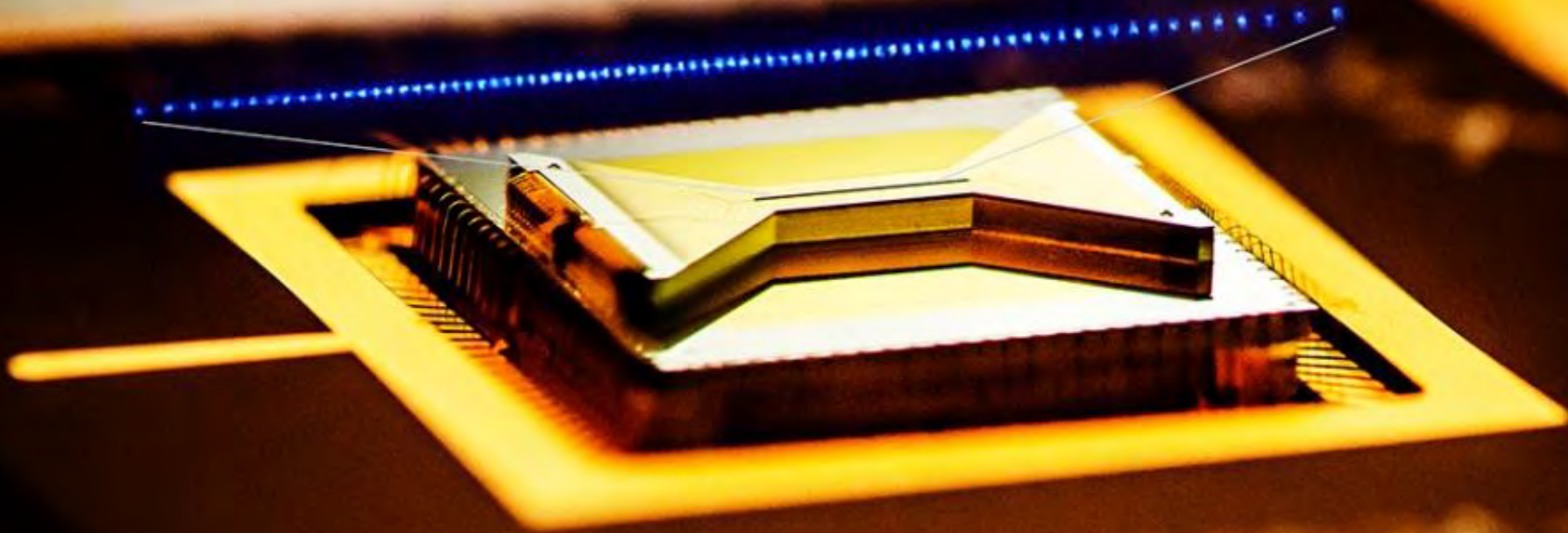


# Quantum Circuits and Simulation with Individual Atoms

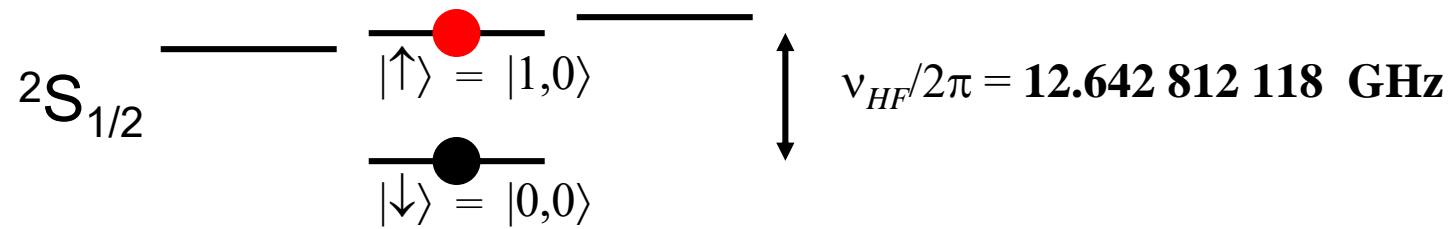


Christopher Monroe  
*Univ. Maryland, JQI, QuICS, and IonQ*

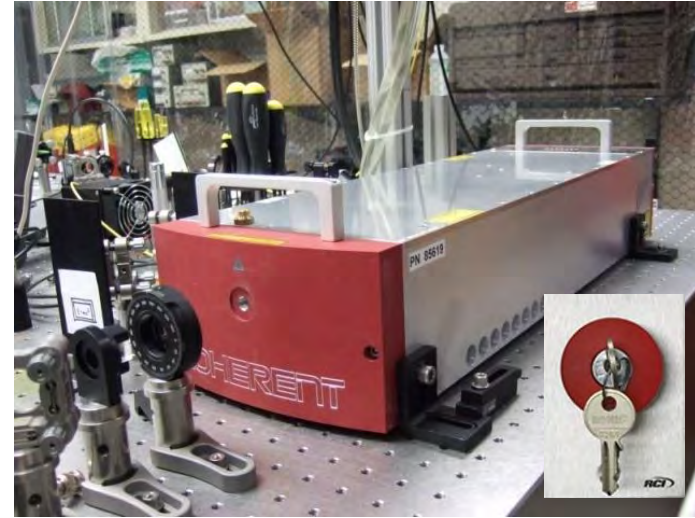
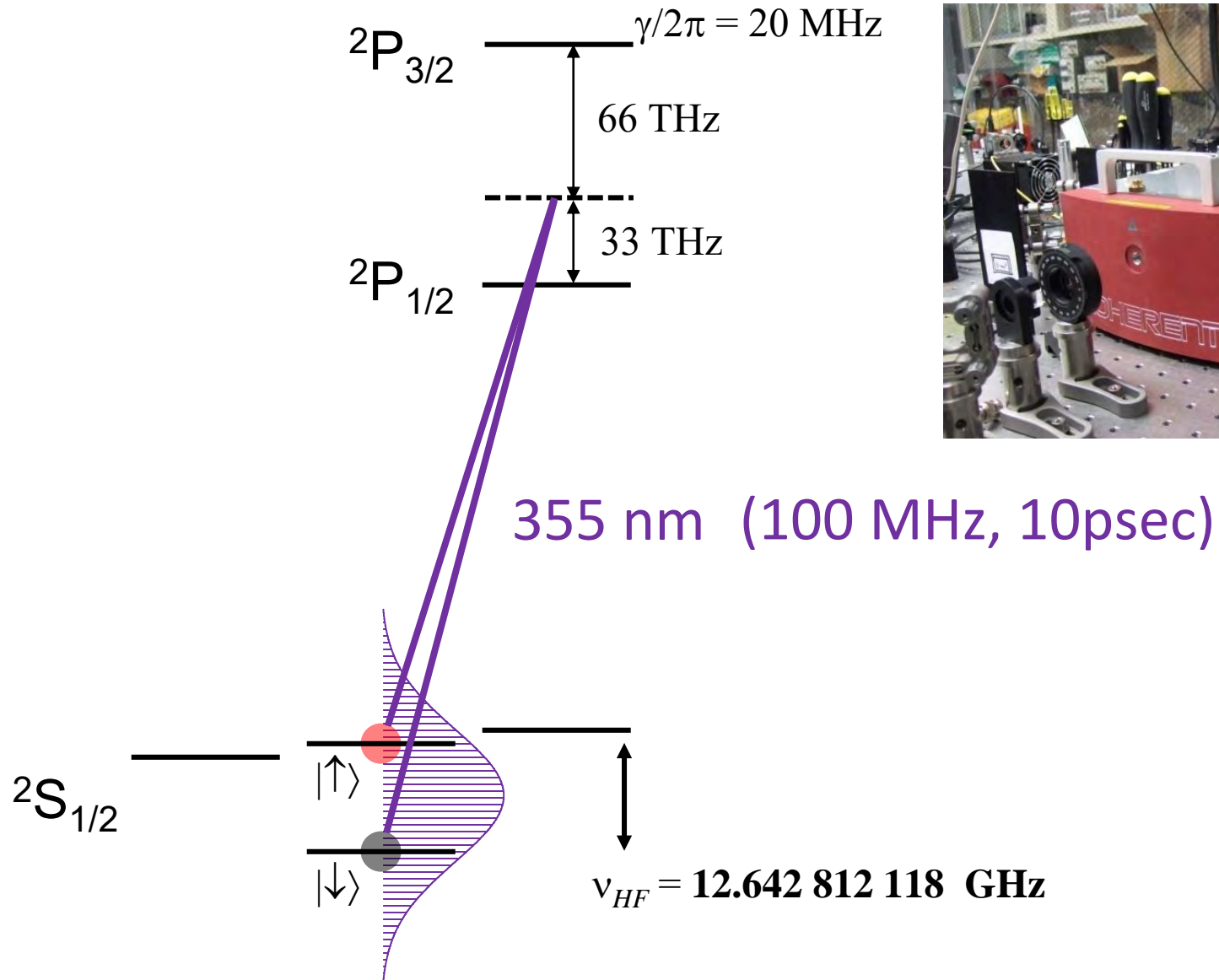


JOINT CENTER FOR  
QUANTUM INFORMATION  
AND COMPUTER SCIENCE

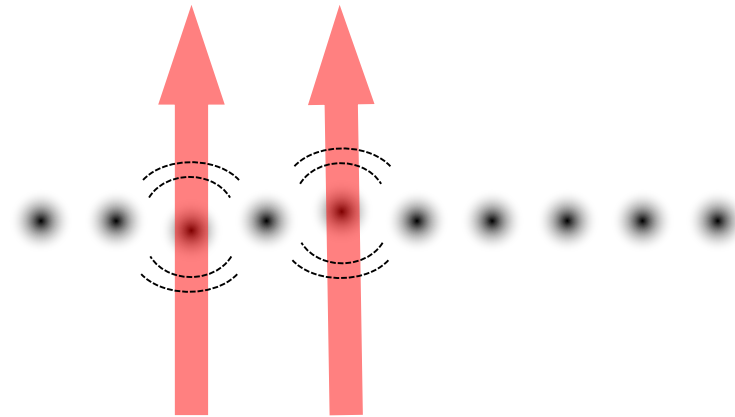
# Atomic Qubit ( $^{171}\text{Yb}^+$ )



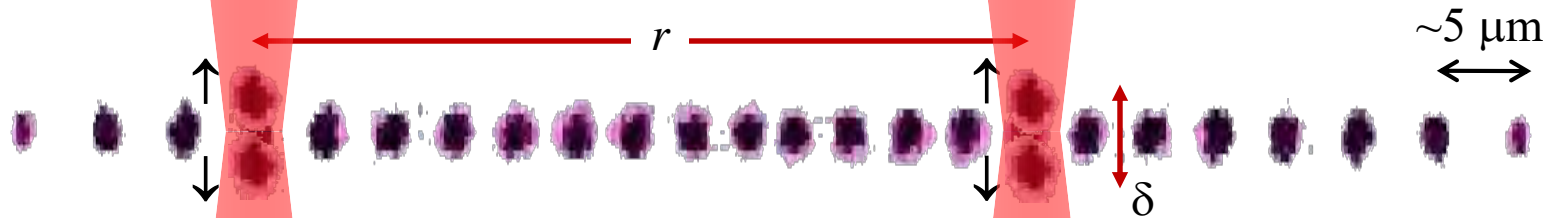
# $^{171}\text{Yb}^+$ Qubit Manipulation



# Quantum Circuits and Algorithms



# Quantum Entanglement of Trapped Ions



dipole-dipole coupling  $\Delta E = \frac{e^2}{\sqrt{r^2 + \delta^2}} - \frac{e^2}{r} \approx -\frac{(e\delta)^2}{2r^3}$   $\delta \sim 10 \text{ nm}$   
 $e\delta \sim 500 \text{ Debye}$

$$\begin{array}{l}
 |\downarrow\downarrow\rangle \rightarrow |\downarrow\downarrow\rangle \\
 |\downarrow\uparrow\rangle \rightarrow e^{-i\varphi} |\downarrow\uparrow\rangle \\
 |\uparrow\downarrow\rangle \rightarrow e^{-i\varphi} |\uparrow\downarrow\rangle \\
 |\uparrow\uparrow\rangle \rightarrow |\uparrow\uparrow\rangle
 \end{array}
 \longrightarrow
 \varphi = \frac{\Delta E t}{\hbar} = \frac{e^2 \delta^2 t}{2\hbar r^3} = \frac{\pi}{2}$$

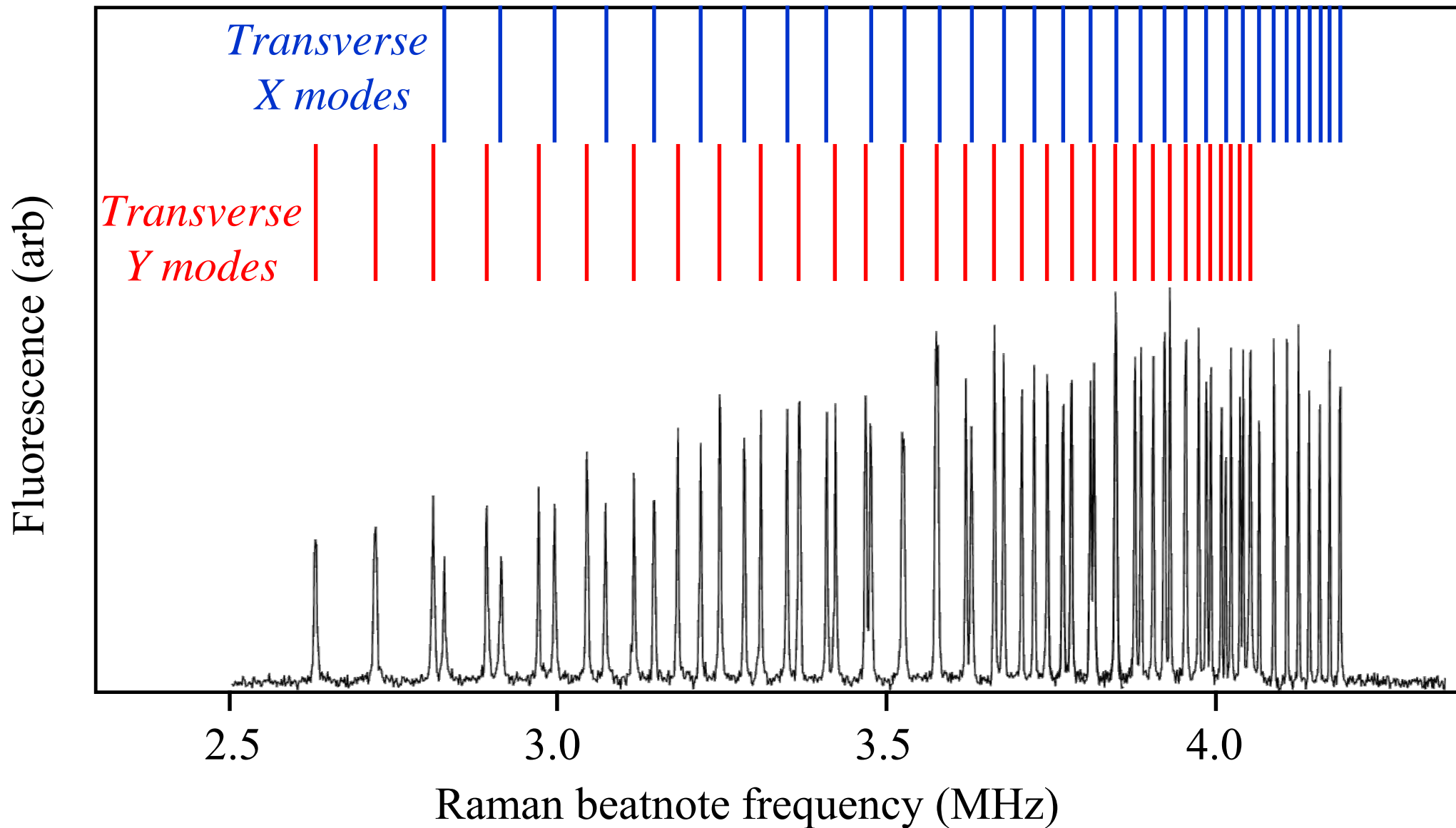
for full entanglement

Native Ion Trap Operation: "Ising" gate

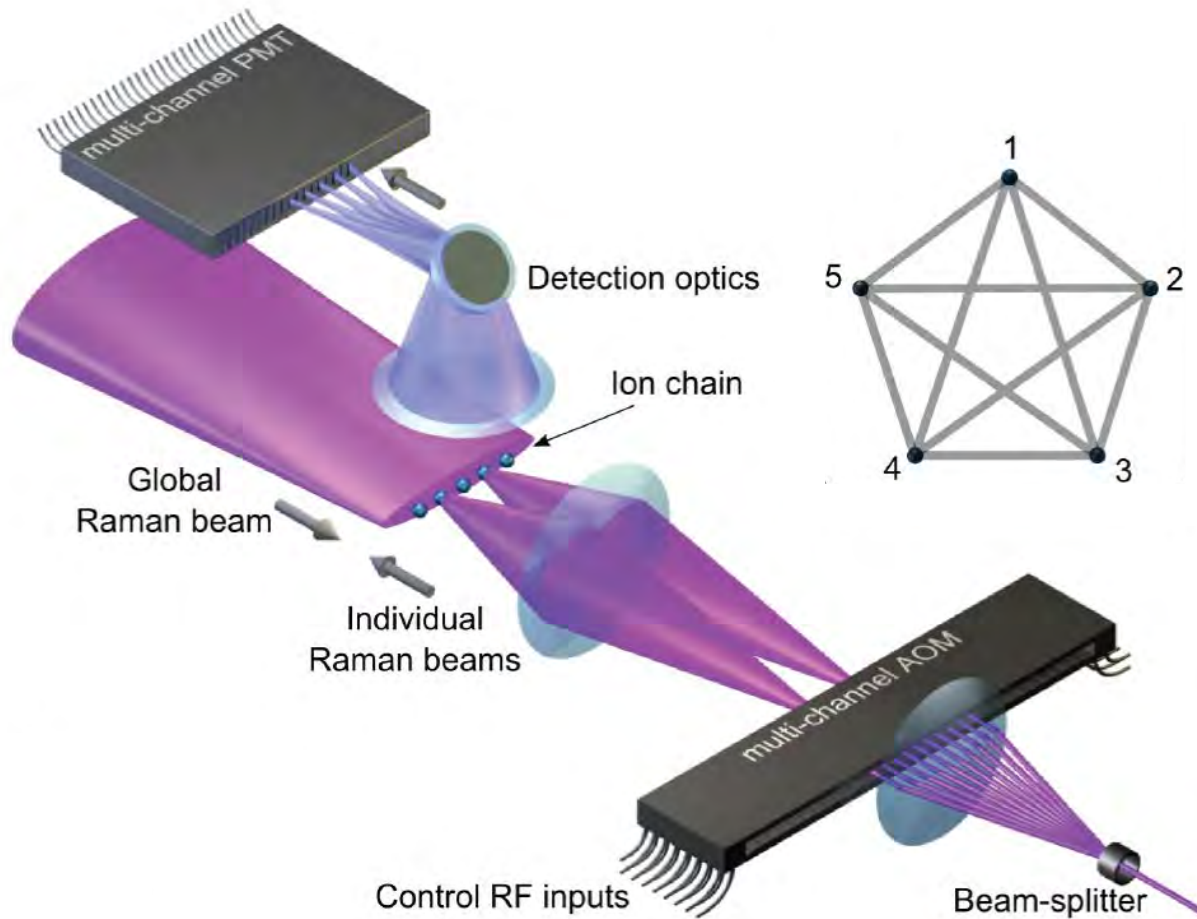
$$XX[\varphi] = e^{-i\sigma_x^{(1)}\sigma_x^{(2)}\varphi} \quad T_{gate} \sim 10-100 \mu\text{s} \\
 F \sim 98\% - 99.9\%$$

Cirac and Zoller (1995)  
 Mølmer & Sørensen (1999)  
 Solano, de Matos Filho, Zagury (1999)  
 Milburn, Schneider, James (2000)

# Raman Sideband Spectrum of 32 $^{171}\text{Yb}^+$ ions



# Programmable/Reconfigurable Quantum Computer Module



## Full “Quantum Stack” architecture

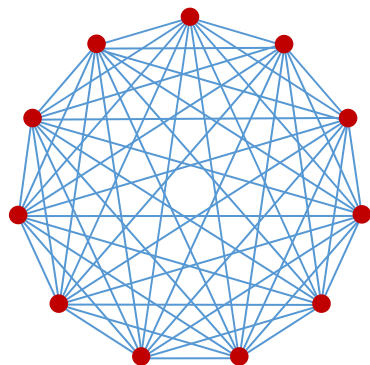
User	<b>Quantum Algorithms:</b> <i>Deutsch-Jozsa, QFT, etc.</i>
Quantum compiler	<b>Universal gates:</b> <i>Hadamard, C-NOT, C-Phase, etc.</i> <b>Native gates:</b> <i>XX-Gates, R-gates</i>
Quantum control	<b>Pulse shaping:</b> <i>Optimization of XX- and R-Gates</i>
Hardware	<b>Optical addressing:</b> <i>Qubit manipulation/ detection</i> <b>Ion trap:</b> <i>Linear ion-chain, optical access, etc.</i>

# Benchmarking 11-qubit register

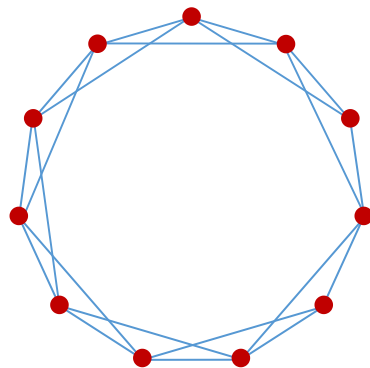


11 Trapped Ions  
fully connected

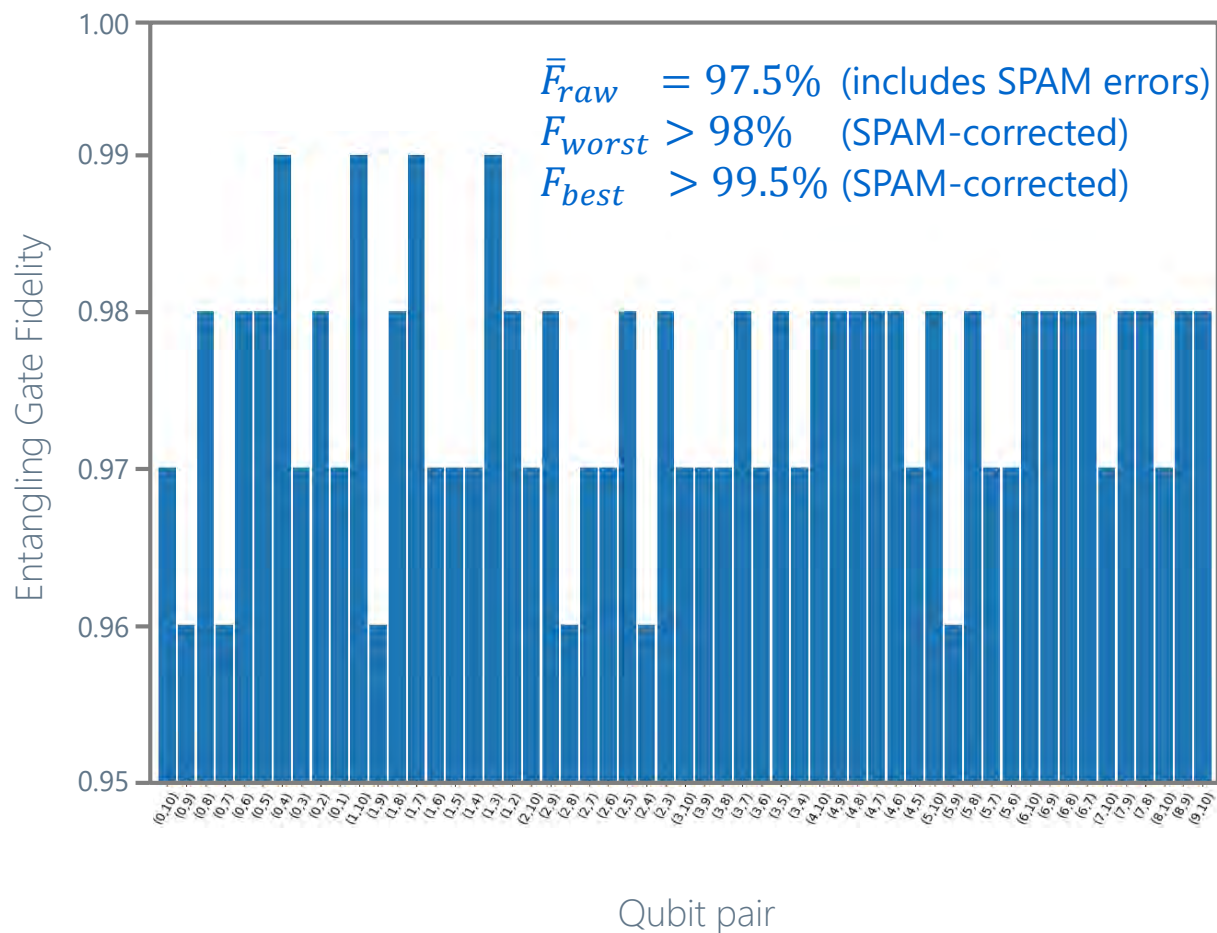
$$\binom{11}{2} = 55 \text{ gates}$$



2D nearest-neighbor



Fidelities of all two-qubit gates





# Benchmarking 11-qubit register



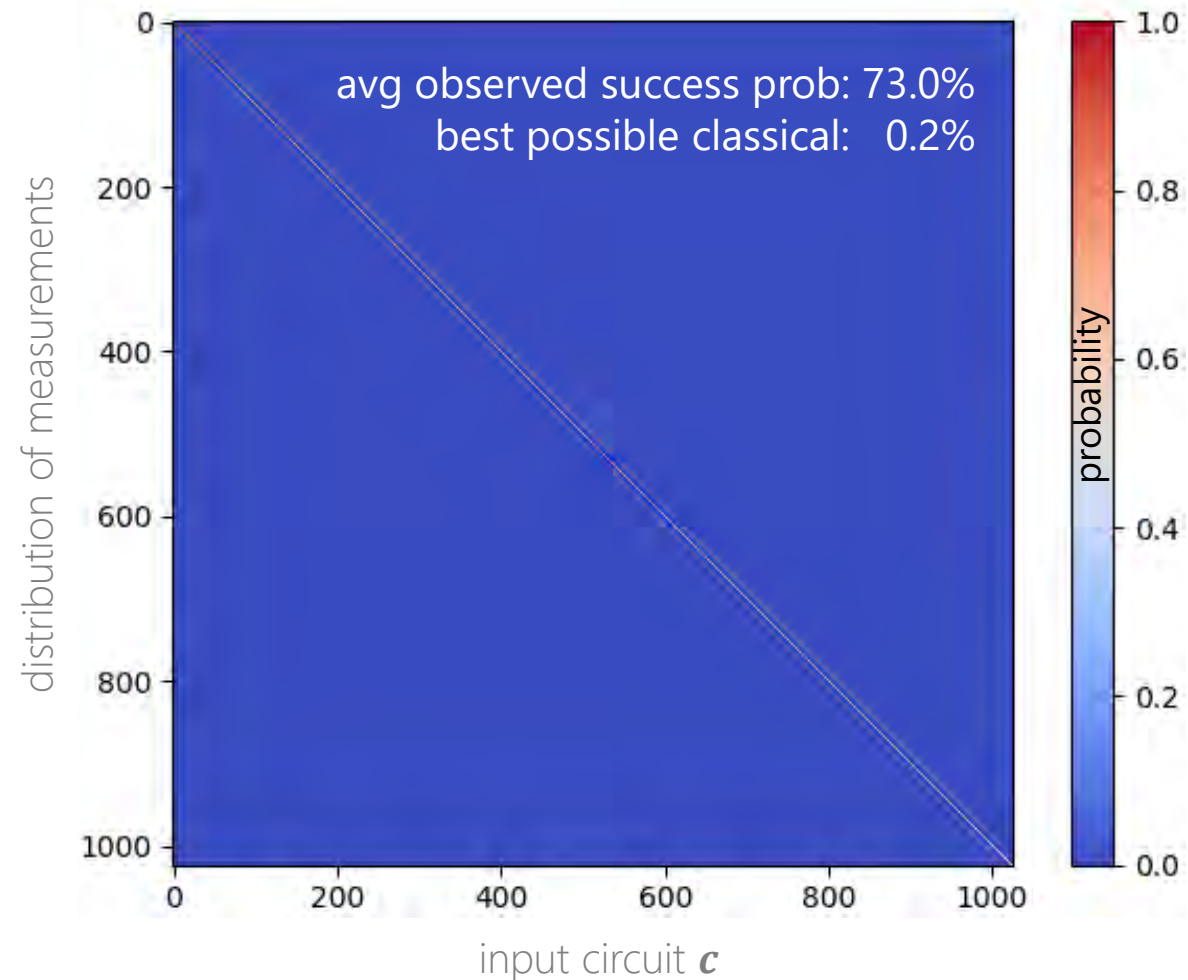
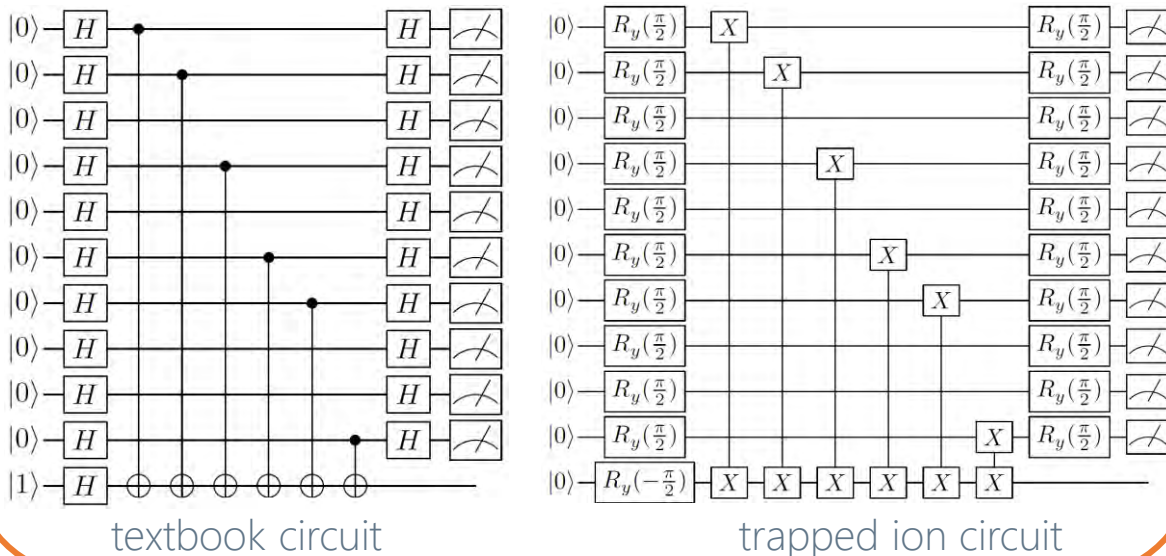
## Bernstein-Vazirani Algorithm

Given  $f(\mathbf{x}) = \mathbf{c} \cdot \mathbf{x}$ , find  $n$ -bit string  $\mathbf{c}$

classical:  $n$  queries

quantum: 1 query

example:  $\mathbf{c} = 1101011001$



# Build it and they will come!

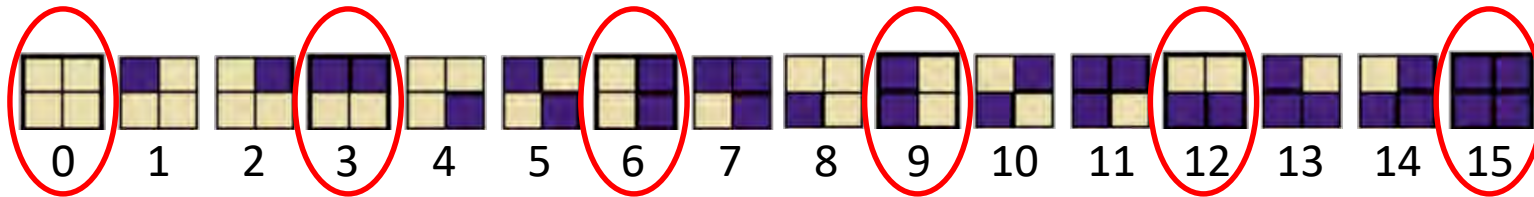
application	#qubits	# 2Q gates	# 1Q gates	fidelity	reference	collaborator
CNOT	2	1	3	99%	Nature 536, 63 (2016)	
QFT Phase est.	5	10	70-75	61.9%	Nature 536, 63 (2016)	
QFT period finding	5	10	70-75	695-97%	Nature 536, 63 (2016)	
Deutsch-Jozsa	5	1-4	13-34	93%-97%	Nature 536, 63 (2016)	
Bernstein-Vazirani	5	0-4	10-38	90%	Nature 536, 63 (2016)	
Hidden Shift	5	4	42-50	77%	PNAS 114, 13 (2017)	Microsoft
Grover Phase	3	10	35	85%	Nat. Comm. 8, 1918 (2017)	NSF
Grover Boolean	5	16	49	83%	Nat. Comm. 8, 1918 (2017)	NSF
Margolus	3	3	11	90%	PNAS 114, 13 (2017)	Microsoft
Toffoli	3	5	9	90%	PNAS 114, 13 (2017)	Microsoft
Toffoli-4	5	11	22	71%	Debnath Thesis	NSF
Fredkin Gate	3	7	14	86%	arXiv:1712.08581 (2017)	Intel
Fermi-Hubbard Sim.	5	31	132		arXiv:1712.08581 (2017)	Intel
Scrambling Test	7	15	30	75%	arXiv: 1806.02807 (2018)	Perimeter, UCB
Bayesian Games	5	5	15		Qu. Sci. Tech 3, 045002 (2018)	Army Res. Lab.
Machine Learning (detection)	5	n/a	n/a		arXiv:1801.07686 (2018)	JQI
Machine Learning (state synth)	4	5*N	30*N	90%	arXiv 1812.08862 (2018)	NASA
[[4,2,2]] Error Det.	5	6-7	20-25	98%-99.9%	Sci. Adv. 3, e1701074 (2017)	Duke
Full Adder	4	4	16	83%	In preparation (2018)	NSF
Simultaneous CNOT	4	2	8	94%	In preparation (2018)	NSF
Deuteron Simulation	3	35	30	<0.5% error	In preparation (2019)	ORNL
Circuit QAOA	7-9	42	50		In preparation (2019)	Perimeter, Intel

# Dynamical Circuits for Machine Learning

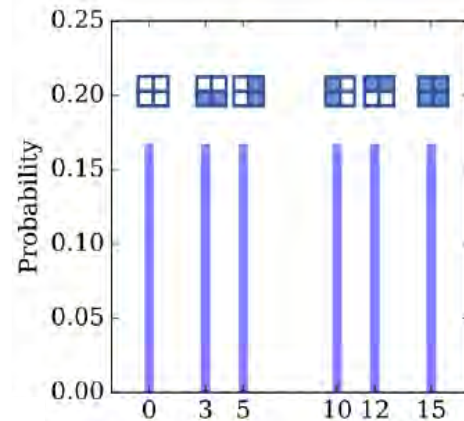
arXiv 1812.08862 (2018)  
with A. Perdomo-Ortiz (NASA)  
M. Benedetti (UC London)

see also E. Martinez et al., New J. Phys. 18, 063029 (2016)

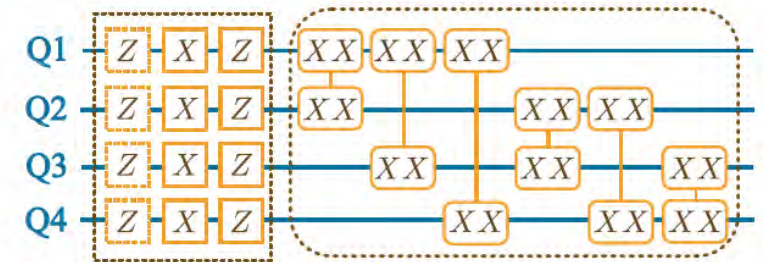
N=4 qubits encodes "Bars and Stripes" patterns



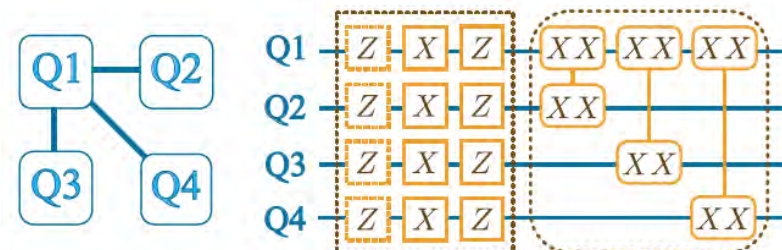
**Our task:**  
prepare equal  
superposition of  
all B&S states



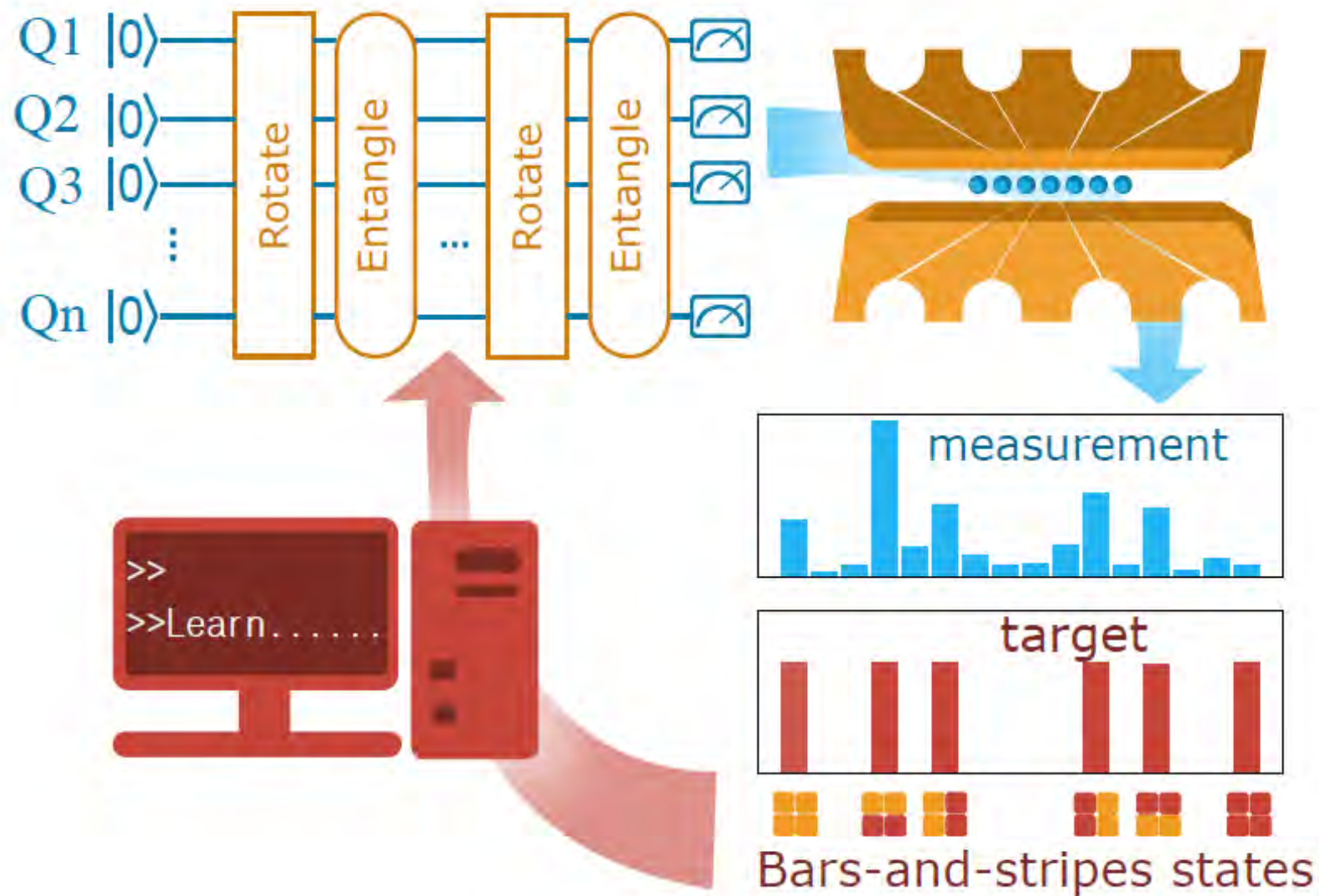
14 parameters



11 parameters

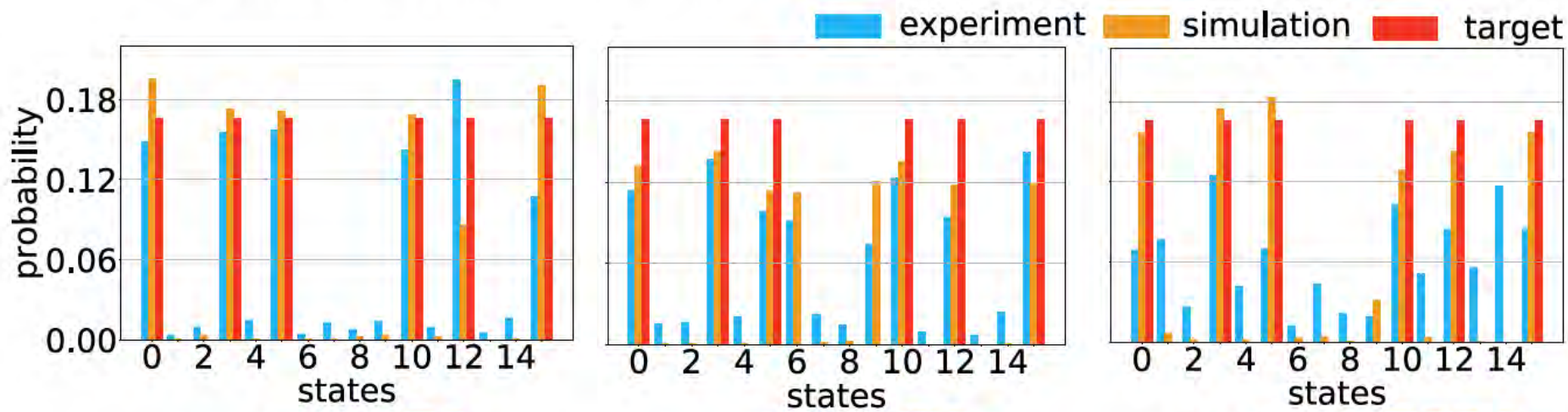
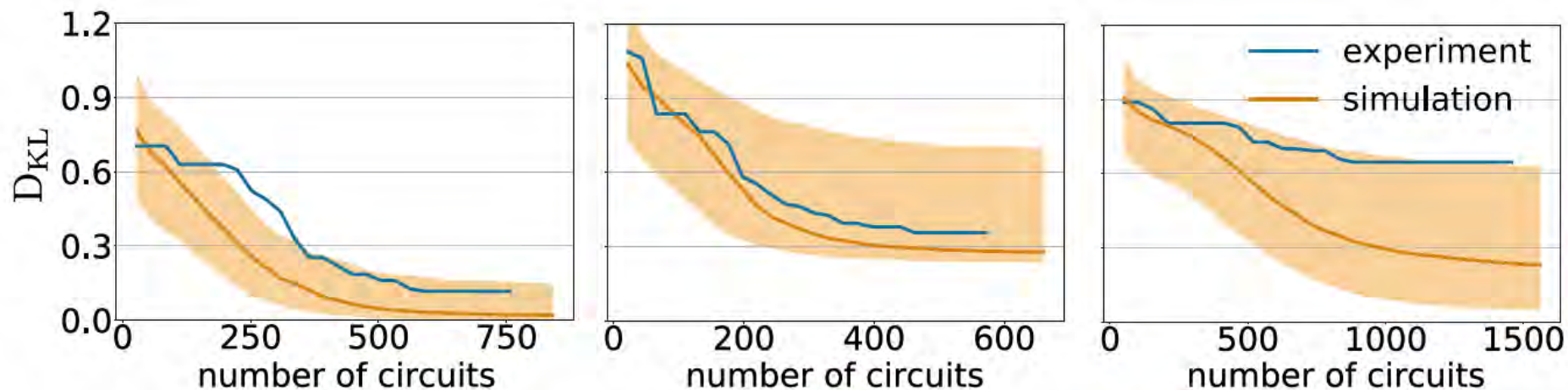


# Hybrid Quantum-Classical Learning Loop



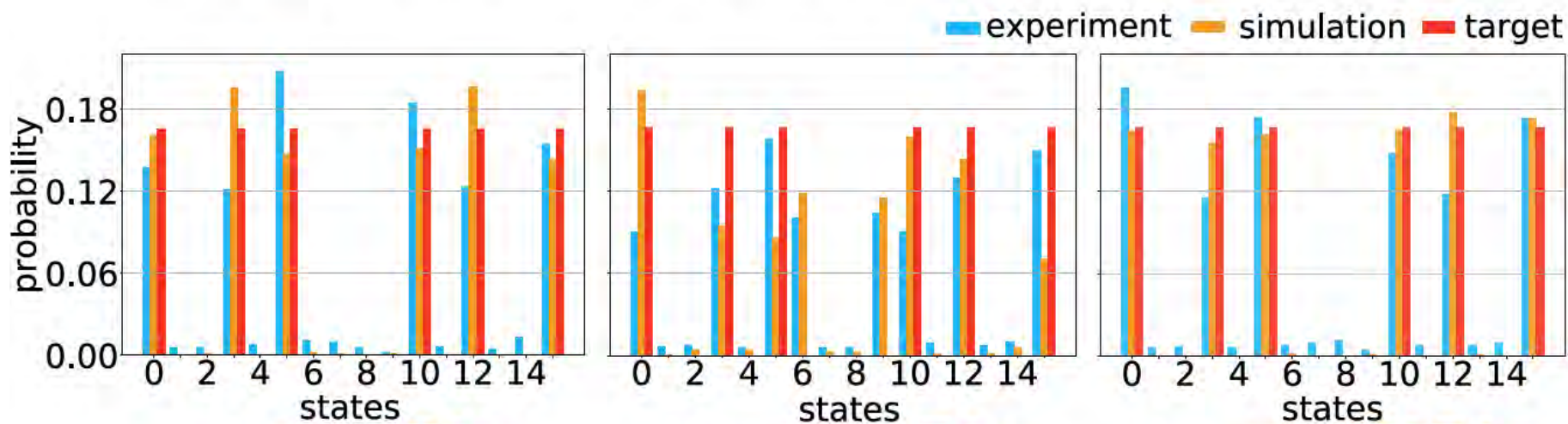
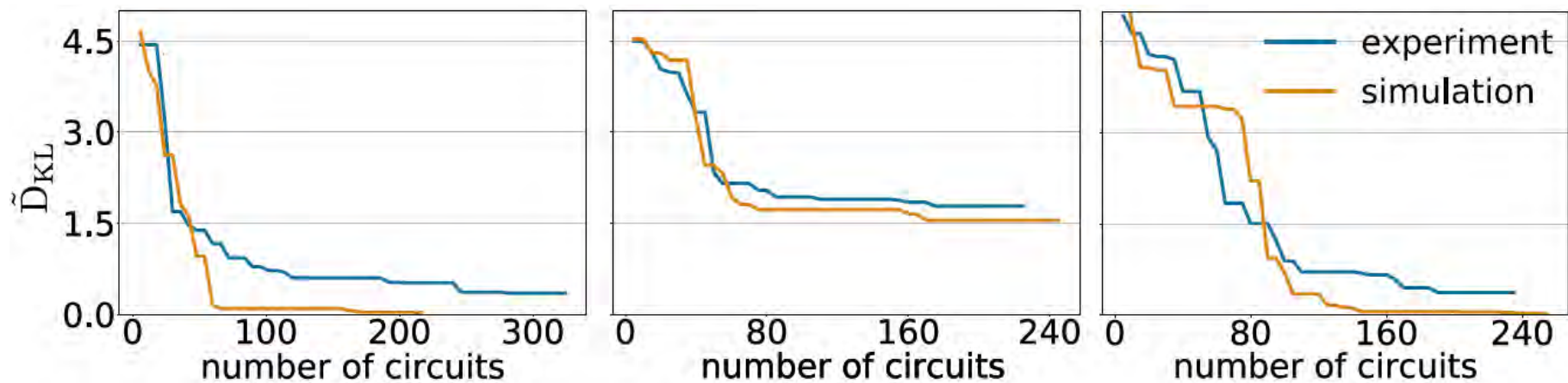
# Particle Swarm (classical) optimization

$\bar{D}_{KL}$ : Kullback-Leibler divergence



# Bayesian (classical) optimization

$\bar{D}_{KL}$ : Kullback-Leibler divergence

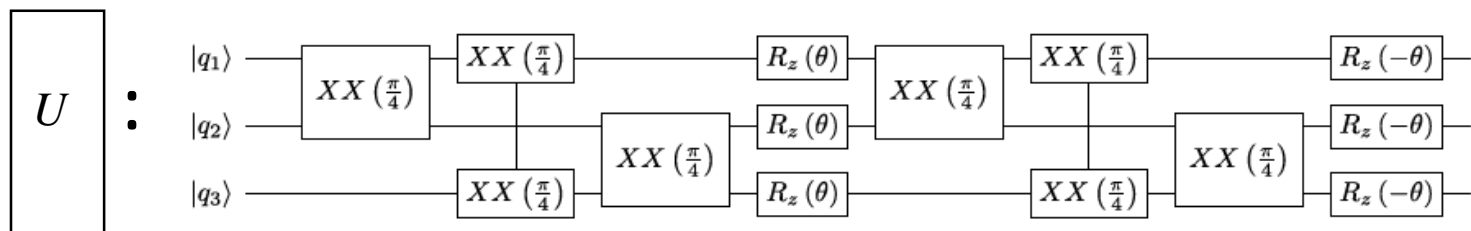
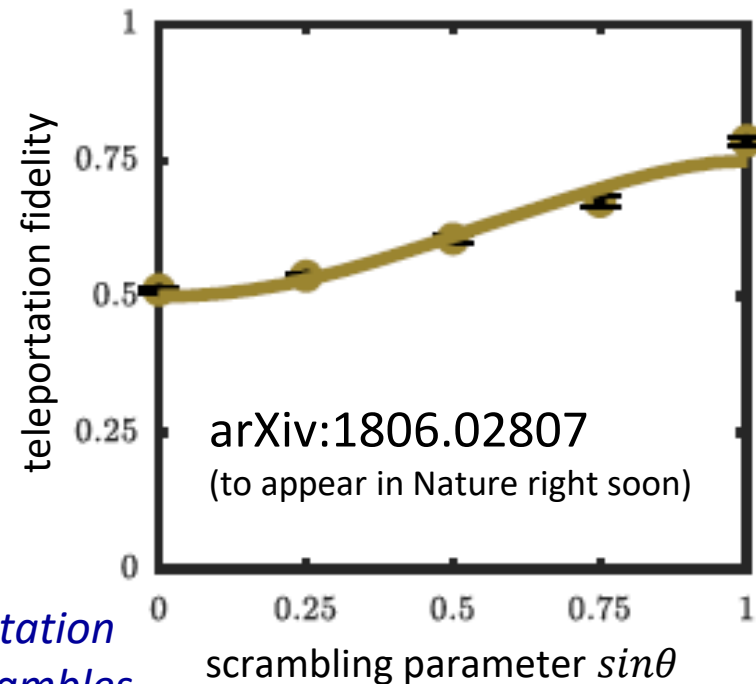
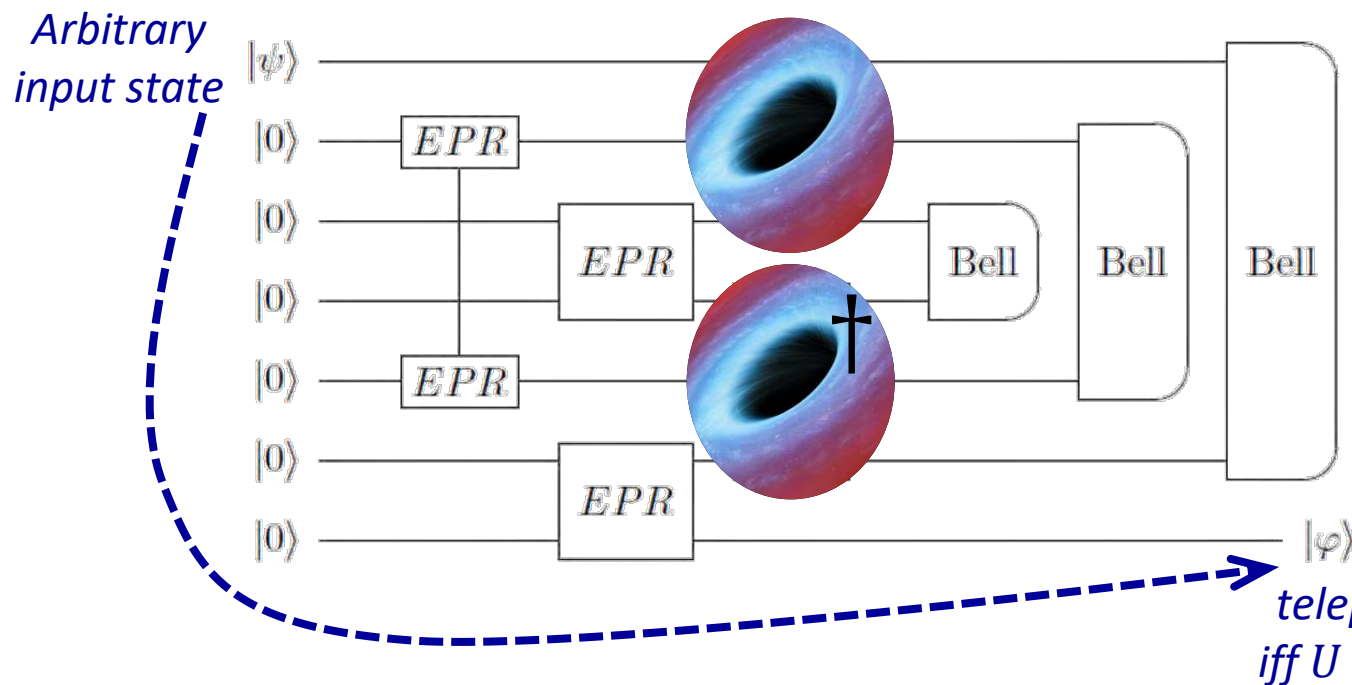


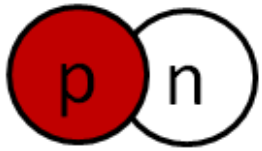
# Quantum Scrambling Litmus Test (7 qubit circuit)

N. Yao (UC Berkeley)  
 B. Yoshida (Perimeter)  
 arXiv:1803.10772

## Quantum scrambling

- The “complete diffusion” of entanglement within a system
- Relevant to information evolution in black holes  
*Hayden and Preskill, J. HEP 9, 120 (2007); Susskind and Zhao, arXiv:1707.04354 (2017)*
- OTOC measurements can be ambiguous





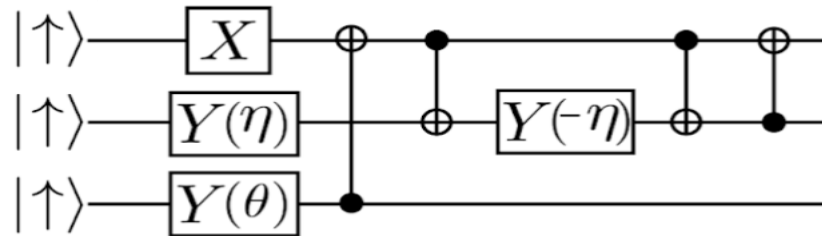
# Simulating the Ground State of the Deuteron

ORNL (R. Pooser, E. Dumitrescu, P. Lougovski, A. McCaskey)

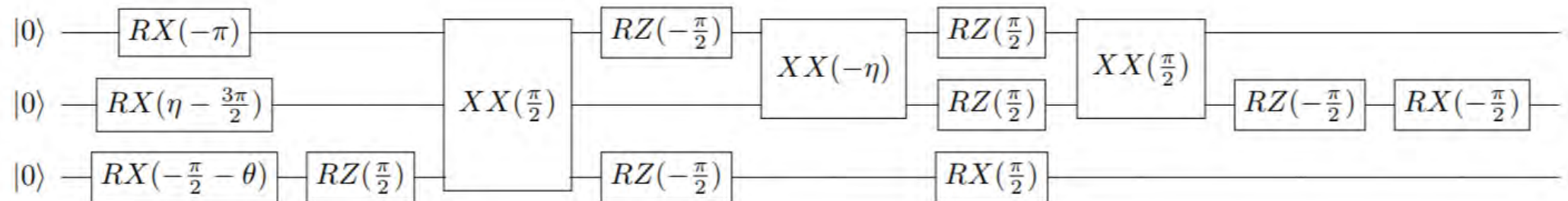
UMD (K. Landsman, N. Linke, D. Zhu, CM)

IonQ (Y. Nam, O. Shehab, CM)

canonical  
UCC ansatz

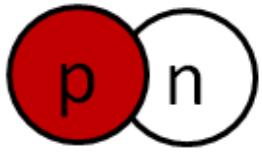


... compiled  
to our native  
gate set



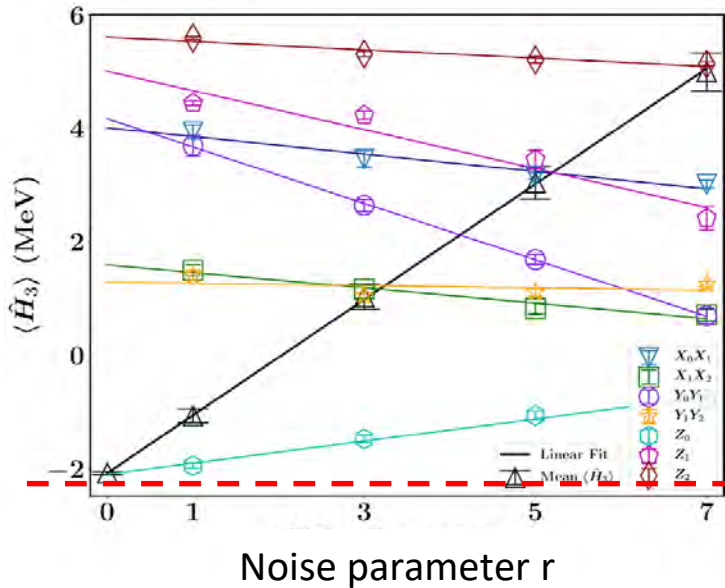
$$\begin{aligned}
 H = & (15.531709)I + (0.218291)Z_0 - (6.125)Z_1 - (9.625)Z_2 \\
 & - (2.143304)X_0X_1 - (2.143304)Y_0Y_1 - (3.913119)X_1X_2 - (3.913119)Y_1Y_2
 \end{aligned}$$





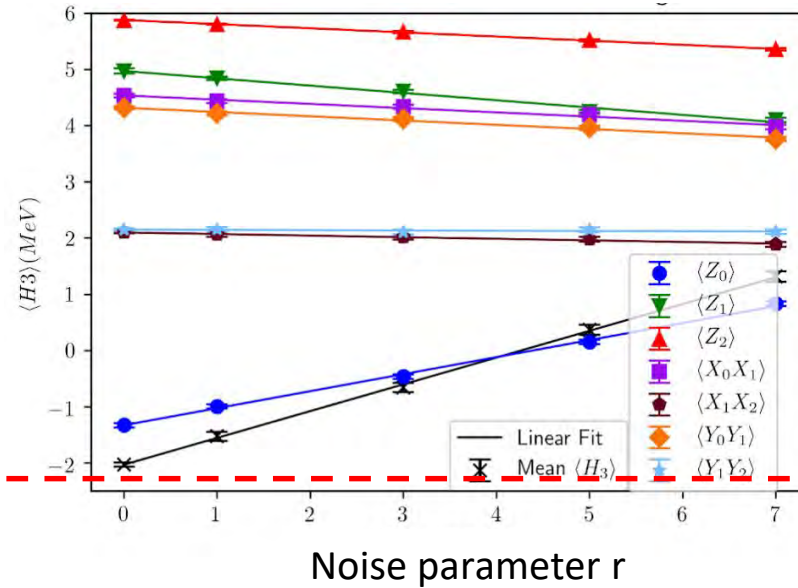
# Simulating the Ground State of the Deuteron

Extrapolated ground state energy for theoretically determined optimal angles (exact: -2.22 MeV):



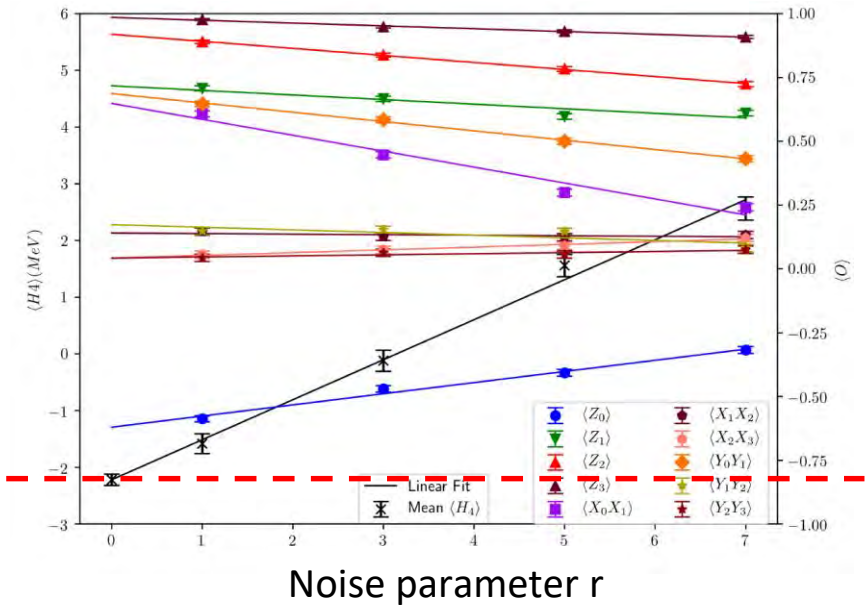
IBM 3-qubit ansatz  
3% error

E.F. Dumitrescu, et al., *Phys. Rev. Lett.* **120**, 210501 (2018)



UMD 3-qubit ansatz  
0.7% error

O. Shehab, et al. (in preparation)



UMD 4-qubit ansatz  
<0.5% error

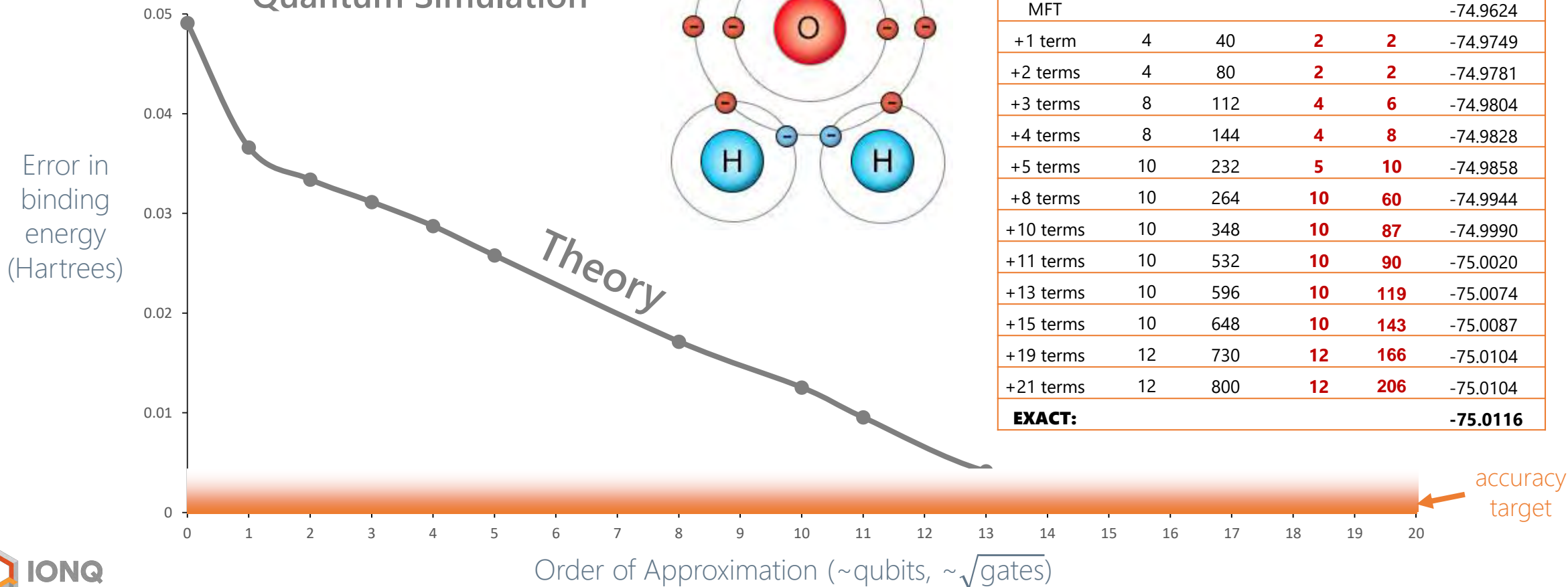
O. Shehab, et al. (in preparation)

(Note: implementing 3-qubit ansatz on Rigetti system was not possible)

# Variational Circuit Simulation of H<sub>2</sub>O

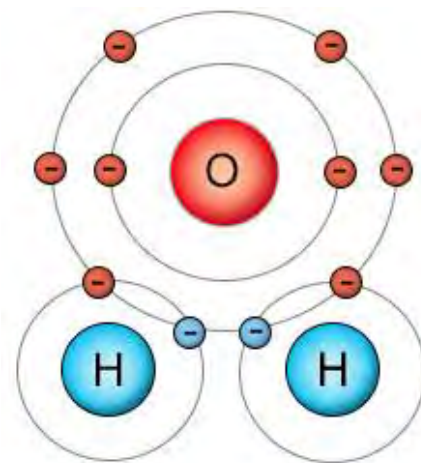
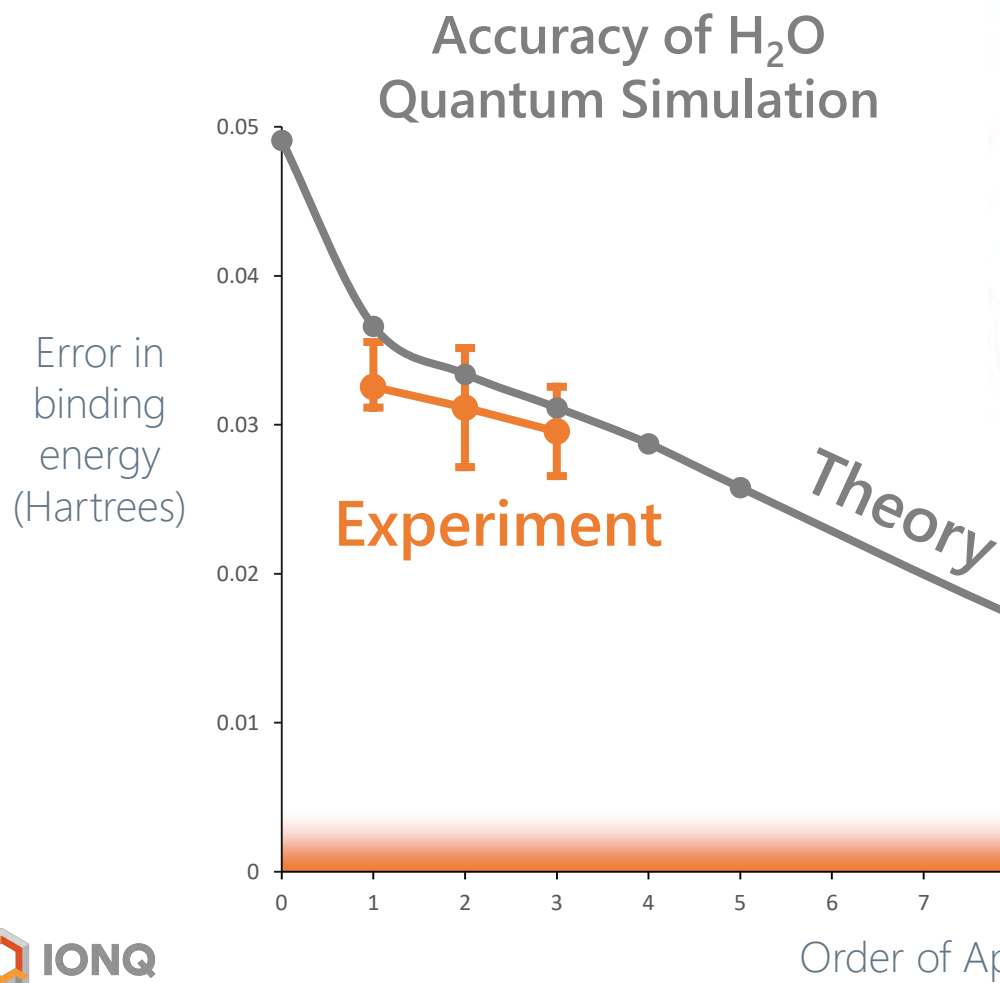
*The Theory of Variational Hybrid Quantum-Classical Algorithms*, New J. Phys. **18**, 023023 (2016) [Aspuru-Guzik group]

Accuracy of H<sub>2</sub>O  
Quantum Simulation



# Variational Circuit Simulation of H<sub>2</sub>O

*The Theory of Variational Hybrid Quantum-Classical Algorithms*, New J. Phys. **18**, 023023 (2016) [Aspuru-Guzik group]

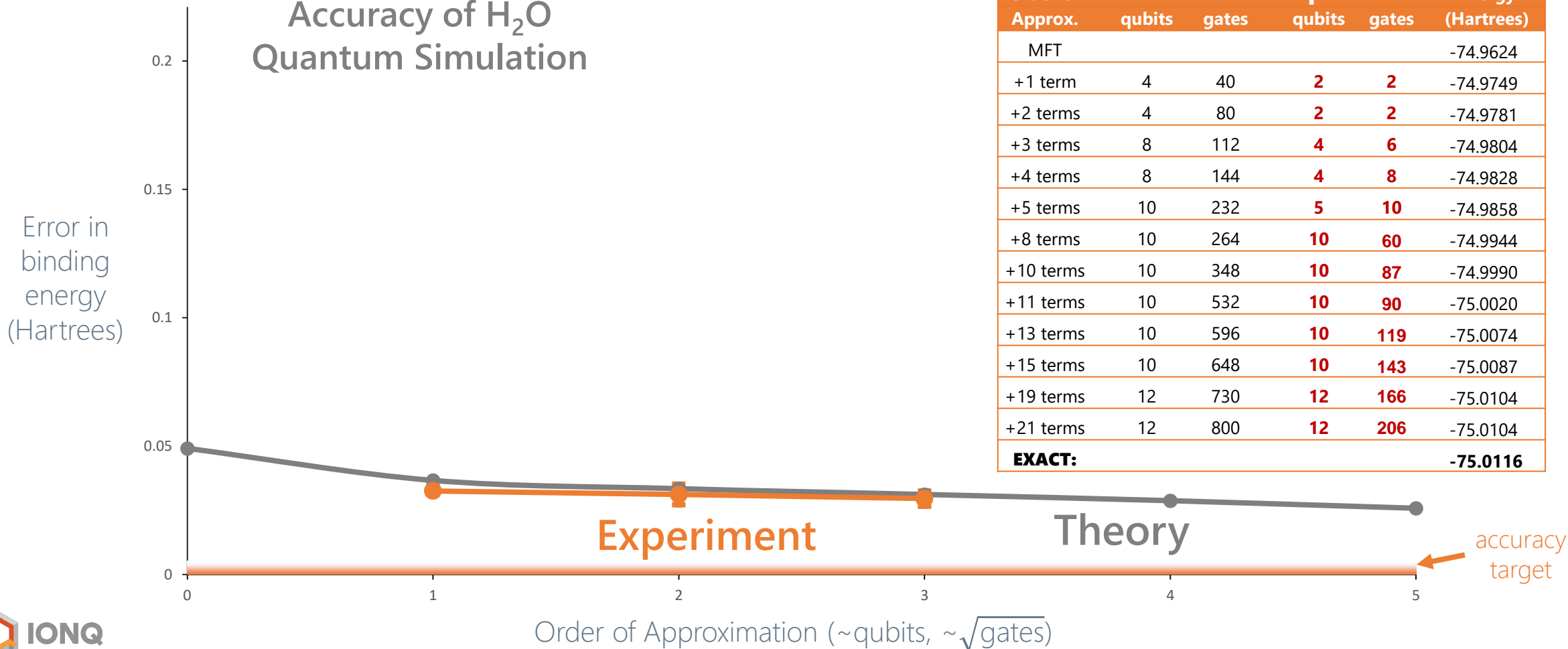


Order of Approx.	Naive qubits	Naive gates	Optimized qubits	Optimized gates	Binding Energy (Hartrees)
MFT					-74.9624
+1 term	4	40	2	2	-74.9749
+2 terms	4	80	2	2	-74.9781
+3 terms	8	112	4	6	-74.9804
+4 terms	8	144	4	8	-74.9828
+5 terms	10	232	5	10	-74.9858
+8 terms	10	264	10	60	-74.9944
+10 terms	10	348	10	87	-74.9990
+11 terms	10	532	10	90	-75.0020
+13 terms	10	596	10	119	-75.0074
+15 terms	10	648	10	143	-75.0087
+19 terms	12	730	12	166	-75.0104
+21 terms	12	800	12	206	-75.0104
<b>EXACT:</b>					<b>-75.0116</b>

# Variational Circuit Simulation of H<sub>2</sub>O

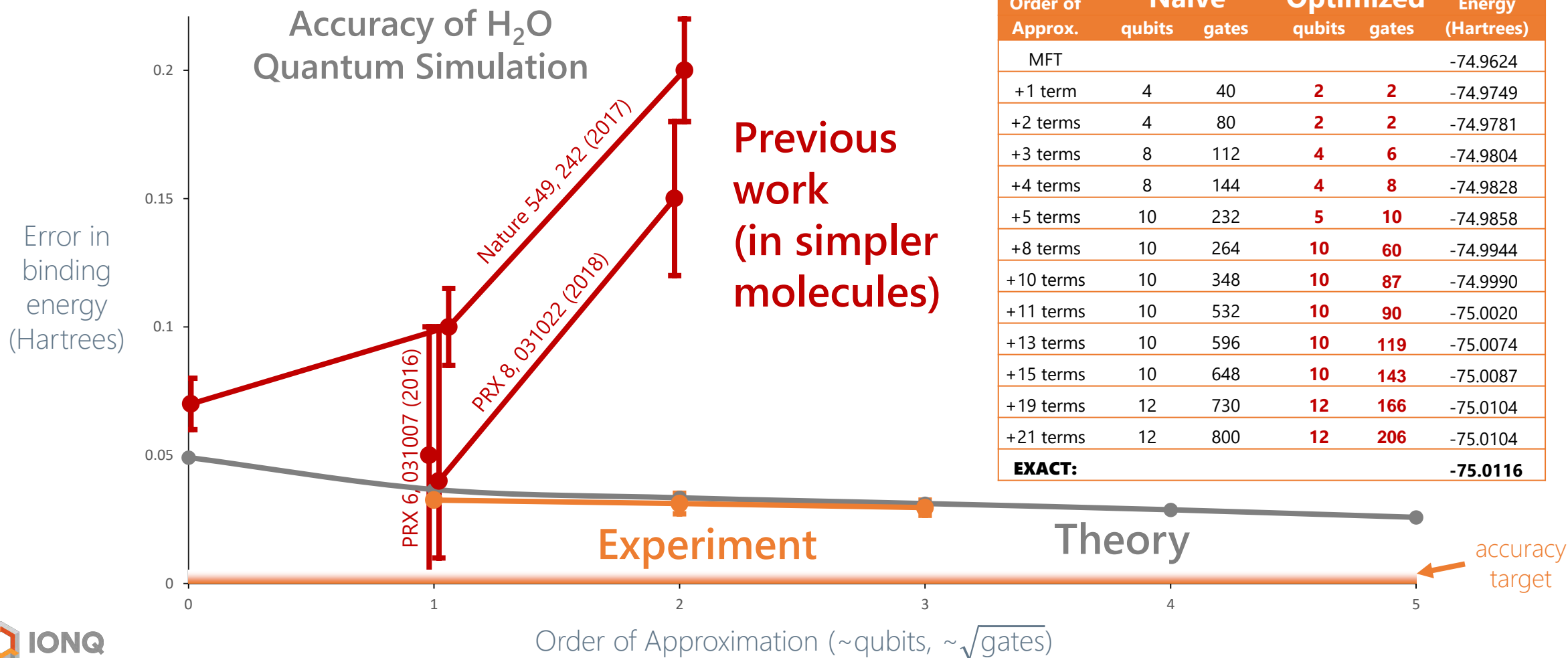
*The Theory of Variational Hybrid Quantum-Classical Algorithms*, New J. Phys. **18**, 023023 (2016) [Aspuru-Guzik group]

### Accuracy of H<sub>2</sub>O Quantum Simulation



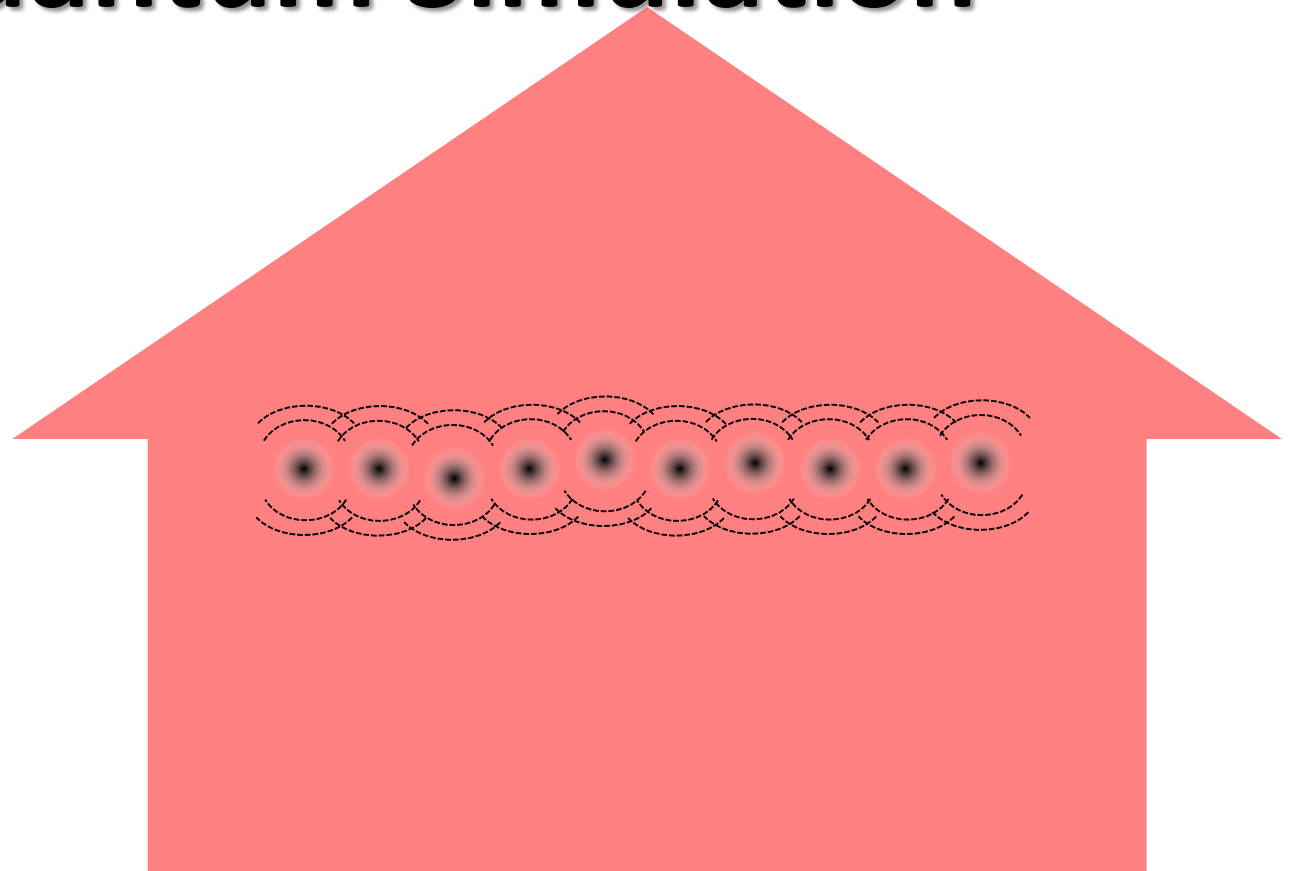
# Variational Circuit Simulation of H<sub>2</sub>O

*The Theory of Variational Hybrid Quantum-Classical Algorithms*, New J. Phys. **18**, 023023 (2016) [Aspuru-Guzik group]

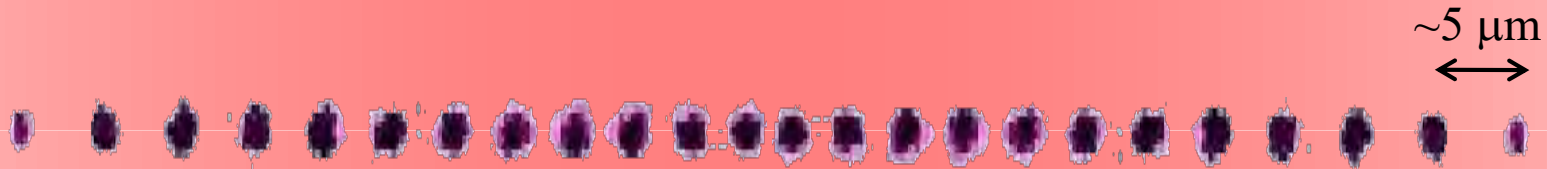


Order of Approx.	Naive qubits	Naive gates	Optimized qubits	Optimized gates	Binding Energy (Hartrees)
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+5 terms	10	232	5	10	-74.9858
+8 terms	10	264	10	60	-74.9944
+10 terms	10	348	10	87	-74.9990
+11 terms	10	532	10	90	-75.0020
+13 terms	10	596	10	119	-75.0074
+15 terms	10	648	10	143	-75.0087
+19 terms	12	730	12	166	-75.0104
+21 terms	12	800	12	206	-75.0104
<b>EXACT:</b>					<b>-75.0116</b>

# **(Analog) Quantum Simulation**



# Global Entanglement of Trapped Ion Qubits



Long-range Ising Hamiltonian

$$H = \sum_{i < j} \frac{J_0}{|i - j|^\alpha} \sigma_x^i \sigma_x^j + B \sum_i \sigma_y^i \quad J_{ij} = \frac{J_0}{|i - j|^\alpha} \quad \begin{array}{l} 0 < \alpha < 3 \\ J_0 \sim 2\pi(1 \text{ kHz}) \\ J_0\tau \sim 50 \end{array}$$

Porras and Cirac (2003)  
Schaetz group [2 ions] (2008)  
UMD [3-50 ions] (2008-)  
Innsbruck [5-20 ions] (2012-)

# Quantum Simulations

$$H = \sum_{i < j} \frac{J_0}{|i - j|^\alpha} \sigma_x^i \sigma_x^j + \sum_i B_i \sigma_y^i$$

## FM and AFM order

R. Islam, et al., *Science* **340**, 583 (2013)

## Breakup of Ising ordering: Devil's Staircase

P. Richerme et. al., *Phys. Rev. Lett.* **111**, 100506 (2013)

## Propagation of correlations and entanglement

P. Richerme et. al., *Nature* **511**, 198 (2014)

P. Jurcevic et al., *Nature* **511**, 202 (2014)

## Many-Body Spectroscopy

C. Senko et. al., *Science* **345**, 430 (2014)

P. Jurcevic, et al., *Phys. Rev. Lett.* **115**, 100501 (2015)

## Spin-1 Dynamics

C. Senko, et al., *Phys. Rev. X* **5**, 021026 (2015)

## Quantum Prethermalization/Manybody Localization

J. Smith, et al., *Nature Physics* **12**, 894 (2016)

B. Neyenhuis, et al., *Science Adv.* **3**, e1700672 (2017)

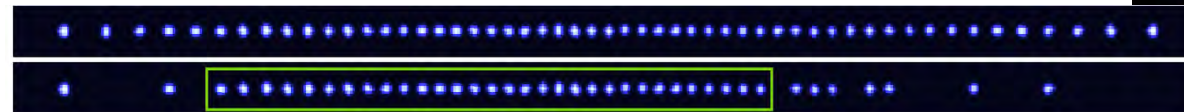
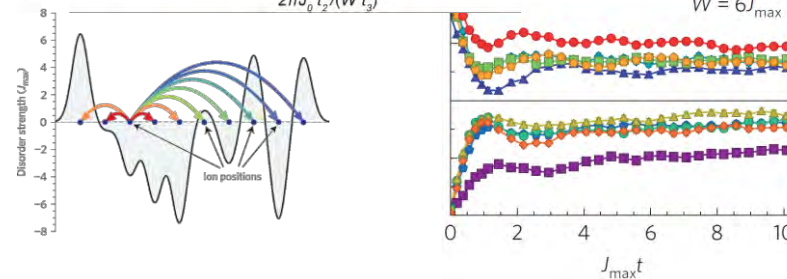
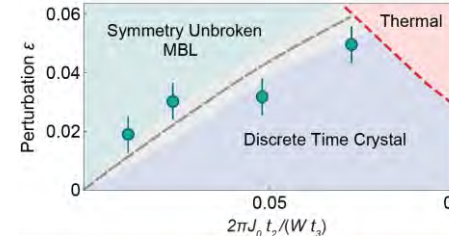
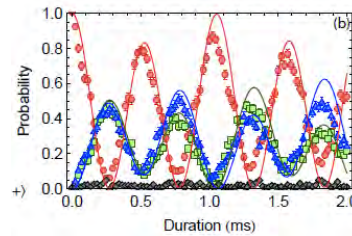
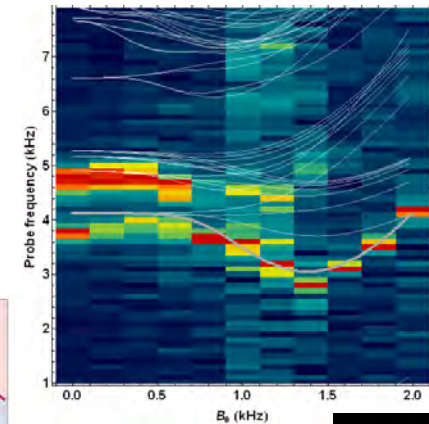
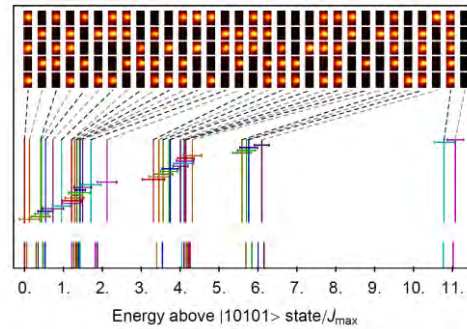
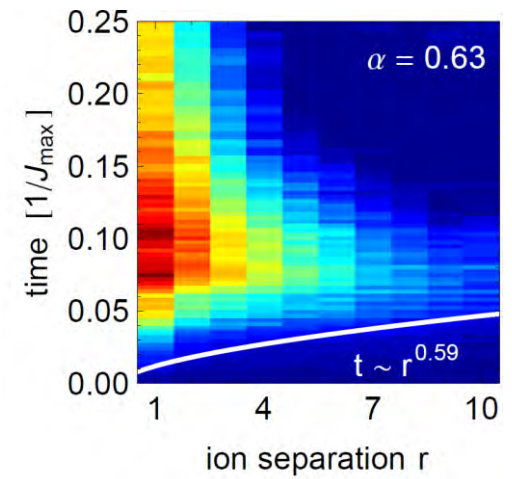
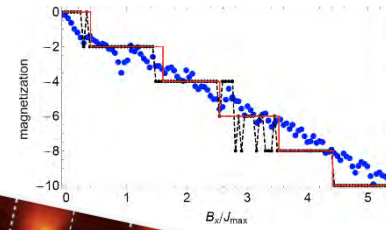
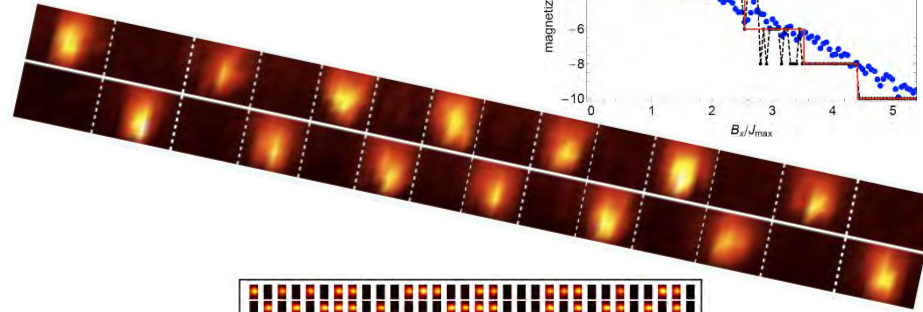
## Observation of a Time Crystal

J. Zhang, et al., *Nature* **543**, 217 (2017)

## Dynamical Phase Transition

P. Jurcevic, et al., *Phys. Rev. Lett.* **119**, 080501 (2017)

J. Zhang, et al., *Nature* **551**, 601 (2017)





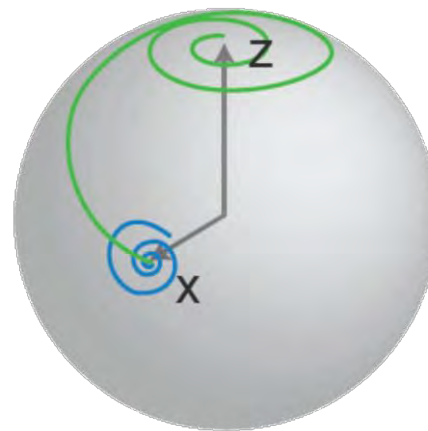
# Dynamical Phase Transition with 50+ Qubits

(1) Prepare spins along  $x$

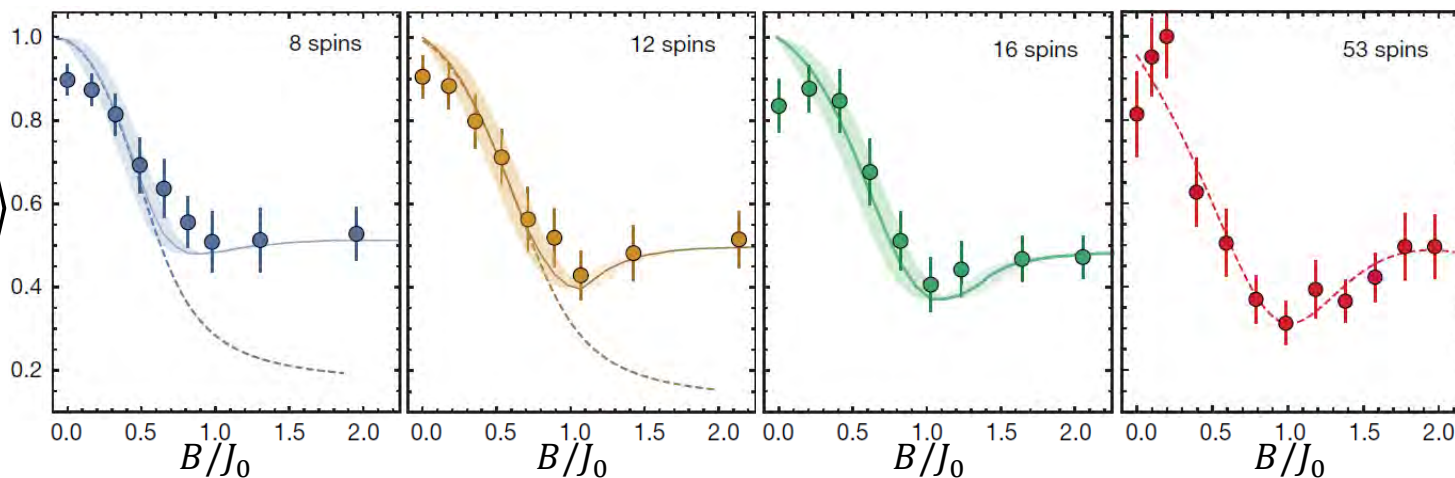
(2) Quench spins to

(3) Measure along  $x$

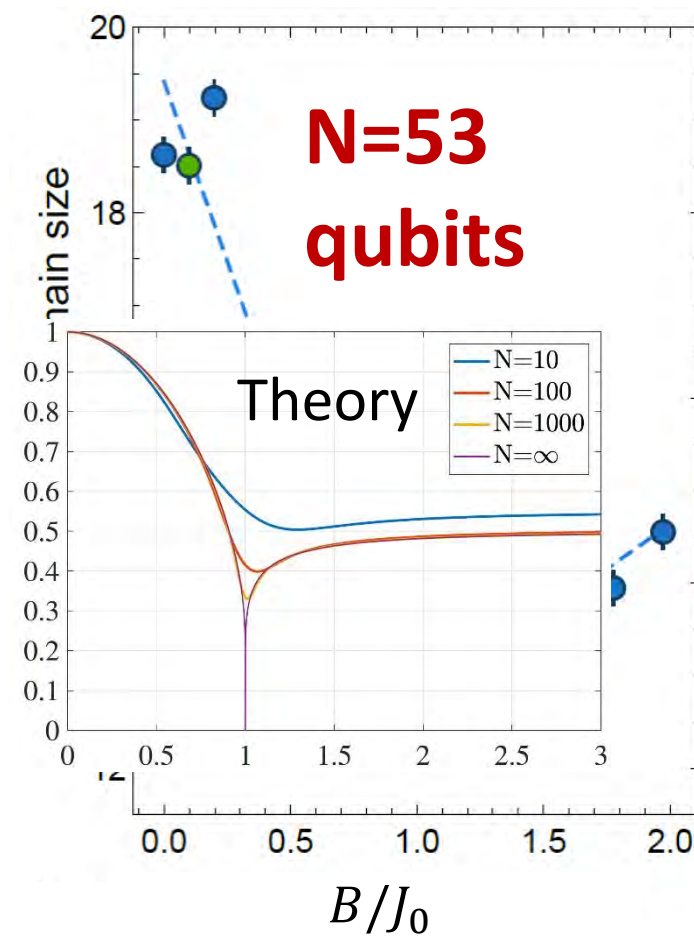
$$H = \sum_{i < j} \frac{J_0}{|i - j|^\alpha} \sigma_x^i \sigma_x^j + B \sum_i \sigma_z^i$$



$$\frac{1}{N^2} \sum_{ij} \langle \sigma_x^i \sigma_x^j \rangle$$



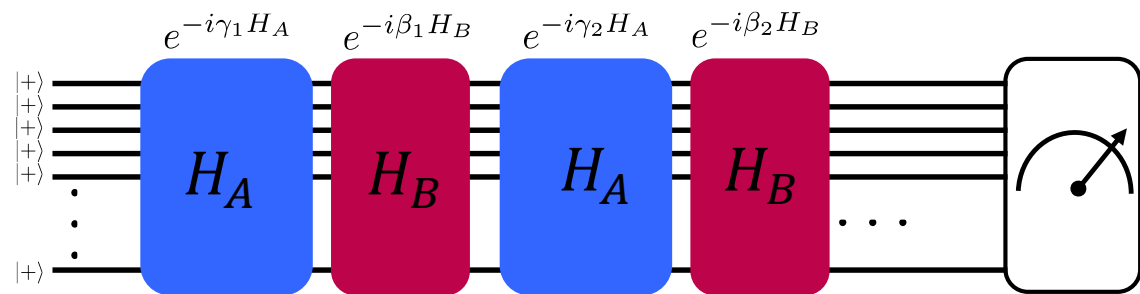
see also: P. Jurcevic, et al., *PRL* **119**, 080501 (2017)



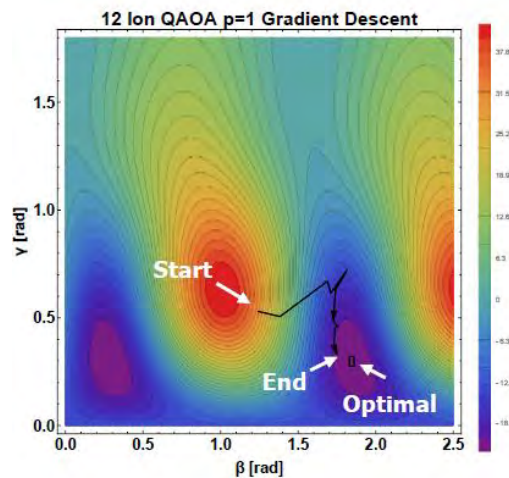
# Quantum Approximate Optimization Algorithm (QAOA)

Goal: create (approximate) ground state of  $H = \underbrace{\sum_{i<j} \frac{J_0}{|i-j|^\alpha} \sigma_x^i \sigma_x^j}_{H_A} + B \underbrace{\sum_i \sigma_y^i}_{H_B}$

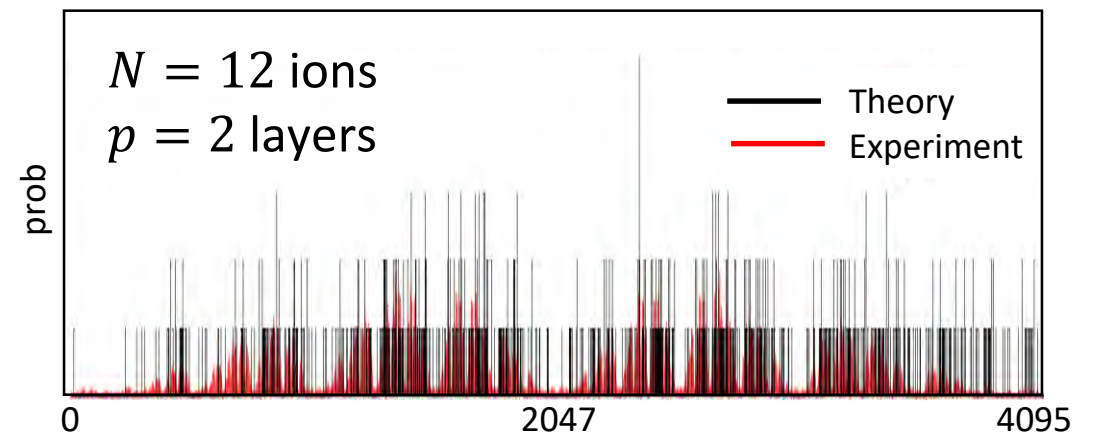
- (1) Prepare the ground state of  $H_B$
- (2) Alternate  $H_A$  and  $H_B$  for  $p$  "layers" with evolution angles  $\{\vec{\gamma}, \vec{\beta}\}$
- (3) Measure the the energy or complete state distribution
- (4) Optimize  $\{\vec{\gamma}, \vec{\beta}\}$  to minimize  $\langle H \rangle$



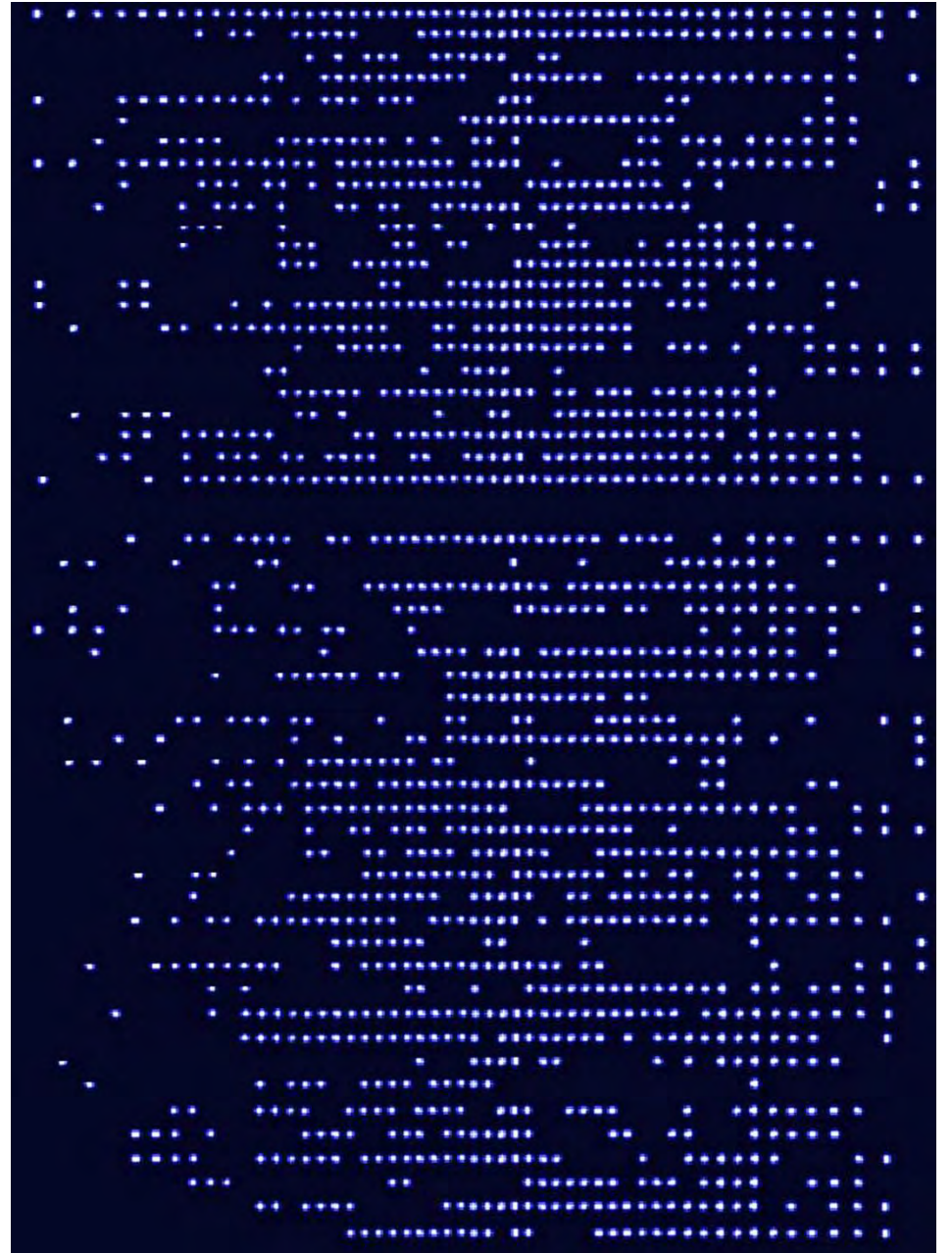
$N = 12$  ions  
 $p = 1$  layer



State distribution

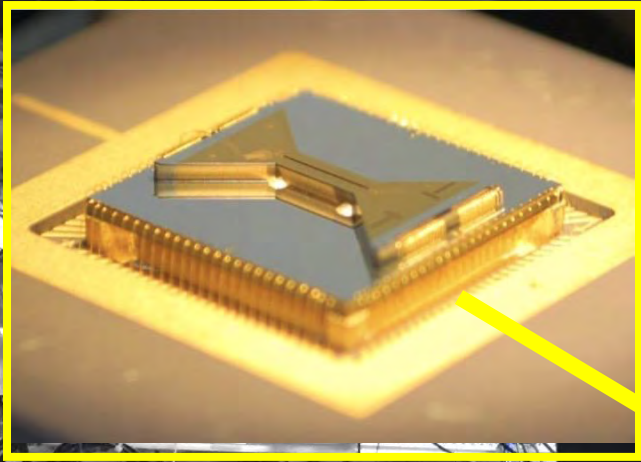


# Scaling the System



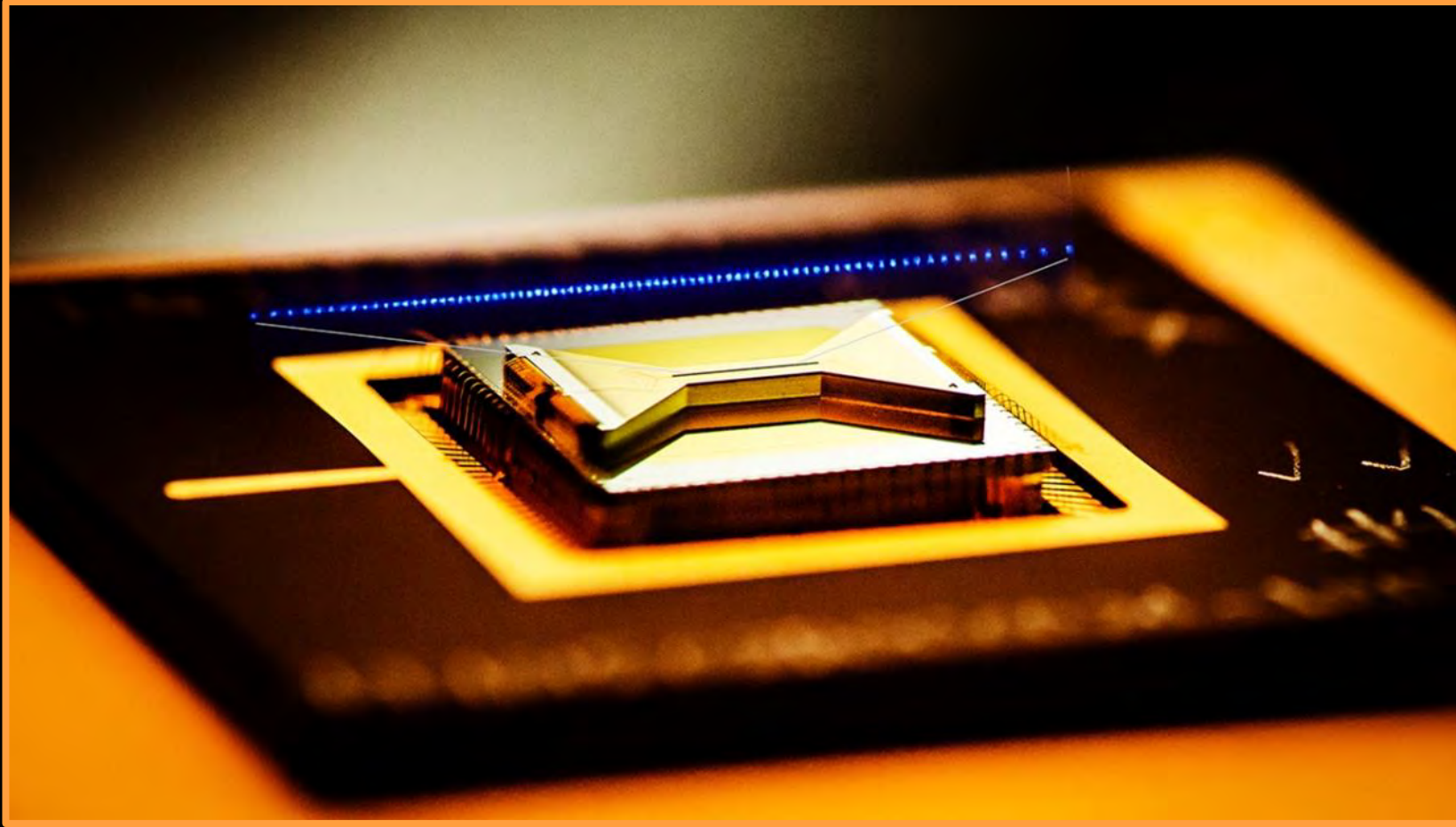
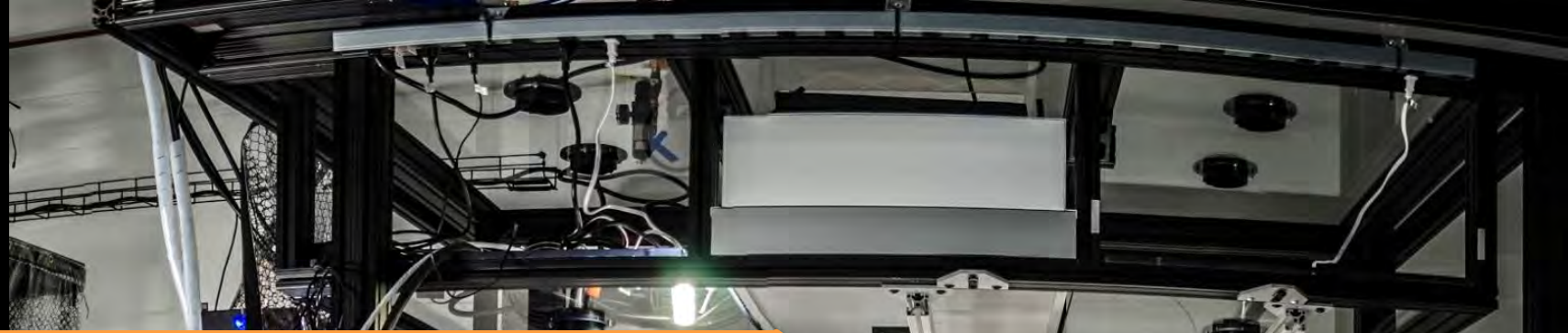


Ion Trap Lab at  
JQI-Maryland





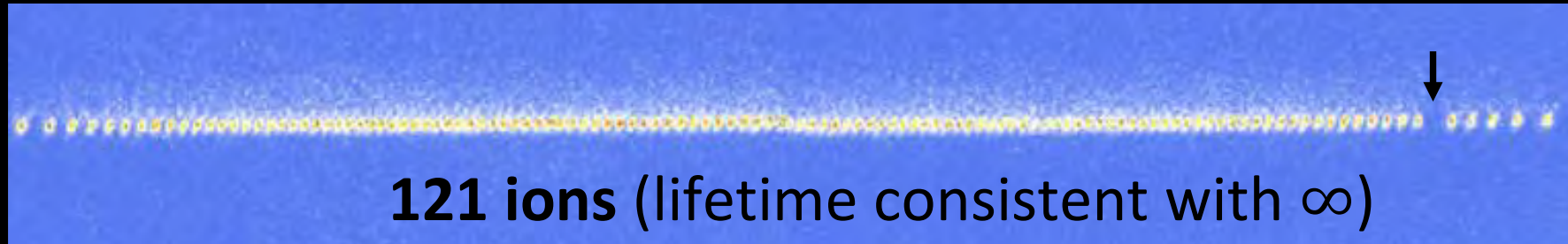
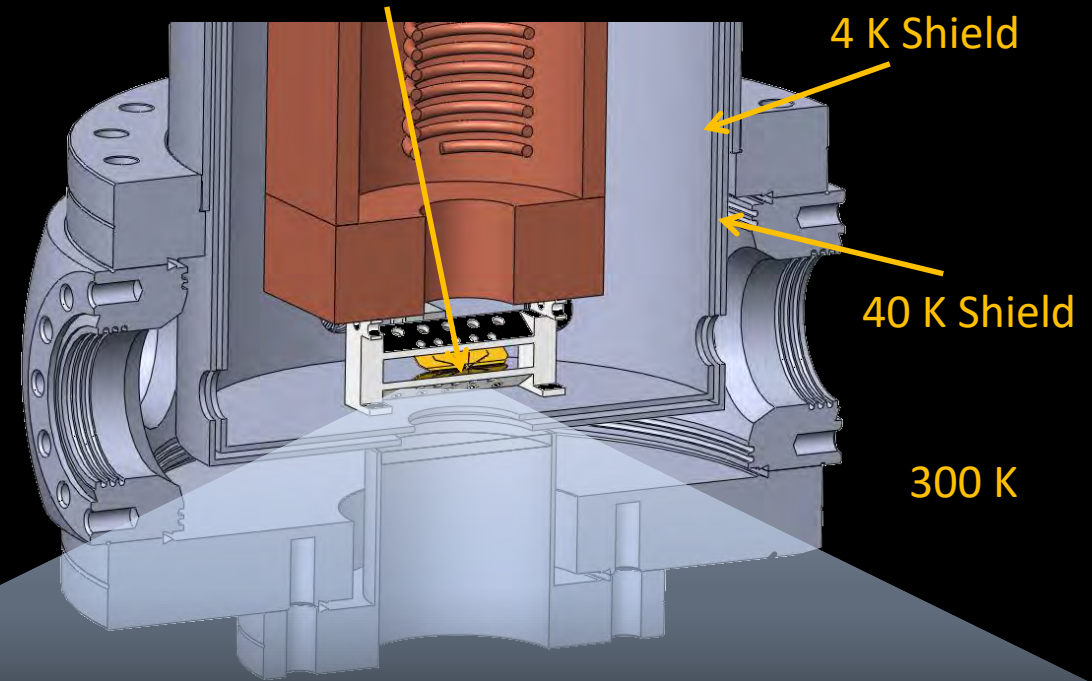
# IONQ System1



# 4K environment (better vacuum!)

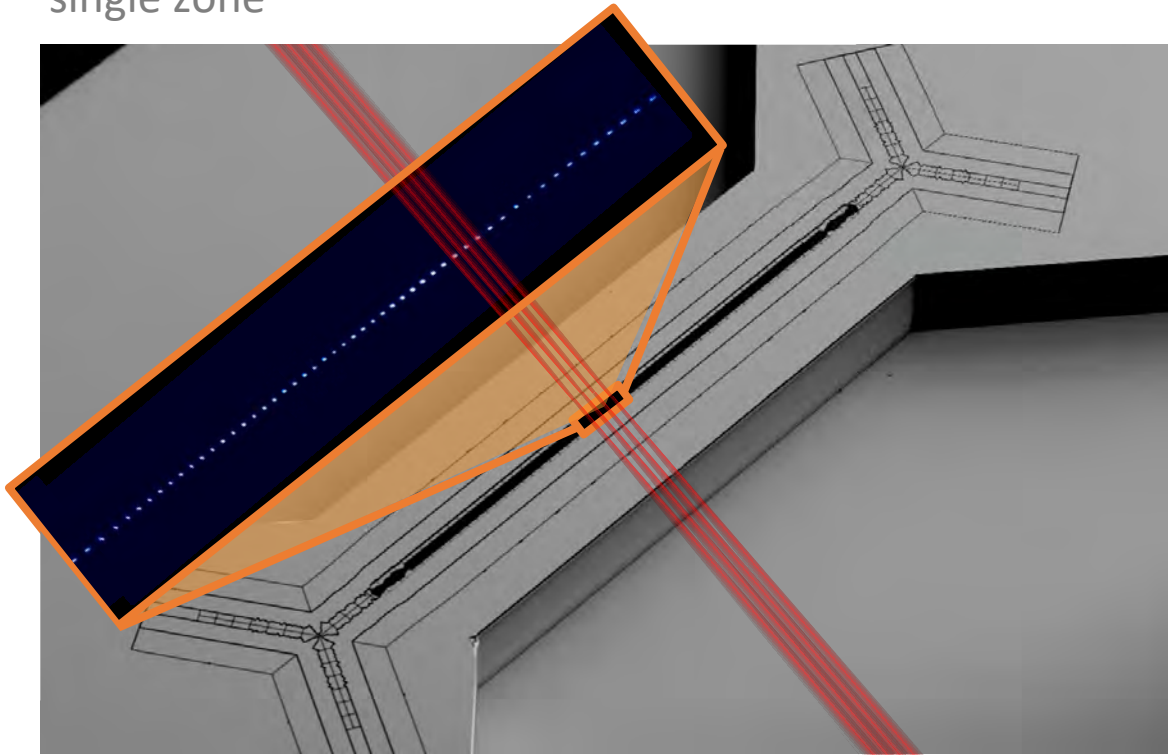


5-segment linear rf ion trap  
(Au on  $\text{Al}_2\text{O}_3$  blades,  $200\mu\text{m}$ )

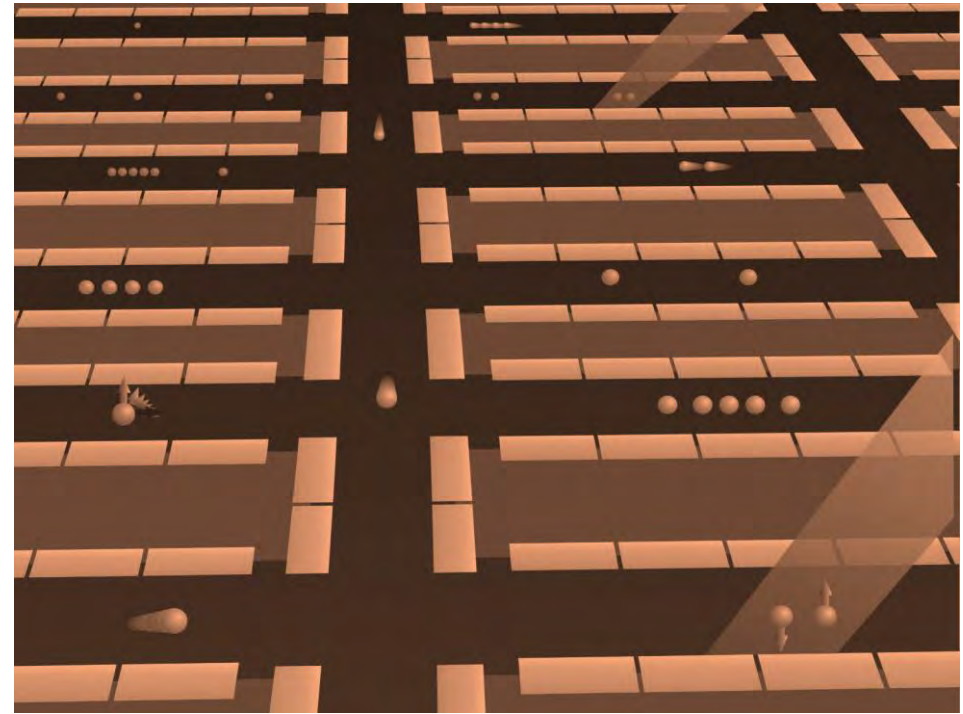


# Scaling to 100-1000s of Qubits

Linear shuttling through single zone



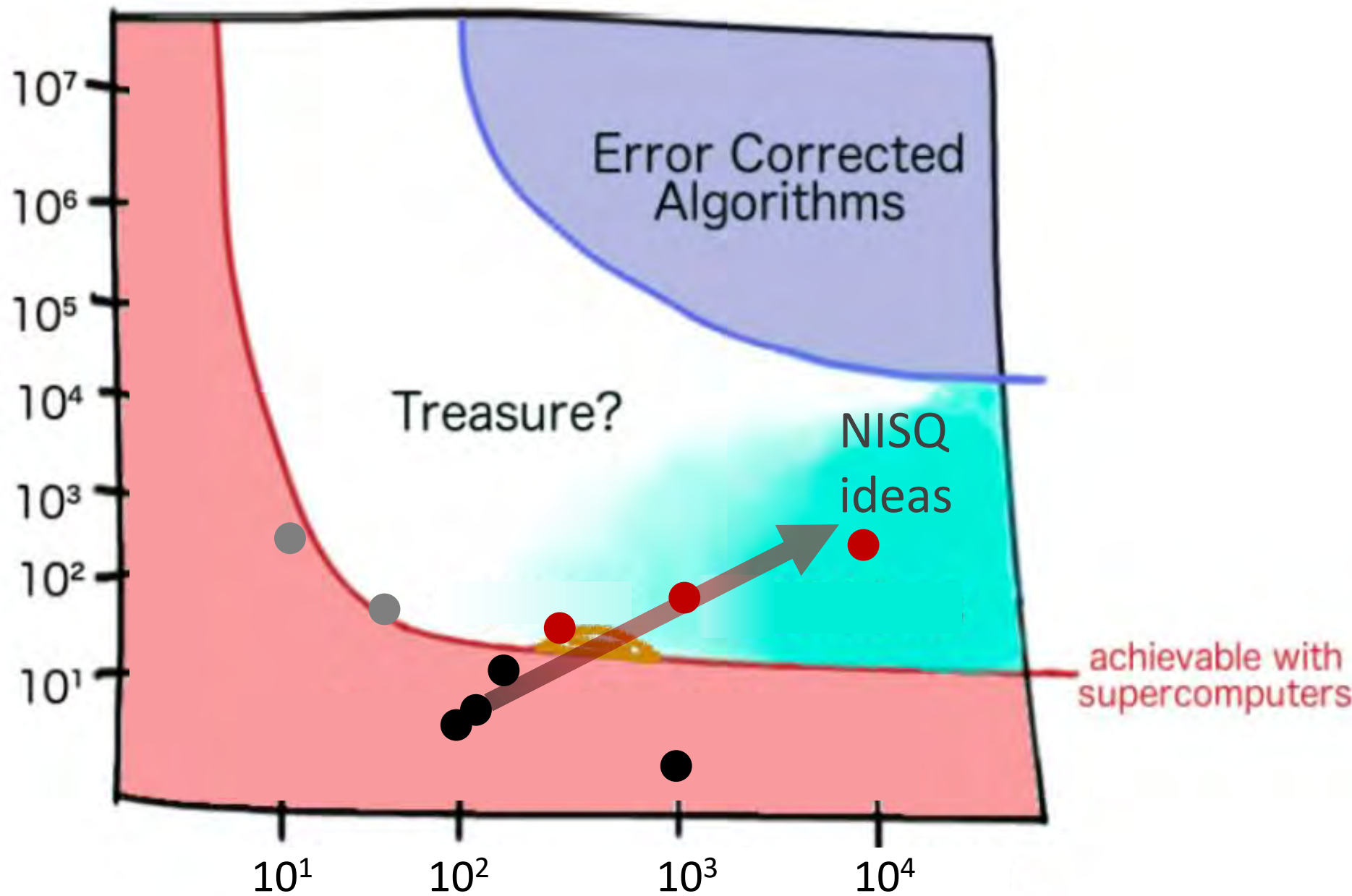
Modular shuttling between multiple zones



Kielpinski, Monroe, Wineland, Nature 417, 709 (2002)  
Leikesh, et al., Science Advances 3, e1601540 (2017)



Qubits



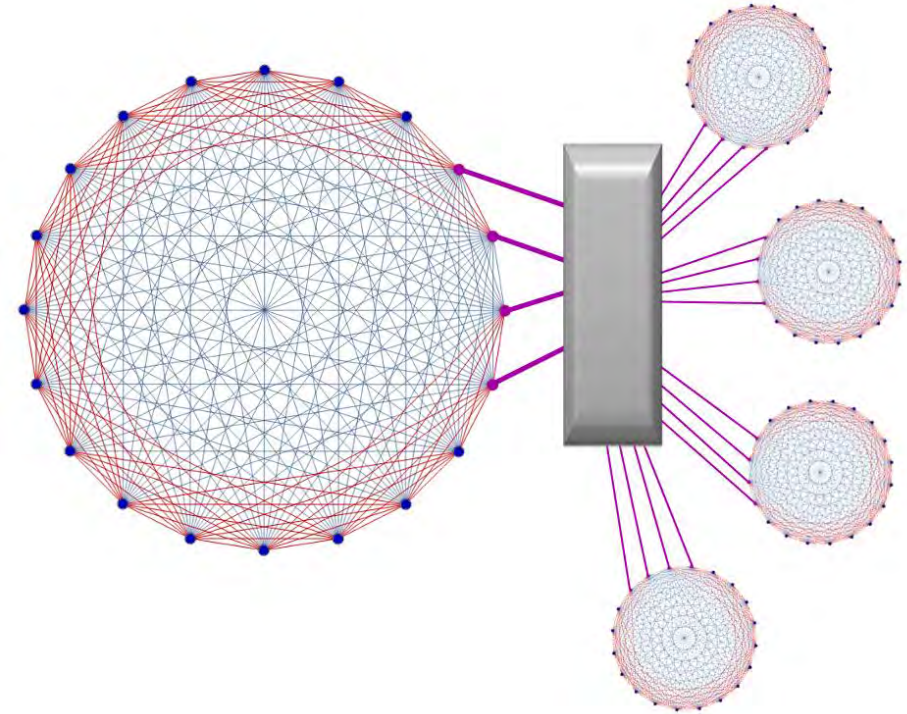
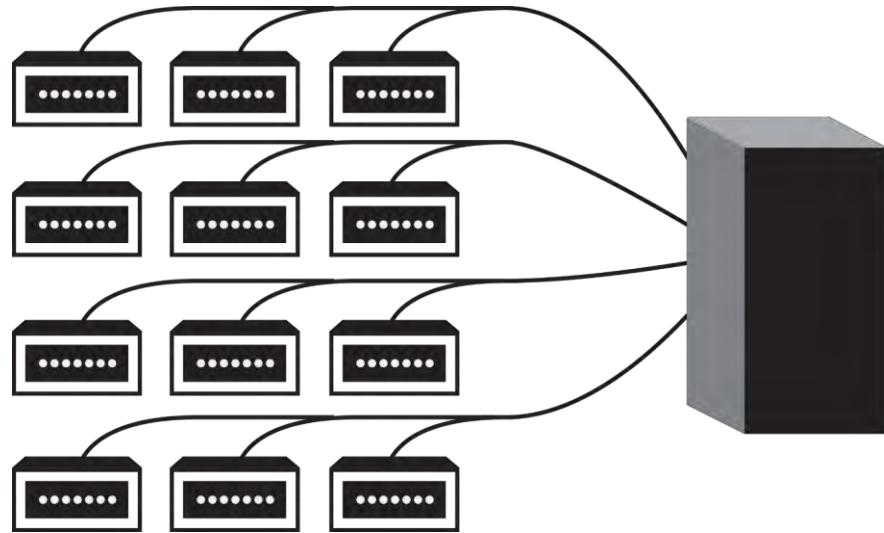
- ion trap (existing)
- Ion trap (limited control)
- ion trap (projected)

Circuit Depth

Background pic from H. Neven (Google)

# Scaling beyond 1000s of Qubits: photonic

## Modular optical interconnects



Duan and Monroe, *Rev. Mod. Phys.* **82**, 1209 (2010)

Li and Benjamin, *New J. Phys.* **14**, 093008 (2012)

Monroe, et al., *Phys. Rev. A* **89**, 022317 (2014)



# Trapped Ion

[www.iontrap.umd.edu](http://www.iontrap.umd.edu)

# Quantum Information



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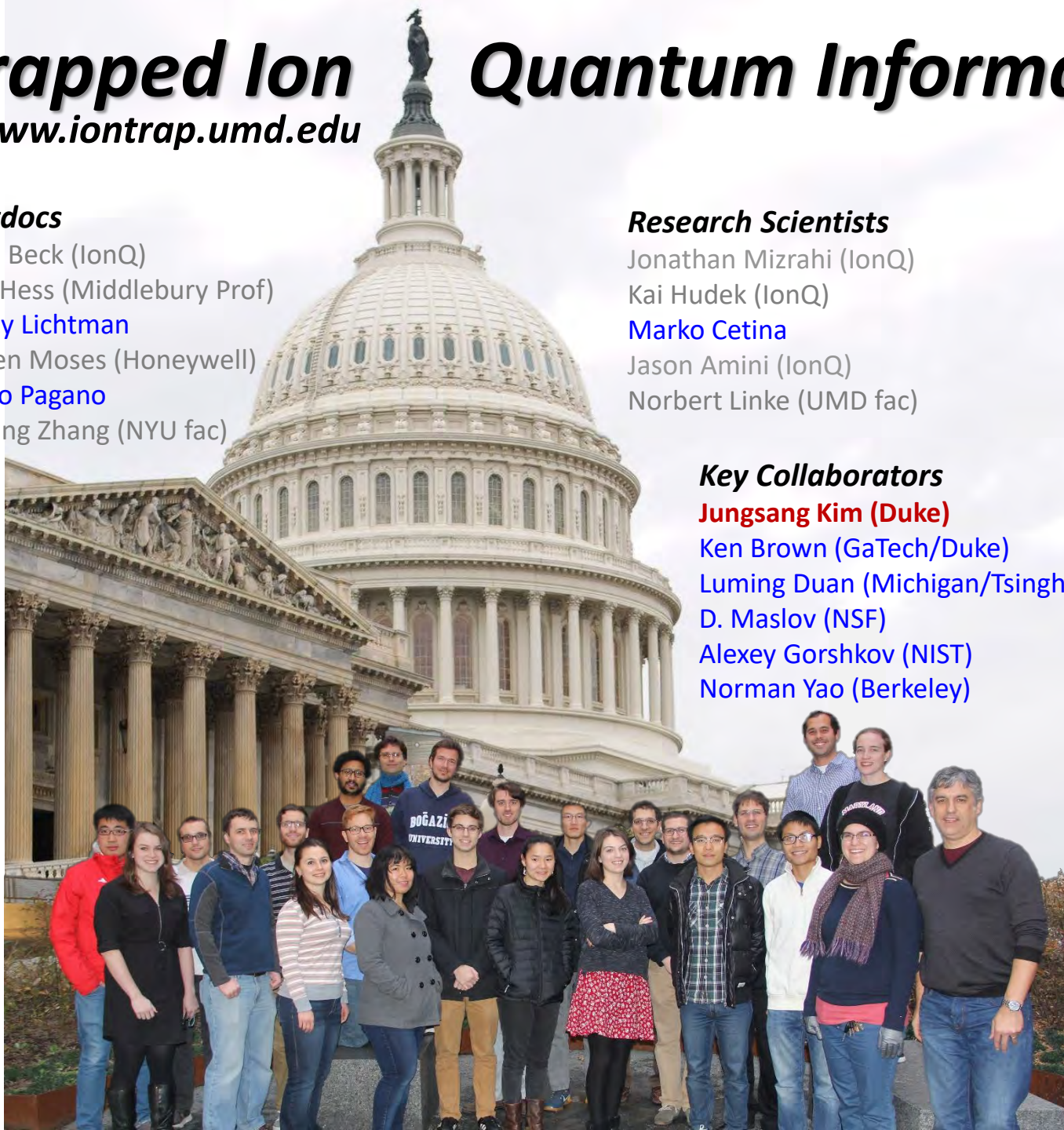
- Kristi Beck (IonQ)
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