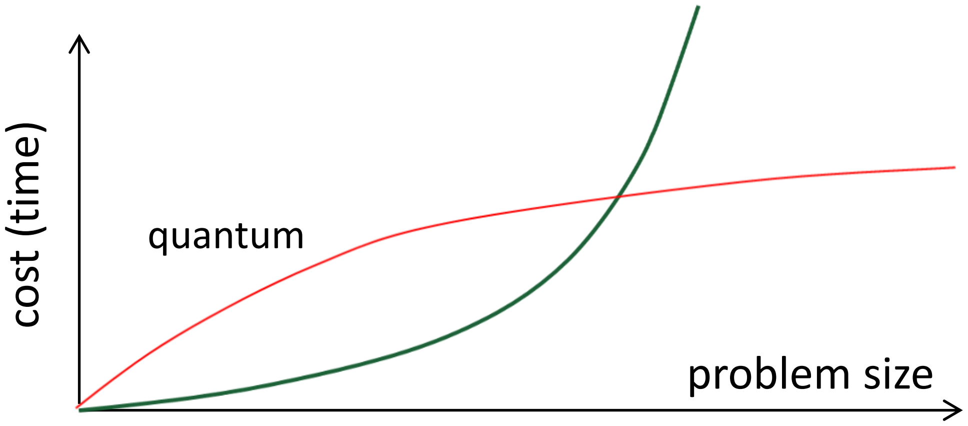
The difference between quantum and classical



10 qubits

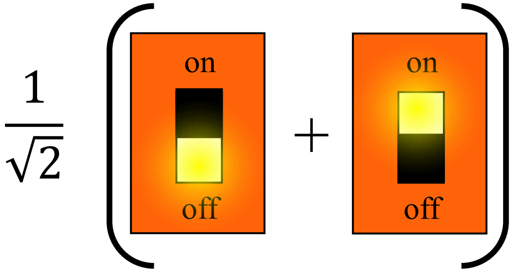


10 bits



Qubits

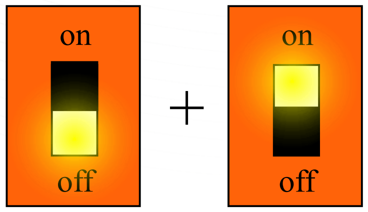
First, consider a quantum bit of information (qubit):



A qubit can be in a **superposition** of both on and off

Qubits

First, consider a quantum bit of information (qubit):

$\frac{1}{\sqrt{2}}$ ()

$|0\rangle$ $|1\rangle$

$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$|0\rangle$ labels one eigenvector

$|1\rangle$ labels the other

Vectors describe quantum state of two level system

Qubits

Quantum gates manipulate the state of two level systems

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}$$

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

Qubits

Quantum gates manipulate the state of two level systems

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$ bit flip

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$ phase flip

Quantum gates

$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$; bit flip

$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$; phase flip

$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$; Hadamard

$P = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$; 90^o phase

$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$

$R_z(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$

$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$; can entangle

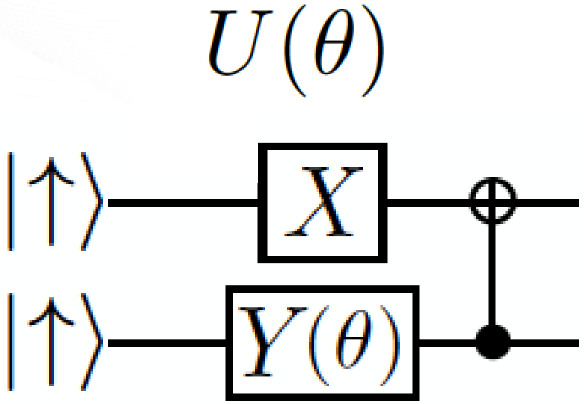
Quantum programming

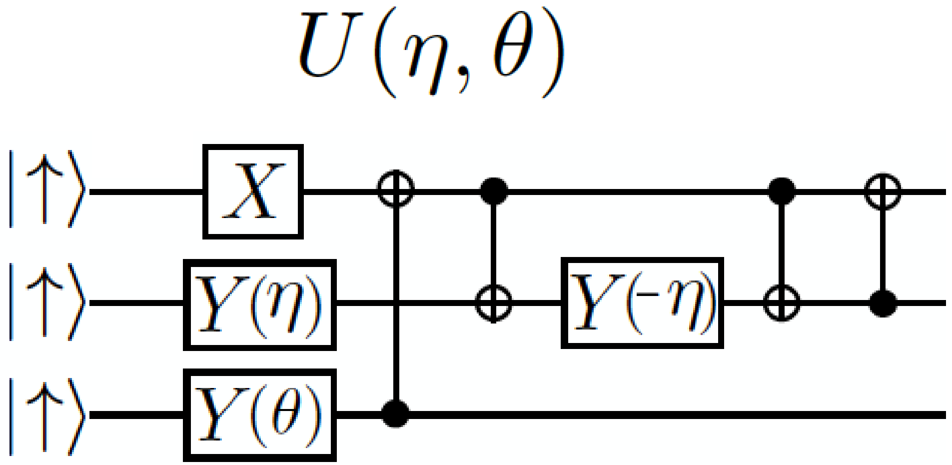
$$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}$$

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$|\psi_f\rangle = XHPCNOTTHX|\psi_i\rangle$$

Quantum programming

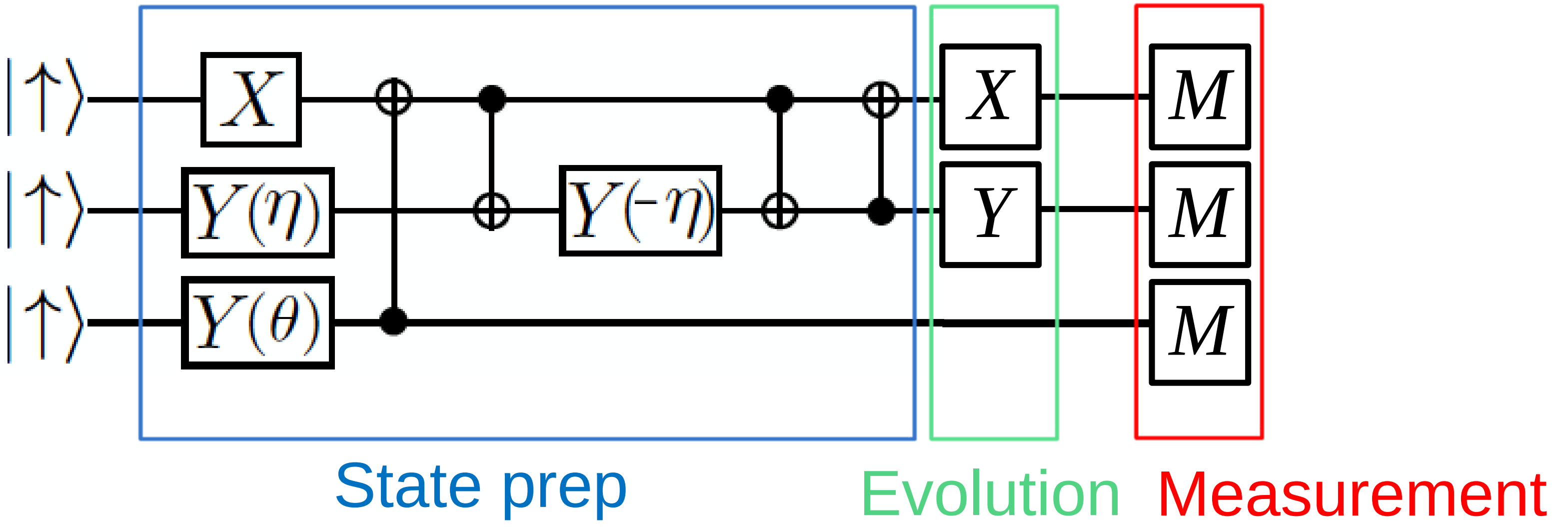




"sheet music" – quantum circuits

Prototype of a quantum simulation

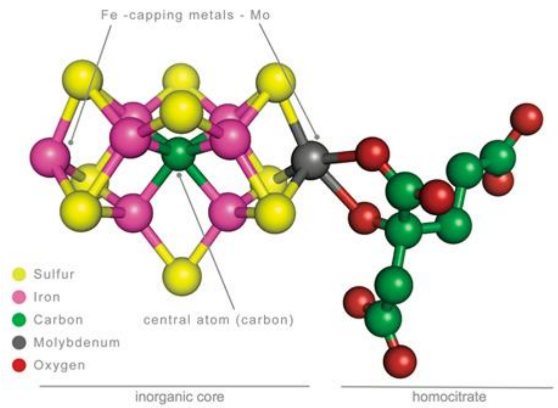
- State preparation (e.g., for initial scattering amplitude)
- Hamiltonian evolution
- Observable measurement
  – Sample from probability distribution of scattering outcomes



Quantum Simulation Examples

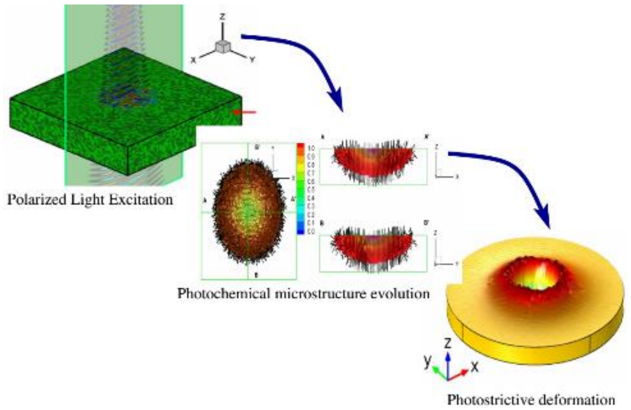
- Scientific discovery and cyber security with quantum computing

Physical Sciences: Chemistry, Materials Sciences, Physics



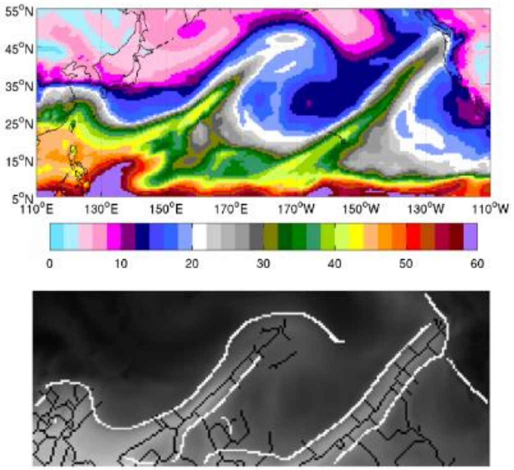
Electronic structure calculations of nitrogenase will support methods for fertilizer production, food security

Applied Sciences: Energy, Medicine, Engineering



Finite-element methods for multi-scale models will support integrated computational materials engineering

Data Sciences: Applied Math, Analytics, Artificial Intelligence,



Machine learning methods will support data analytics and artificial intelligence for situational awareness

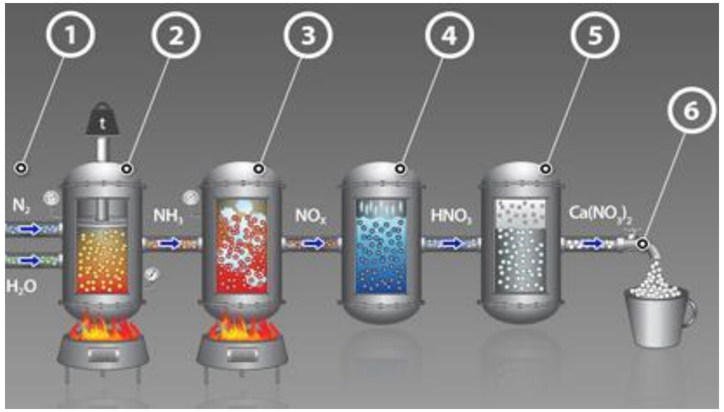
The Impact on Energy

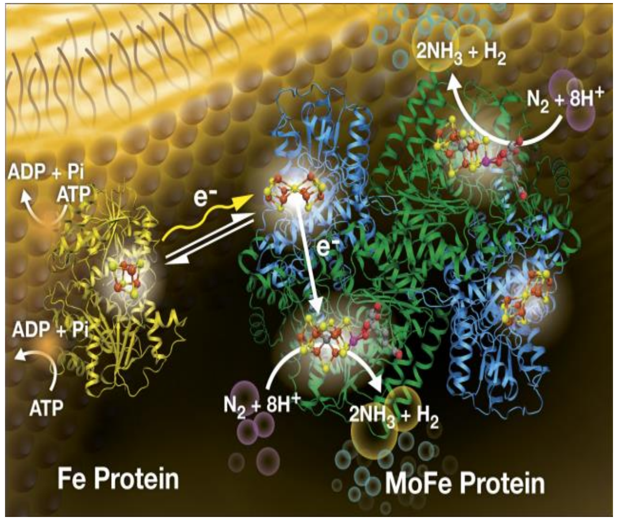
- Protein Folding
- Fertilizer production consumes ~5% of global natural gas supplies and 2% of global energy production
  - This is necessary to meet food requirements worldwide
  - The artificial Haber-Bosch process requires extremely high heat and pressure to achieve efficient ammonia production
- The nitrogenase enzyme operates at STP and is used by bacteria for ammonia production

$$N_2 + 8\,H^+ + 8\,e^- \rightarrow 2\,NH_3 + H_2$$

- Quantum computing will enable high fidelity modeling of these complex chemical reactions
  - Quantum algorithms for computational chemistry provide exponential speed ups over conventional approaches

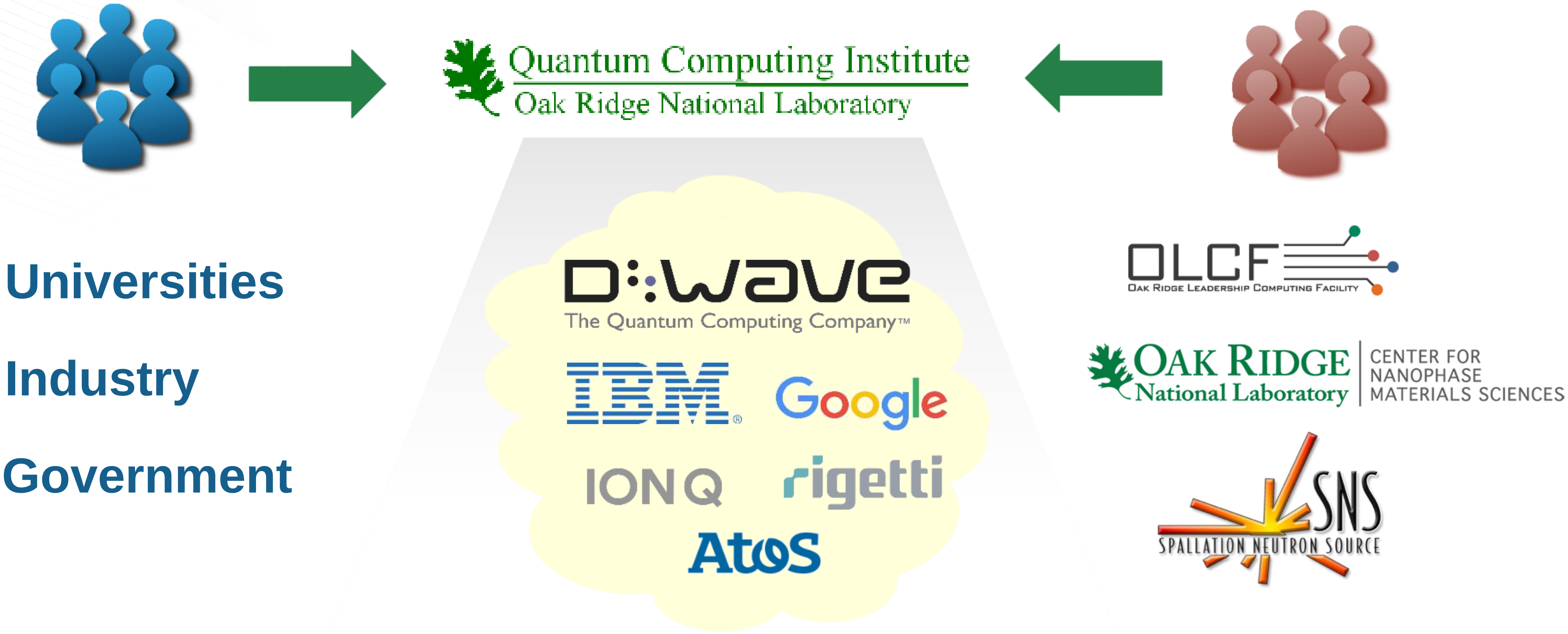
Haber-Bosch Process





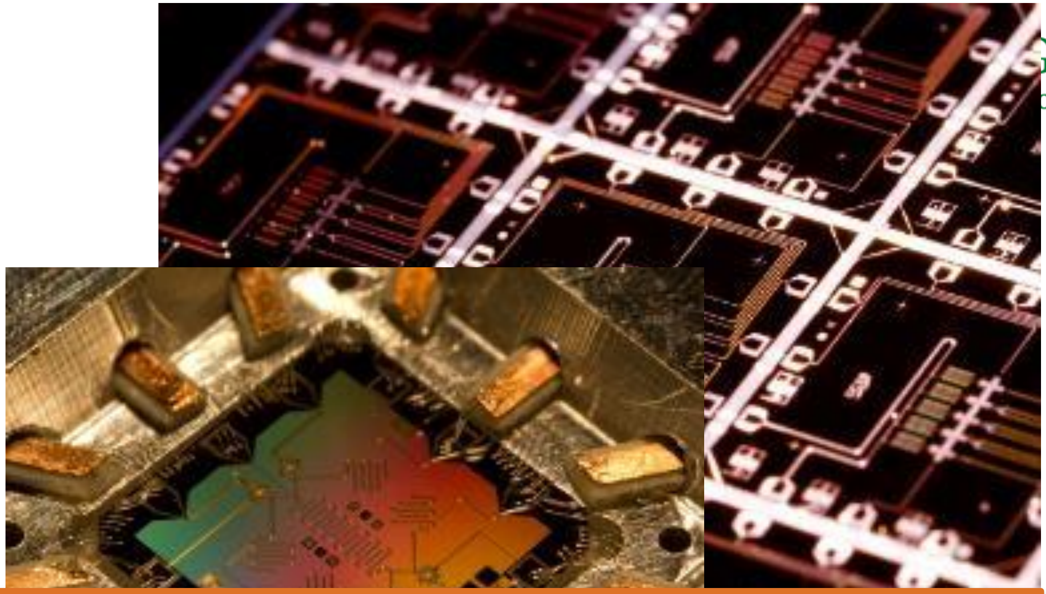
Quantum Computing over the Cloud

- We are providing state-of-the-art quantum computing resources to the user community through strategic partnerships, collaborations, and on-site resources



The NISQ era

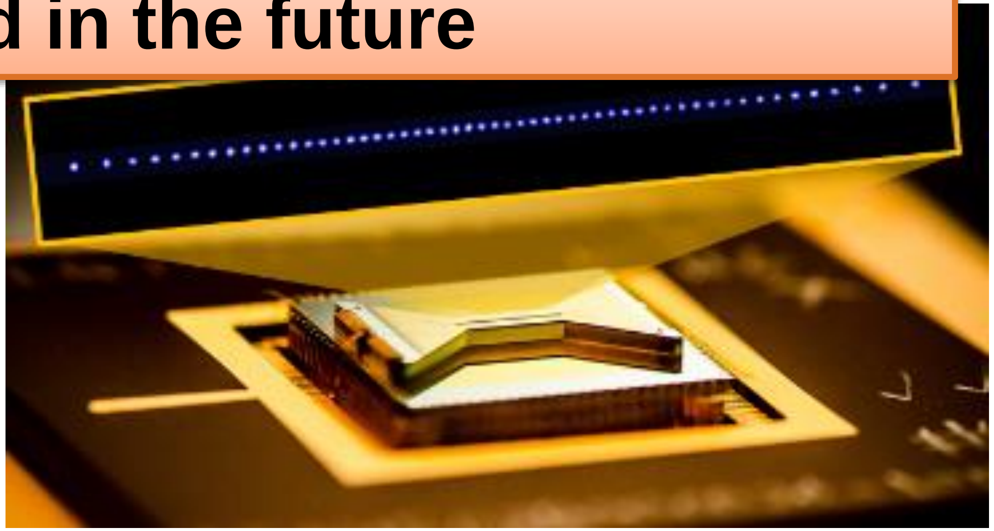
- Can solve a few toy problems
- May reach supremacy in a couple / few years
- Good to study and validate QC now, while it's easy to do in silico



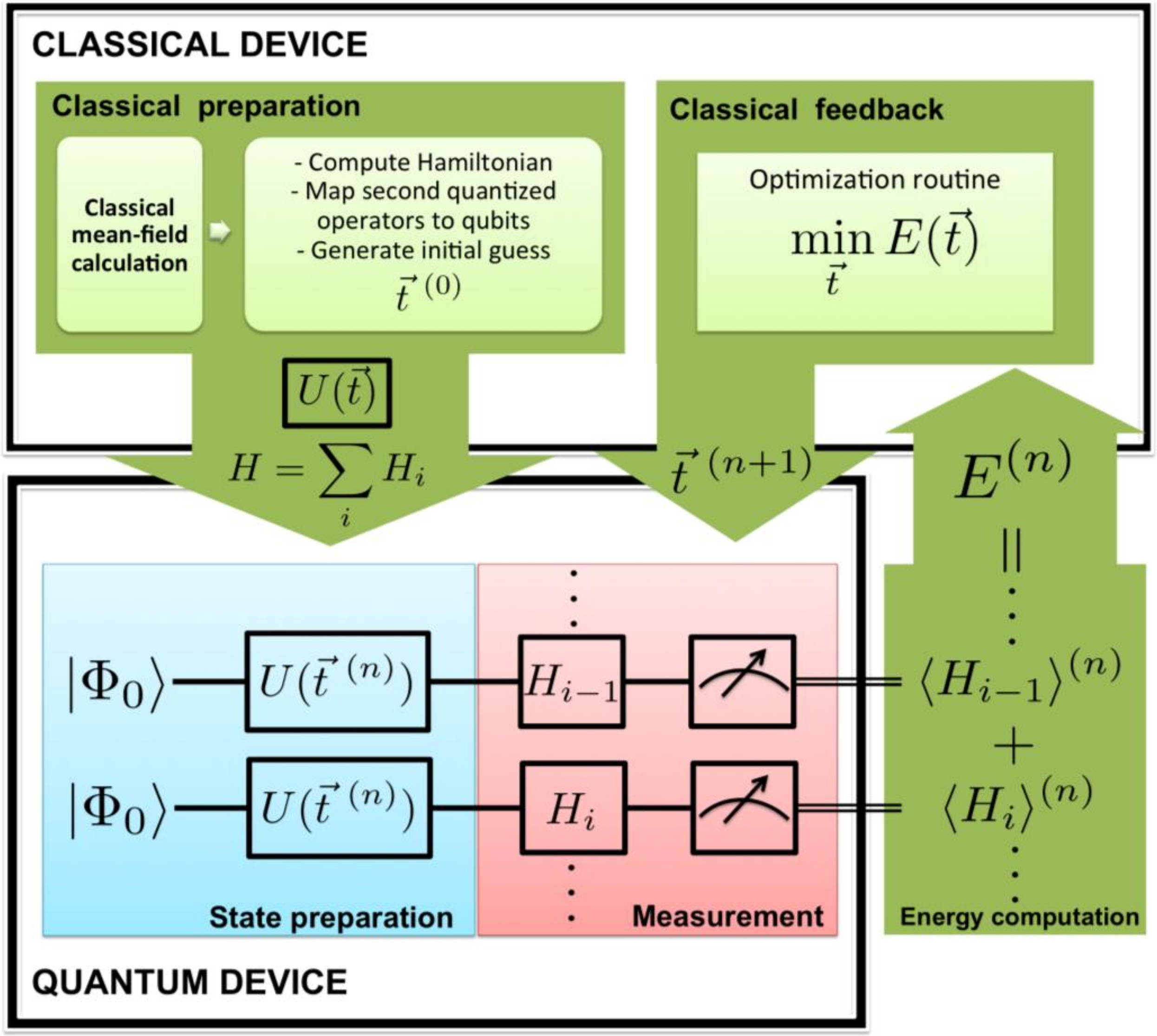
Why? To find out: what Quantum Computers are really good for, now and in the future

Challenges:

- Open system dynamics; Noise and decoherence
- Fixed connectivity, depending on HW
- How to measure performance?



Hybrid quantum simulation



Hello, World

1. Hamiltonian from pionless EFT at leading order; fit to deuteron binding energy; constructed in harmonic-oscillator basis of $^3S_1$ partial wave [à la Binder et al. (2016); Bansal et al. (2017)]; cutoff at about 150 MeV.

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^\dagger a_n$$

$$\langle n'|V|n\rangle = V_0 \delta_n^0 \delta_n^{n'}$$

$$V_0 = -5.68658111 \text{ MeV}$$

2. Map single-particle states |n⟩ onto qubits using |0⟩ = |↑⟩ and |1⟩ = |↓⟩. This is an analog of the Jordan-Wigner transform.

$$a_p^\dagger \leftrightarrow \sigma_-^{(p)} \equiv \frac{1}{2}(X_p - iY_p) \qquad a_p \leftrightarrow \sigma_+^{(p)} \equiv \frac{1}{2}(X_p + iY_p)$$

3. Solve H_1, H_2 (and H_3) and extrapolate to infinite space using harmonic oscillator variant of Lüscher's formula [More, Furnstahl, Papenbrock (2013)]

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k}e^{-2kL} - 4\frac{\gamma^4 L}{k}e^{-4kL}\right) + \frac{\hbar^2 k \gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2w_2 k\gamma^4\right)e^{-4kL}$$

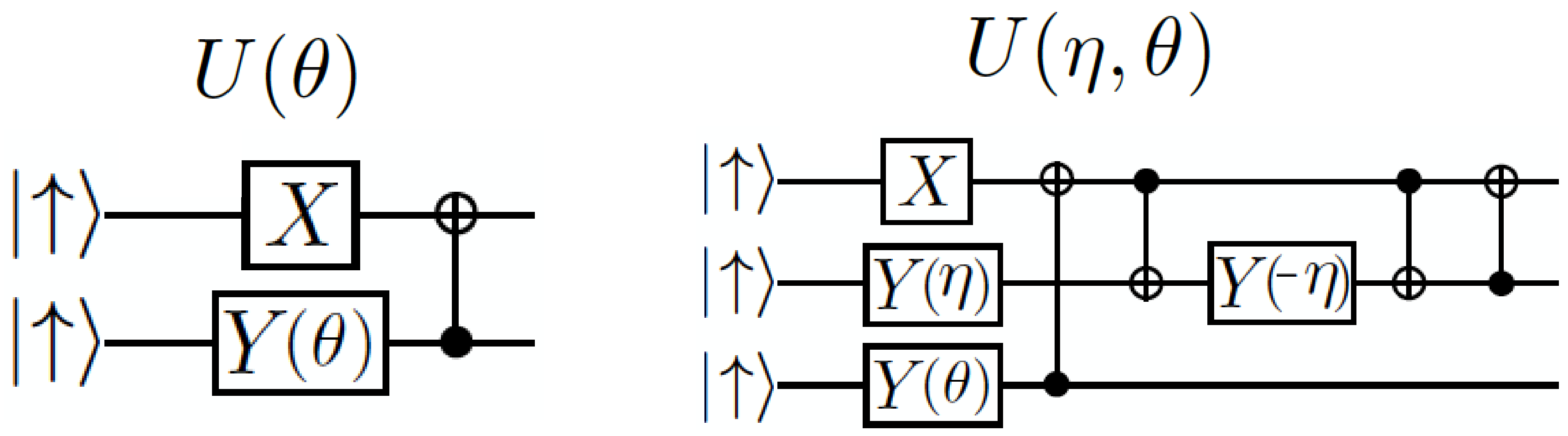
Variational wave function

$$U(\theta)|\downarrow\uparrow\rangle \qquad U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0 Y_1 - X_1 Y_0)}$$

$$U(\eta,\theta)|\downarrow\uparrow\uparrow\rangle \quad U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right) + \theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$$

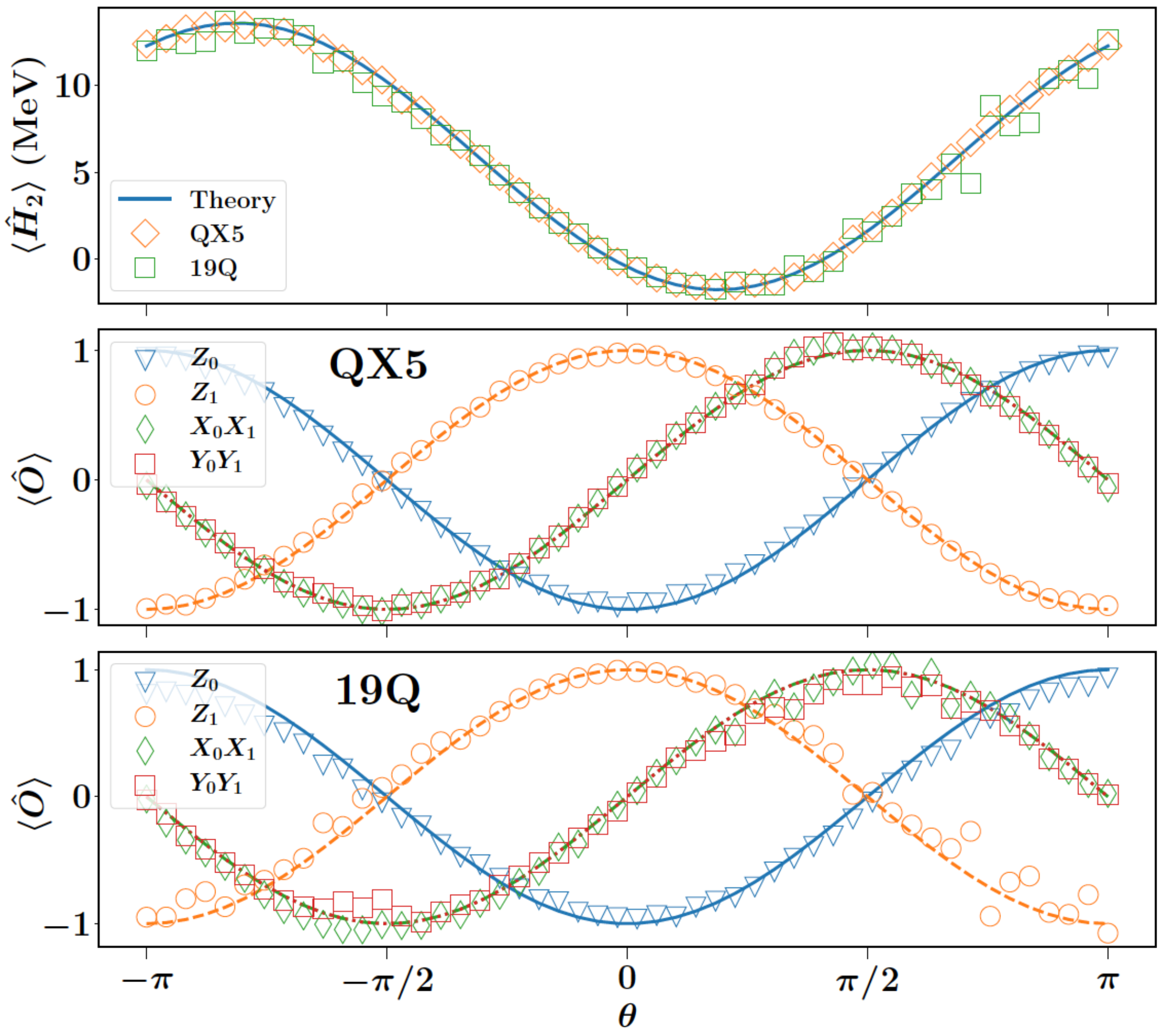
$$\approx e^{i\frac{\eta}{2}(X_0 Y_1 - X_1 Y_0)} e^{i\frac{\theta}{2}(X_0 Z_1 Y_2 - X_2 Z_1 Y_0)}$$

Minimize number of two-qubit CNOT operations to mitigate low two-qubit fidelities (construct a “low-depth circuit”)



Hamiltonian expectation value on two qubits

$$H_2 = 5.906709I + 0.218291Z_0 - 6.125Z_1 - 2.143304\,(X_0X_1 + Y_0Y_1)$$



Quantum-classical hybrid algorithm VQE [Peruzzo et al. 2014; McClean et al 2016]:

Final results

Deuteron ground-state energies from a quantum computer compared to the exact result, E_∞=-2.22 MeV.

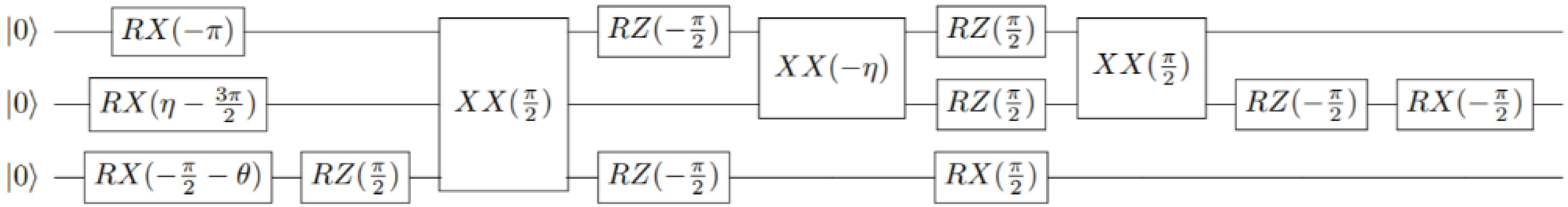
E from exact diagonalization				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	-1.749	-2.39	-2.19	
3	-2.046	-2.33	-2.20	-2.21
E from quantum computing				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	$-1.74(3)$	$-2.38(4)$	$-2.18(3)$	
3	$-2.08(3)$	$-2.35(2)$	$-2.21(3)$	$-2.28(3)$

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k}e^{-2kL} - 4\frac{\gamma^4 L}{k}e^{-4kL}\right) + \frac{\hbar^2 k \gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2w_2 k\gamma^4\right)e^{-4kL}$$

Dumitrescu, McCaskey, Hagen, Jansen, Morris, Papenbrock, Pooser, Dean, Lougovski, Phys. Rev. Lett. **120**, 210501(2018)

And on ion traps

Three qubit ansatz:

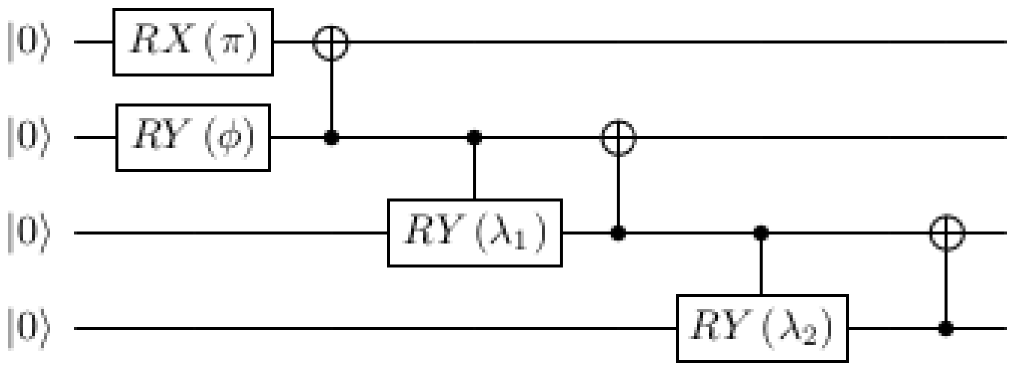


$$\mathrm{XX}(\chi) = e^{-i(\hat{\sigma}_x^{(1)}+\hat{\sigma}_x^{(2)})^2\chi/4} = e^{-i\hat{\sigma}_x^{(1)}\hat{\sigma}_x^{(2)}\chi/2}$$

$$= \begin{pmatrix} \cos(\chi/2) & 0 & 0 & -i\sin(\chi/2) \\ 0 & \cos(\chi/2) & -i\sin(\chi/2) & 0 \\ 0 & -i\sin(\chi/2) & \cos(\chi/2) & 0 \\ -i\sin(\chi/2) & 0 & 0 & \cos(\chi/2) \end{pmatrix}$$

Deuteron on ion traps

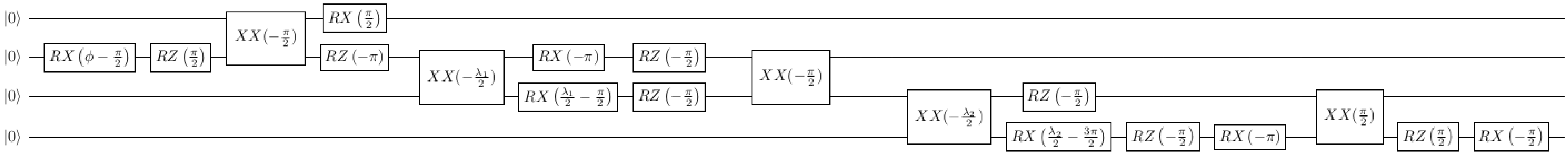
4 qubit ansatz:



…within 1% accuracy

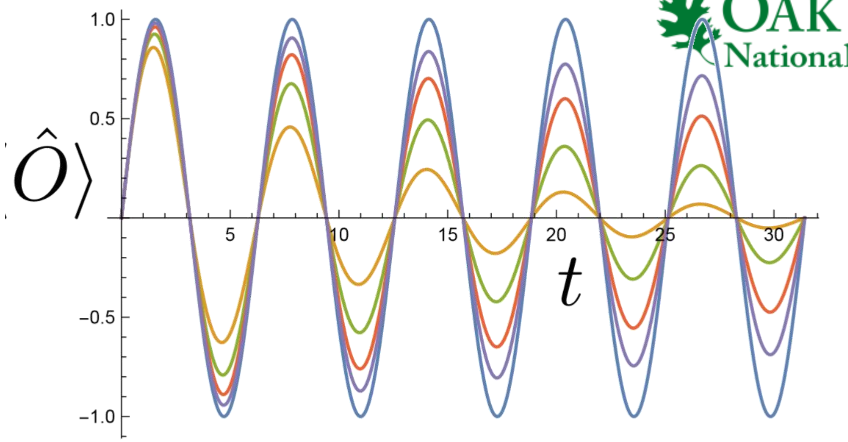
Final results:

-2.2(2) MeV



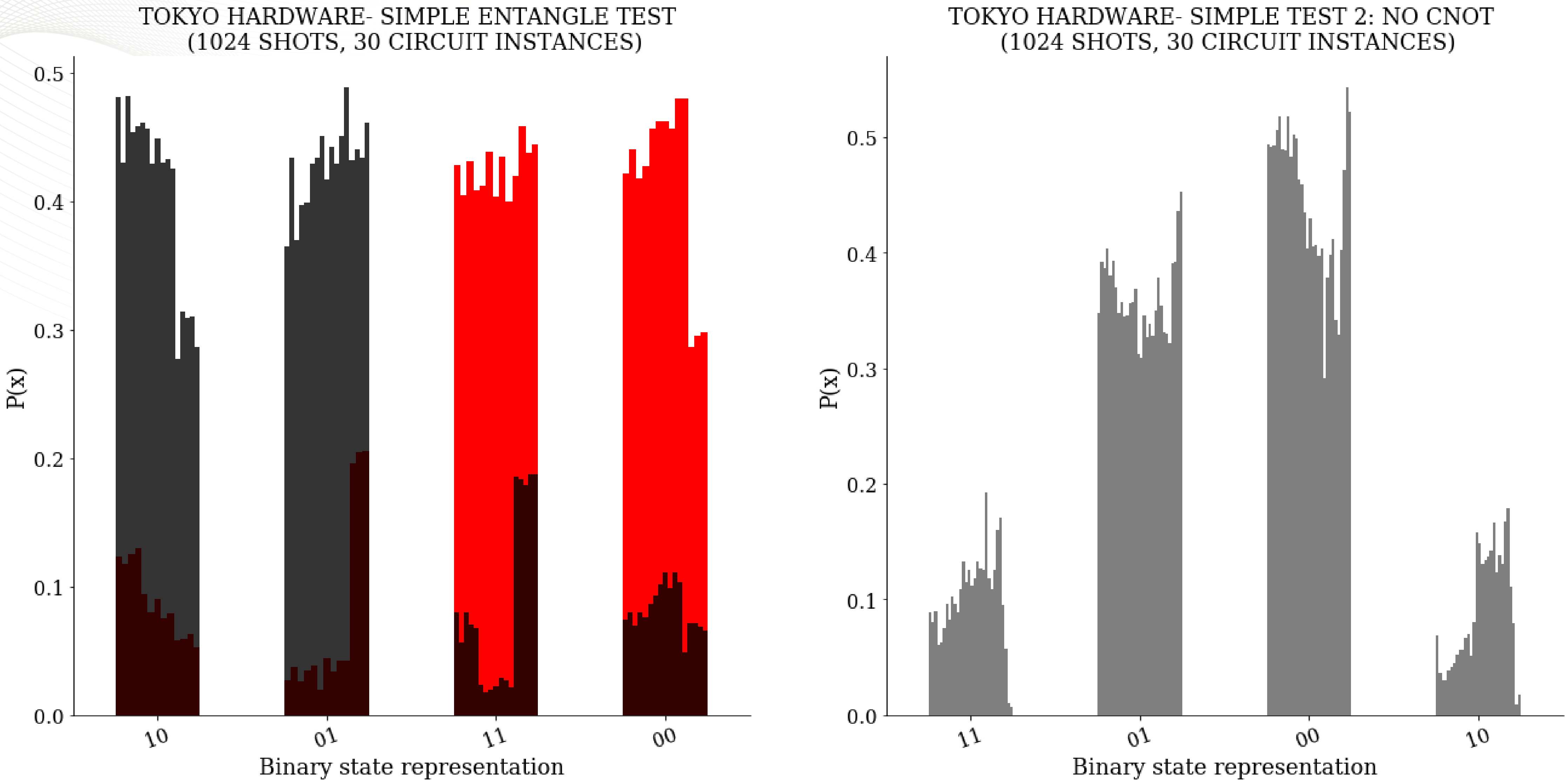
Shehab et al., PRA

Error mitigation



- What is error mitigation(EM)?
- A protocol to “correct” physical noise in post proc.
- How do the protocols work?
- By collecting and post-processing additional quantum data supplementing the logical computation.
- In other words, distilling/decoding logical information from a set of corrupted computations.
- Bad news: Signal to noise ratio deteriorates rapidly. (exponentially in worst case). EM schemes with exponential sample complexity will not be tractable.
- Information distillation may require multiple levels of mitigation. • Steps must be consistent with one another and avoid overfitting!
- 3 Methodologies by (peer-reviewed) anecdote: (i) readout, (ii), extrapolation, (iii) purification

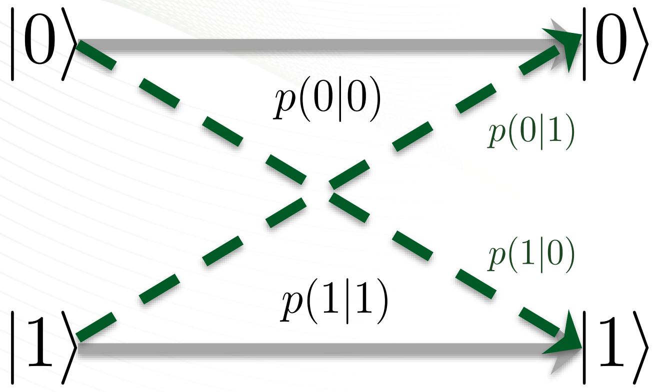
At minimum, measurement error mitigation is required



Error mitigation

Oak Ridge National Laboratory

Calibrating measurement errors:

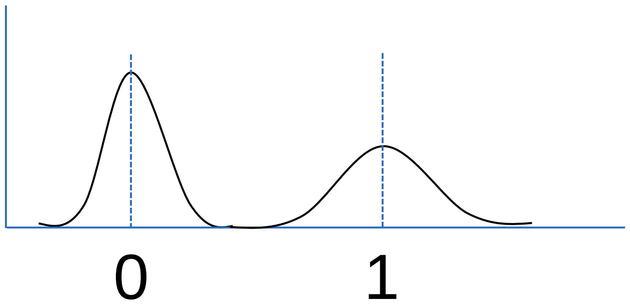


Error model

$$p_i^{\pm} = p(0|1)_i \pm p(1|0)_i$$

$$\langle \hat{p} \rangle = \sum_{x \in \text{counts}} p(x) \prod_{j \in \text{supp}(p)} \left[\frac{(-1)^{x_j} - p_j^{-}}{1 - p_j^{+}} \right]$$

characterization

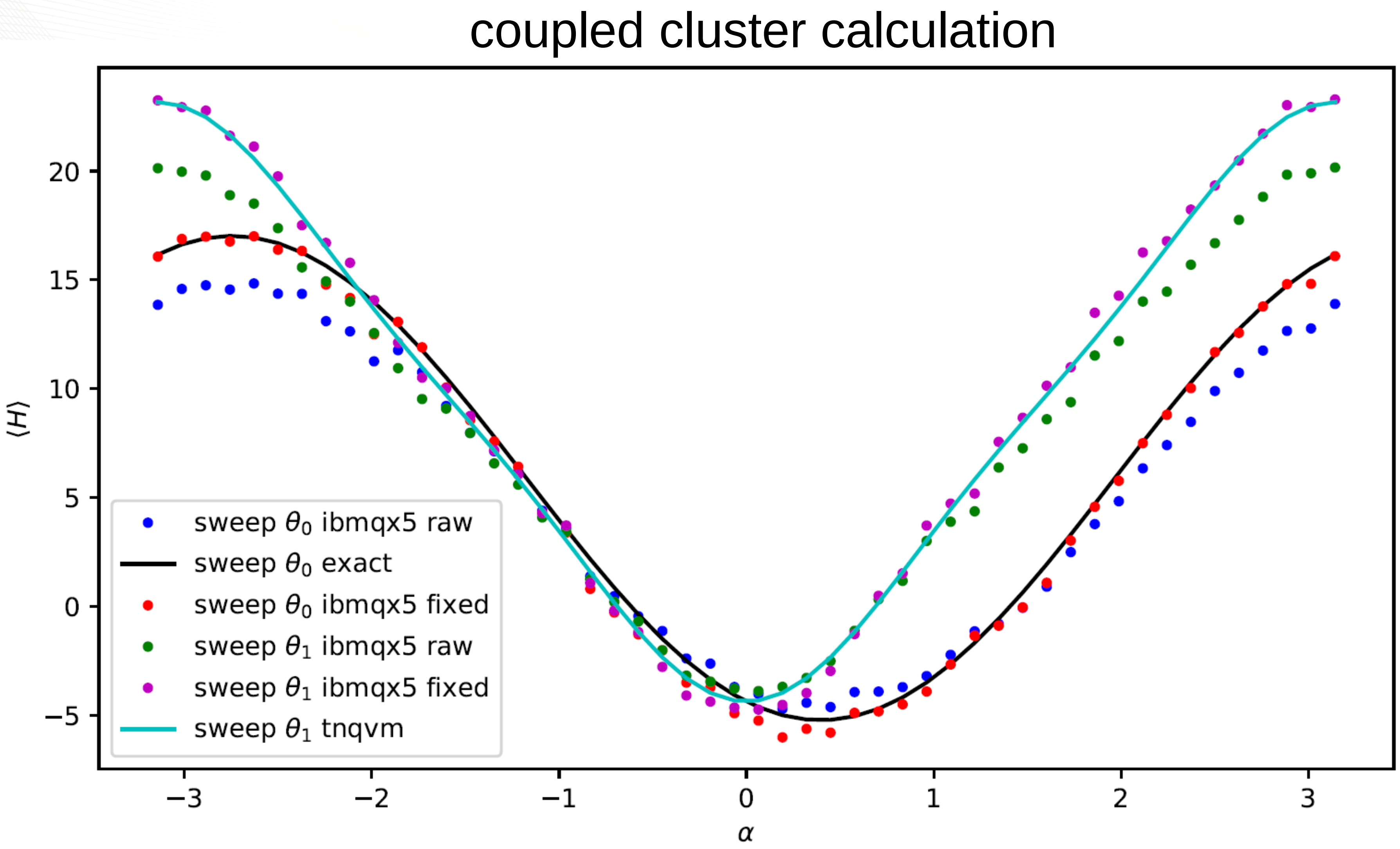


Obtain distribution of measurement outcomes, bound error rate

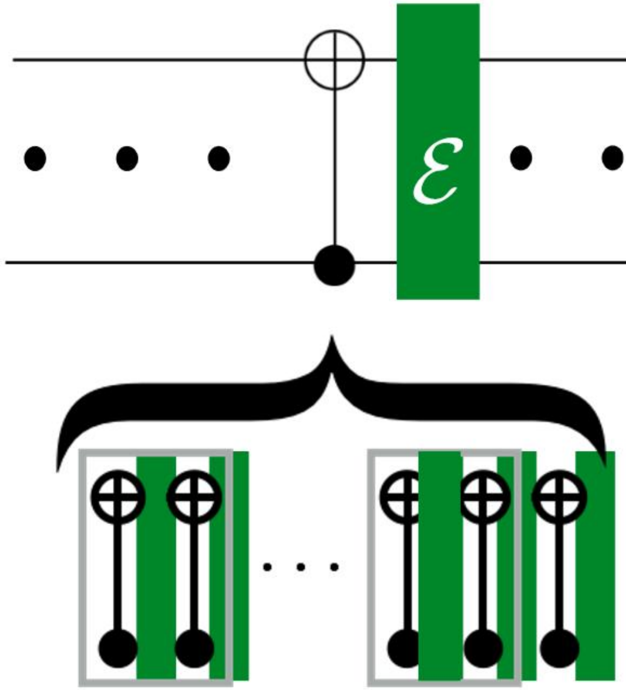
$$\langle \Delta\psi \rangle^2 = \langle \Delta\alpha \rangle^2 + \langle \Delta\beta \rangle^2$$

Systematic error in measurement outcome is converted to statistical error with calibration
Automated in our programming environment, XACC

Example error correction results



Error extrapolation



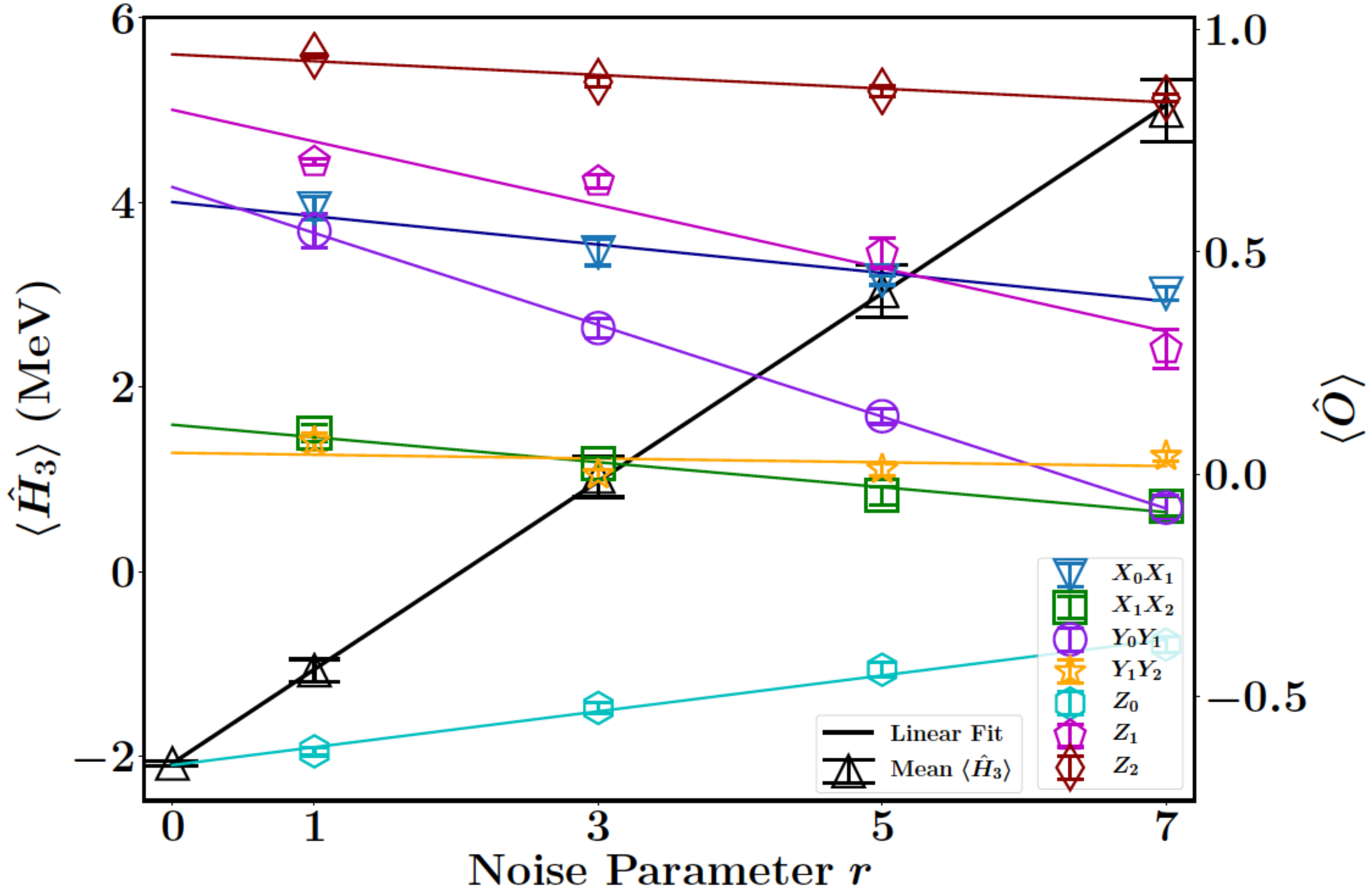
Temme 17, Li 17, Kandala 18,

$$\mathcal{E}(\rho) = (1-\varepsilon)\rho + \varepsilon I$$

$$\begin{aligned} & \mathcal{E} \circ C \circ \ldots \mathcal{E} \circ C \circ \rho \\ = \quad & (1-\varepsilon)^n C \circ \rho + (1-(1-\varepsilon)^n) I \\ = \quad & (1-n\varepsilon) C \circ \rho + n\varepsilon I + \mathcal{O}(\varepsilon^2) \end{aligned}$$

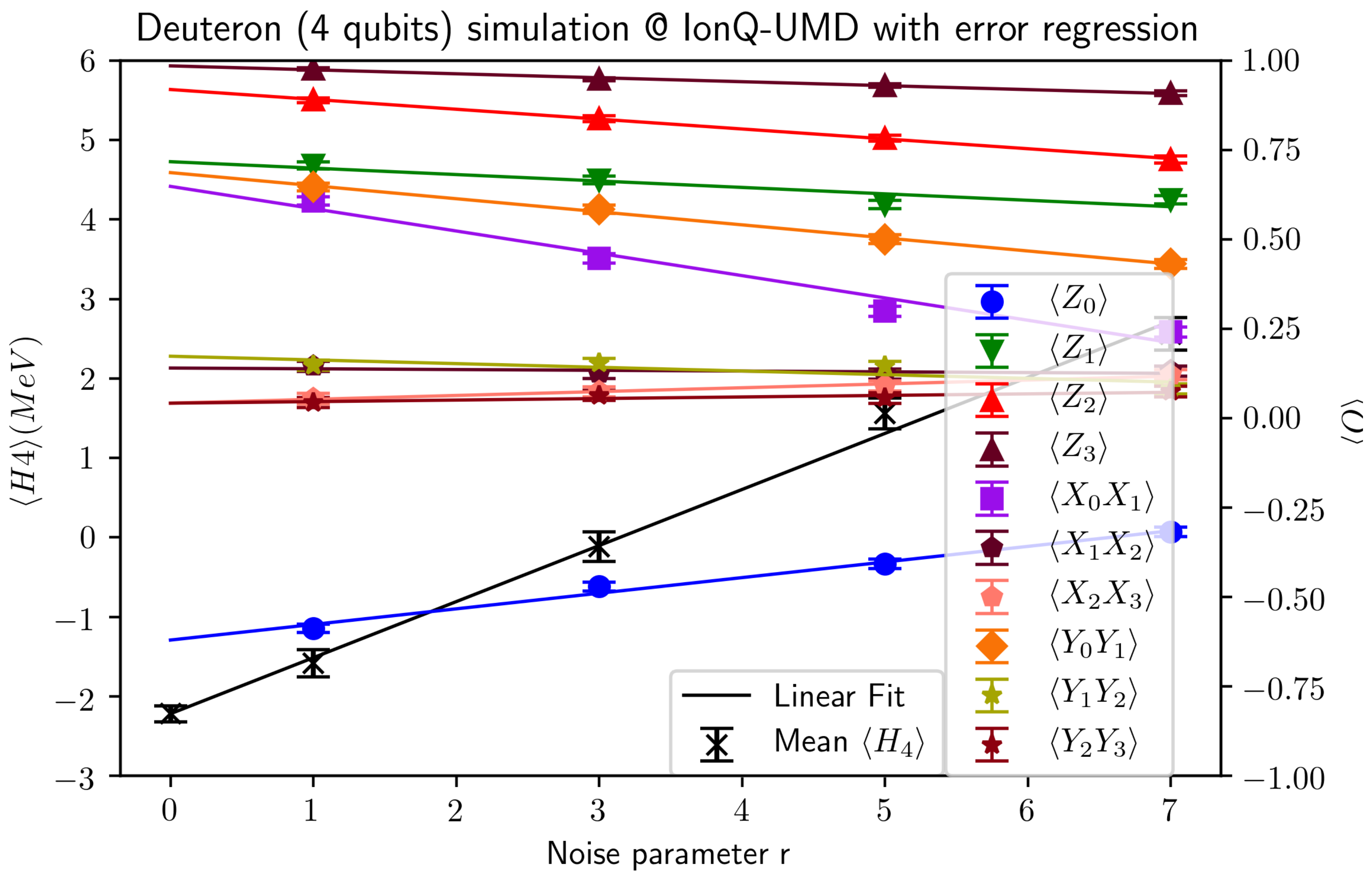
Deuteron CNOT error mitigation on superconductors

$$H_3 = H_2 + 9.625(I - Z_2) - 3.913119\,(X_1X_2 + Y_1Y_2)$$



Three qubits have more noise. Insert *r* pairs of CNOT (unity operators) to extrapolate to *r*=0.
[See, e.g., Ying Li & S. C. Benjamin 2017]

Deuteron CNOT error mitigation on ion traps



Purification – alternative approach

Problem:

$$H_0 = \frac{1}{2}\sum_{x=0}^{L-1}\left[\pi^2(x) + (\nabla\phi(x))^2 + m^2\phi^2(x)\right]$$

$$H_I = \sum_{x=0}^{L-1}\left[\frac{\delta_m}{2}\phi^2(x) + \frac{\lambda}{4!}\phi^4(x)\right]$$

with k = 0, pi and $q^2(k) = \frac{1}{2}\left[a^2(k) + (a^\dagger(k))^2 + 2n(k) + 1\right]$

$$H_I = \frac{\lambda}{48}\left[\frac{q^4(0)}{\omega^2(0)} + \frac{6q^2(0)q^2(\pi)}{\omega(0)\omega(\pi)} + \frac{q^4(\pi)}{\omega^2(\pi)}\right] + \frac{\delta_m}{2}\left[\frac{q^2(0)}{\omega(0)} + \frac{q^2(\pi)}{\omega(\pi)}\right] \qquad \mathbb{Z}_2 \times \mathbb{Z}_2$$

Encoding:

$$\phi(x) = \frac{1}{\sqrt{L}}\sum_k \frac{1}{\sqrt{2\omega(k)}}\left(a^\dagger(k)e^{-ikx} + a(k)e^{ikx}\right)$$

$$\pi(x) = \frac{i}{\sqrt{L}}\sum_k \sqrt{\frac{\omega(k)}{2}}\left(a^\dagger(k)e^{-ikx} - a(k)e^{ikx}\right).$$

$$a = \sum_{n=1}^{\infty}\sqrt{n}|n-1\rangle\langle n|$$

$$|i\rangle\langle j| = \bigotimes_l \left|b_l^{(i)}\right\rangle\left\langle b_l^{(j)}\right|$$

$$\begin{cases} |0\rangle\langle 0|_l \to \frac{\mathbb{I}+Z_l}{2} \\ |0\rangle\langle 1|_l \to \frac{X_l+iY_l}{2} \\ |1\rangle\langle 0|_l \to \frac{X_l-iY_l}{2} \\ |1\rangle\langle 1|_l \to \frac{\mathbb{I}-Z_l}{2} \end{cases}$$

Purification:

Measurement basis

$$\mathbb{P}_2 = \sigma_0^\mu \sigma_1^\nu$$

$$\mu,\nu \in \{I, X, Y, Z\}$$

$$\rho = \sum_{p\in\mathbb{P}_2} c_p p$$

Readout correction, followed by

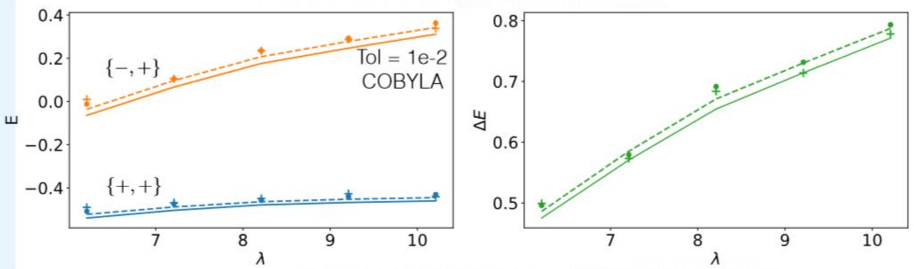
$$\rho_{n+1} = 3\rho^2 - 2\rho^3$$

$$\mathcal{N} = \mathrm{Tr}\left[\rho^2 - \rho\right]$$

$$\epsilon_{\mathcal{N}} < 10^{-4}$$

7

Results:



Yeter-Ayedeniz, et al, PRA arXiv:1811.12332 2018

McWeeny purification

$$E(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})| H |\psi(\boldsymbol{\theta})\rangle = \sum_{p,q} h_{pq} \langle\psi(\boldsymbol{\theta})| a_p^\dagger a_q |\psi(\boldsymbol{\theta})\rangle + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} \langle\psi(\boldsymbol{\theta})| a_p^\dagger a_q^\dagger a_s a_r |\psi(\boldsymbol{\theta})\rangle ,$$

$$\langle\psi(\boldsymbol{\theta})| a_p^\dagger a_q^\dagger a_s a_r |\psi(\boldsymbol{\theta})\rangle \equiv \rho_{pqrs}$$

Two body reduced density matrix

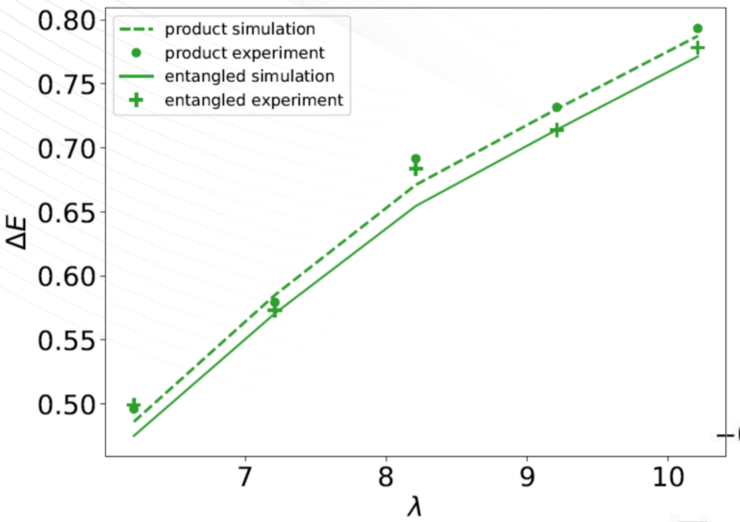
Iteratively purify:

$$\rho_{pqrs} \leftarrow 3(\rho_{pqrs})^2 - 2(\rho_{pqrs})^3$$

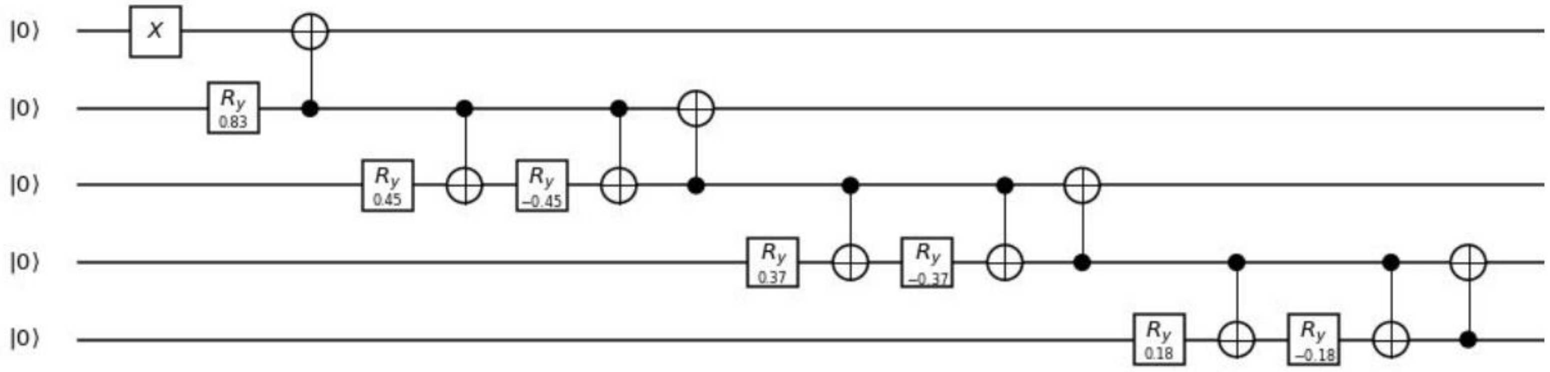
Until:

$$\mathrm{Tr}(\rho_{pqrs}^2 - \rho_{pqrs}) < \epsilon$$

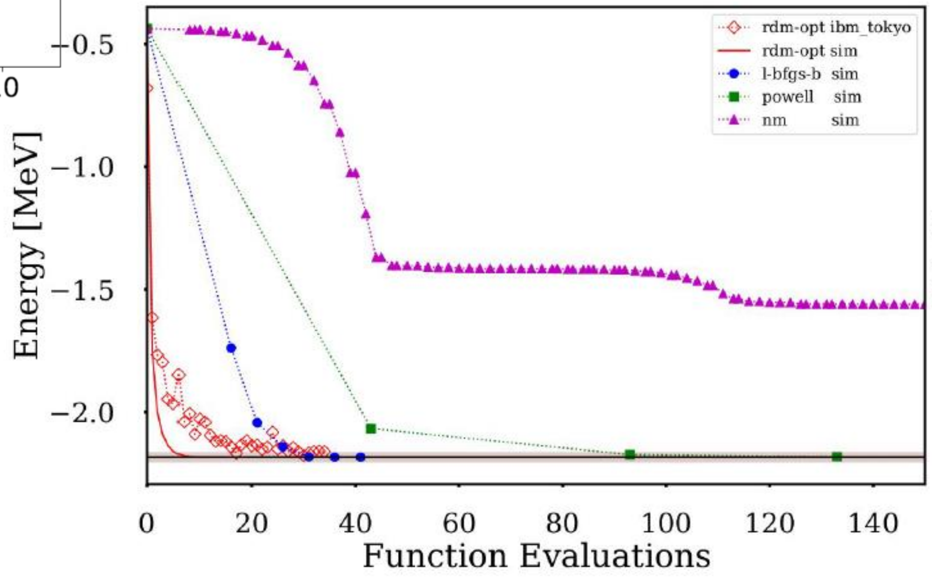
Purification

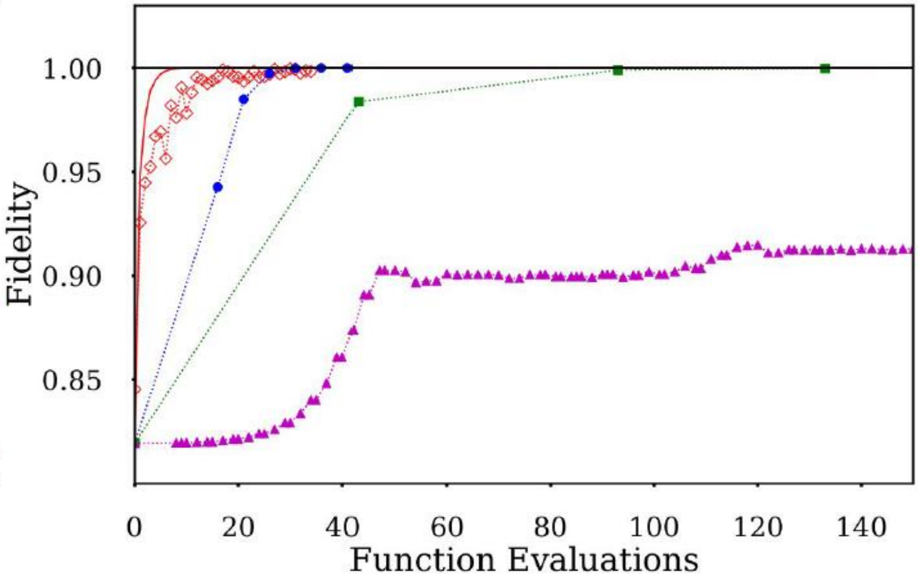


5x5 deuteron



Allows full VQE convergent loop on hardware



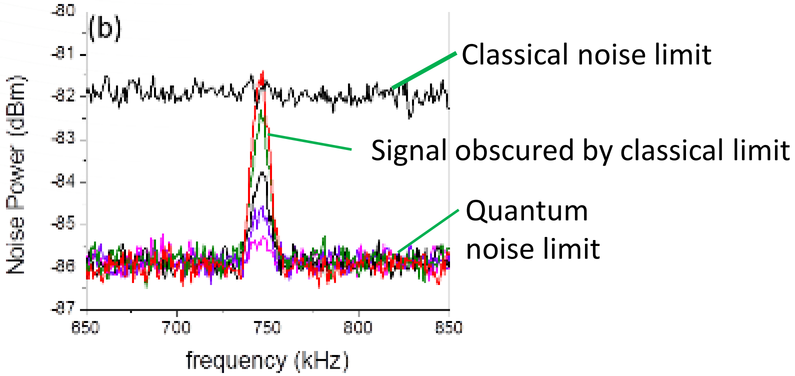


Conclusion

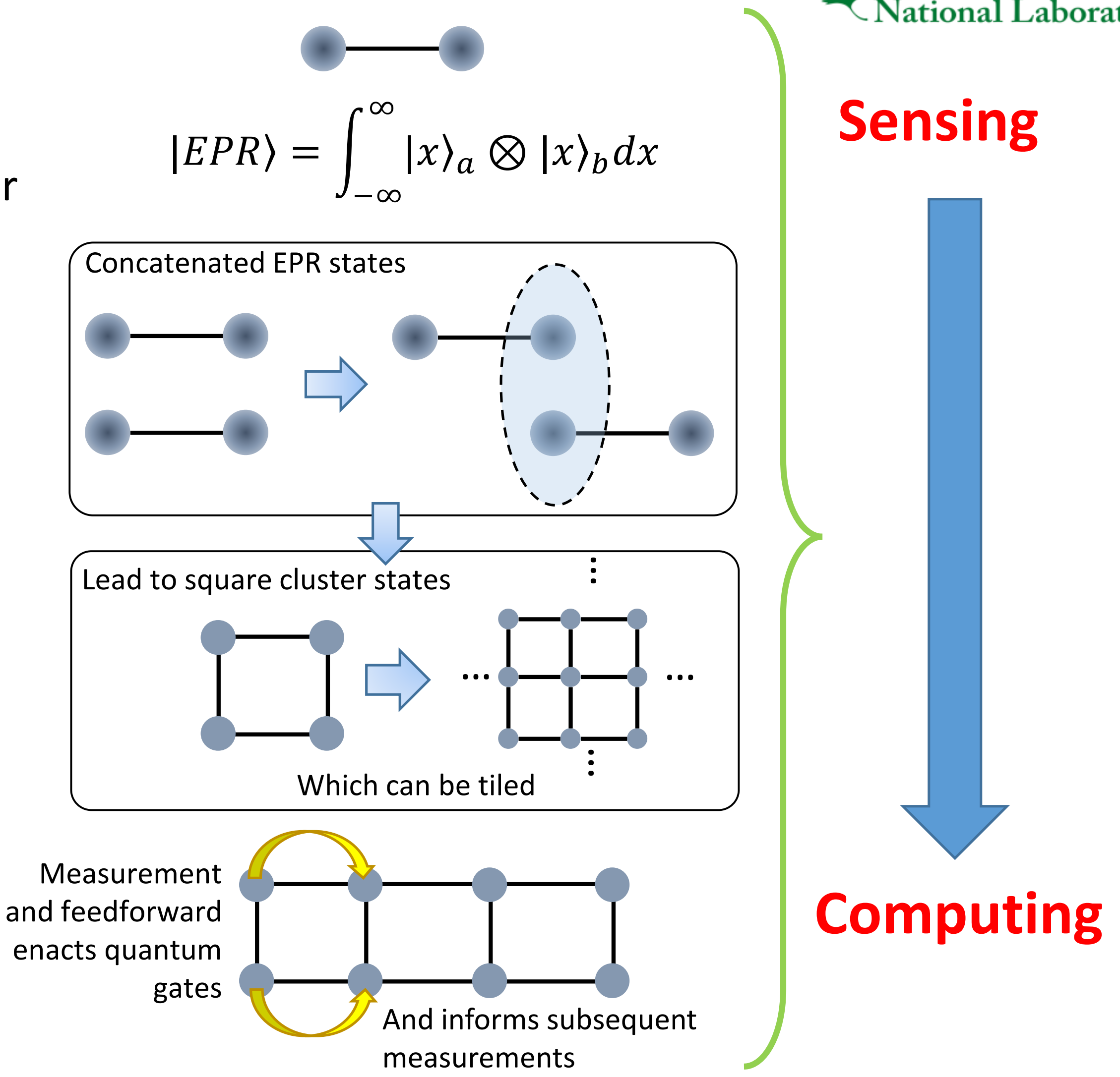
- NISQ devices are very noisy
- Error Mitigation - we can still use them to accomplish useful computations
- Intensive benchmarking required
- Several benchmarks developed
  – Machine learning (BAS test)
  – Chemistry
  – Nuclear physics
  – Field theory
  – Gate constructions
- Combined benchmarking strategy allows us to determine feasibility in the NISQ era

Quantum Sensing and Quantum Computing Across Quantum Networks

- Quantum networks are collections of qubits (nodes) connected by interactions, or quantum gates (edges)
- Simplest quantum network is the two qubit EPR state or Bell state, *which is a workhorse in quantum sensing*
  - The quantum correlations in EPR quantum networks can be used to *reduce the noise floor in measurements* – **quantum metrology**



- Indefinitely large quantum networks can be built by concatenating EPR states – *the same network is a resource for measurement-based quantum computing and distributed quantum sensors*



$$|EPR\rangle = \int_{-\infty}^{\infty} |x\rangle_a \otimes |x\rangle_b dx$$

The know-how in generating long range entanglement for quantum sensing lends itself to building quantum computers. This is because in order to make these quantum sensors, one must build a *quantum network* with a *two qubit gate* interaction between the nodes.