Qiskit workshop for PC5228

Junye Huang

Quantum Developer Advocate

IBM **Quantum**

Schedule

IBM **Quantum**

Date	Start	End	Subject
21 Aug	12:00	13:30	Introduction to Qiskit and IBM Quantum Experience
18 Sep	12:00	14:00	Quantum algorithms: Deutsch-Jozsa and Grover algorithm
6 Nov	12:00	14:00	Quantum applications: Simulating Molecules using Variational Quantum Eigensolver (VQE)

All sessions will be recorded

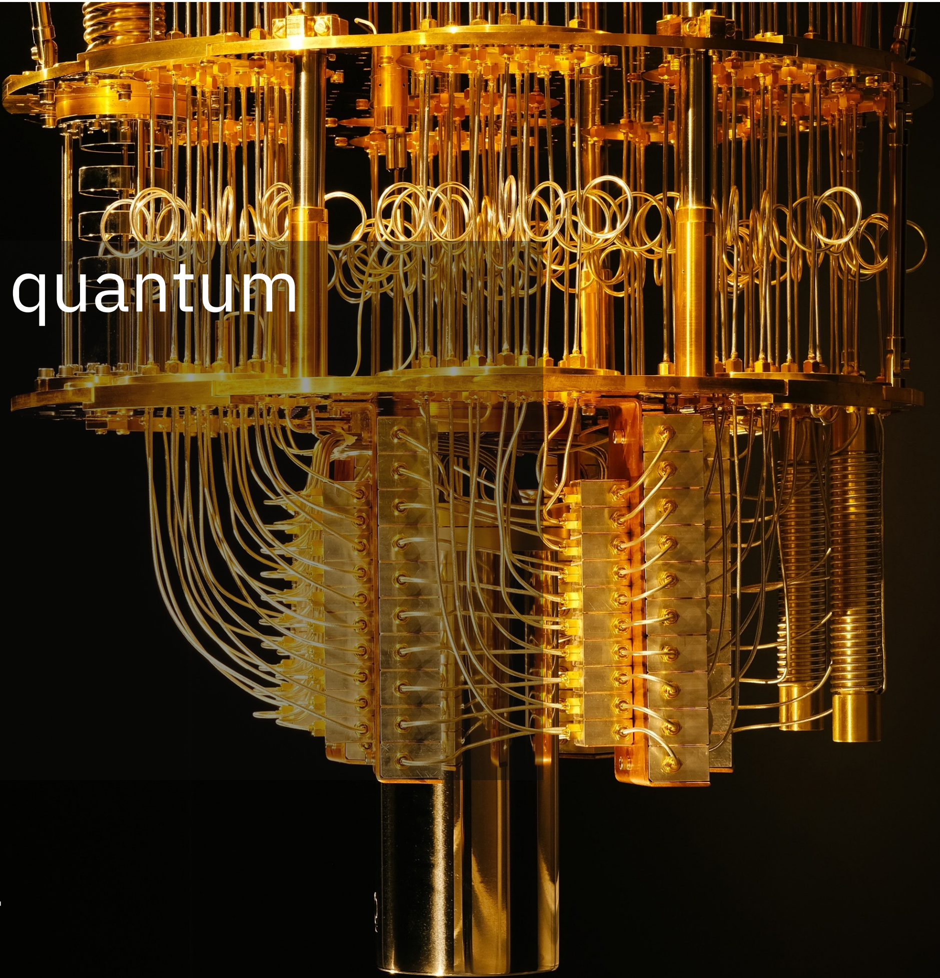
Session 3: Simulating Molecules using Variational Quantum Eigensolver (VQE)

Start	End	Duration	Subject
12:00	12:10	0:10	Opening and Overview
12:10	13:00	0:50	VQE – Theory & Experiment
13:00	13:10	0:10	Break
13:10	13:40	0:30	VQE – Qiskit Implementation
13:40	13:55	0:15	Assignment Office Hour
13:55	14:00	0:05	IBM Quantum Updates: IBM Quantum Challenge

Simulating chemistry on a quantum computer II

Abhinav Kandala
akandala@us.ibm.com

IBM Quantum



QISKIT Global Summer School
July 29, 2020

IBM Quantum

IBM Research Frontiers Institute

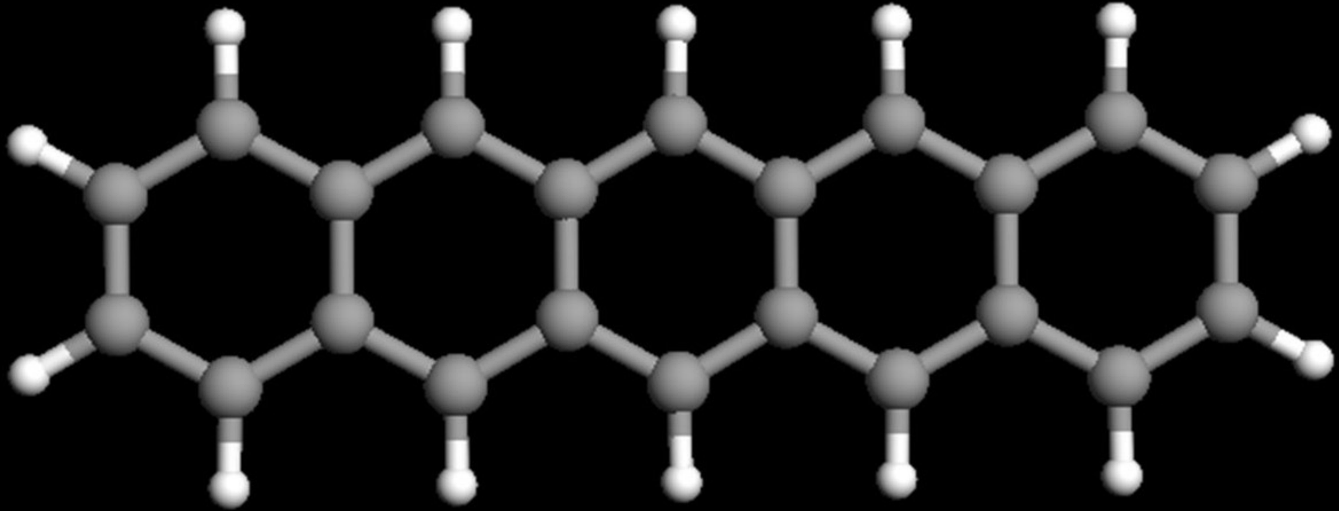
IARPA

Overview

- Motivation for quantum simulations
- Hardware: superconducting qubits
- Variational Quantum Eigensolver
- Error Mitigation

Motivations: Richard Feynman Quote

"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."



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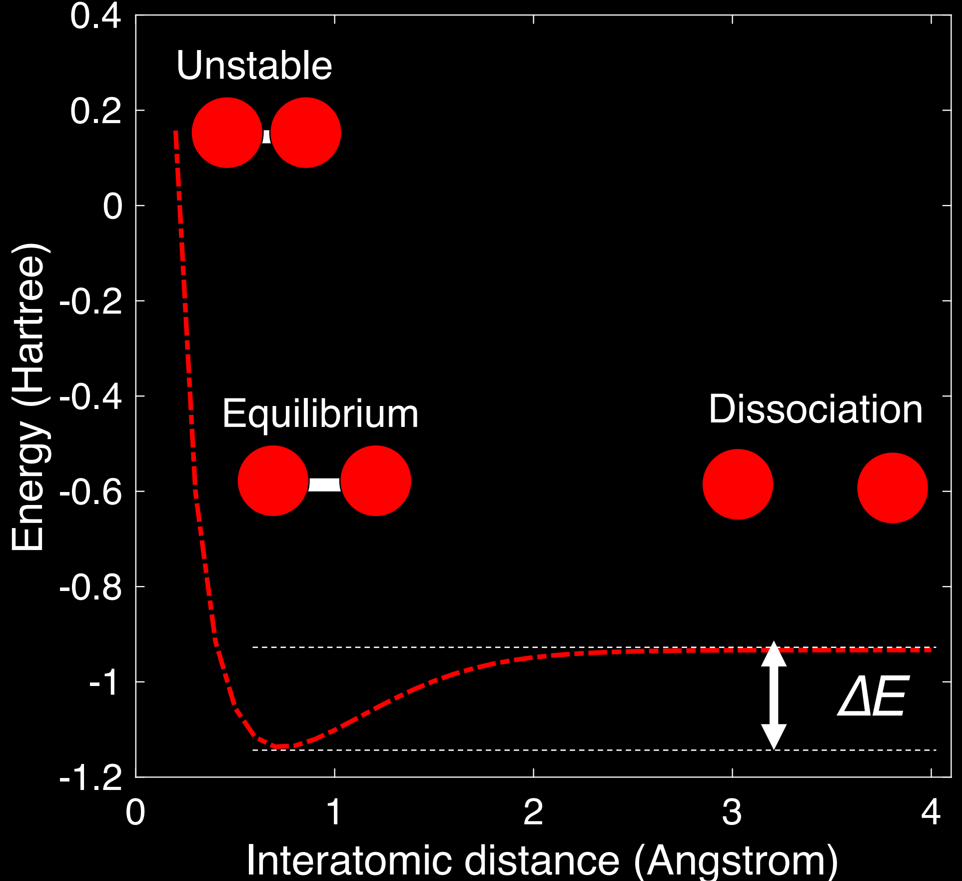
Potential energy curve of a molecule

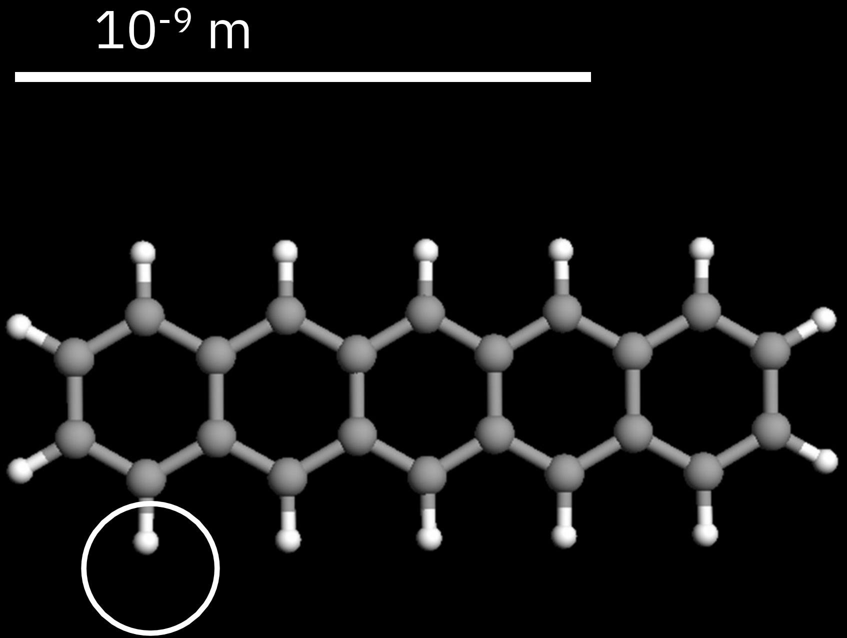


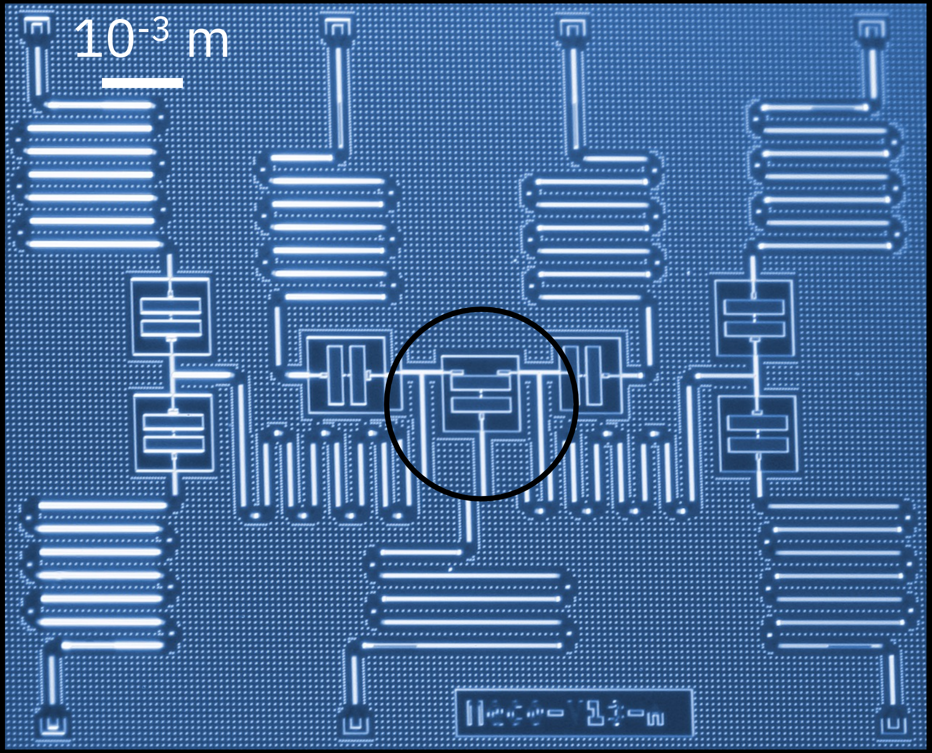
Rate $\propto$ Exp($-\Delta E/kT$)

Can we build a programmable, well-controlled quantum system to simulate the properties of other natural quantum systems, like molecules?

Natural atoms

Artificial Atoms





The Electronic Structure Problem

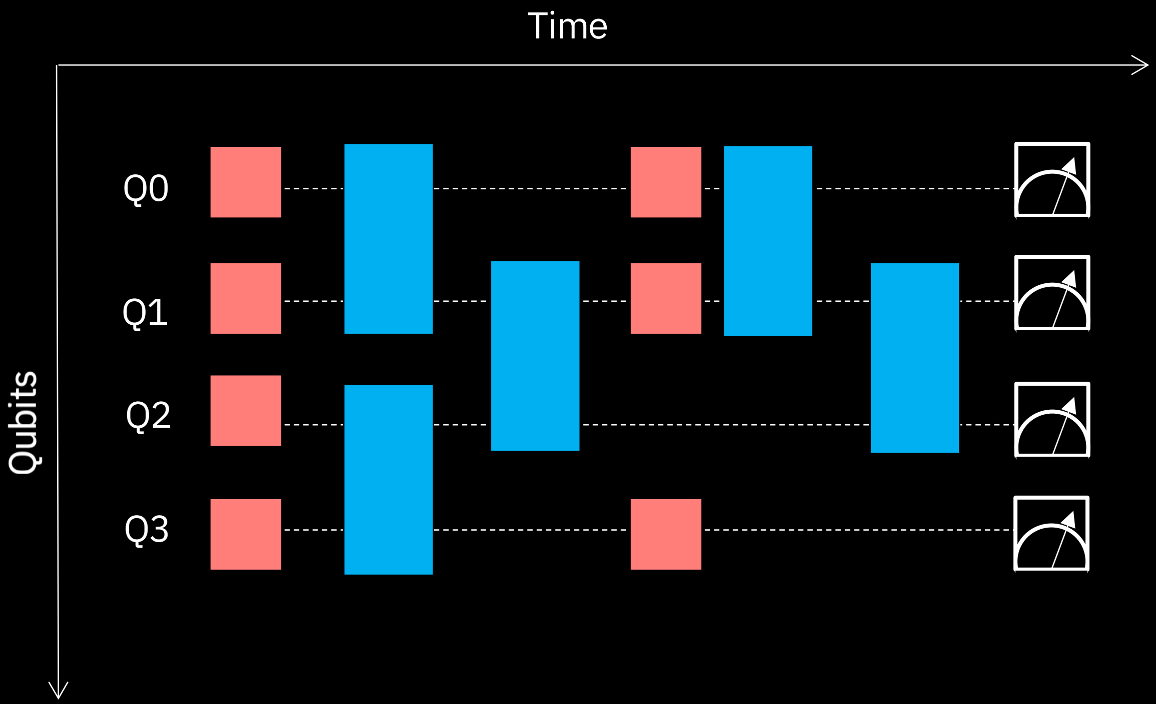
Interacting fermionic problems: A core challenge in modern computational physics and HPC

$$H_{\mathrm{e}} = -\sum_{i=1}^{N} \frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + \sum_{j>i} \frac{1}{r_{ij}}$$

$$H|\psi_G\rangle = E_G|\psi_G\rangle$$

Short depth circuits

Approximate quantum computing with noisy quantum hardware

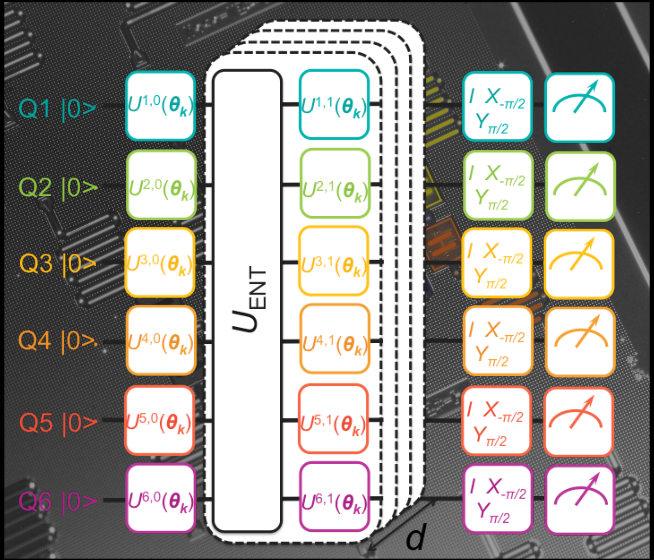


- Near-term quantum hardware is noisy
- Fault tolerant architectures not immediately accessible
- Novel algorithms focused on using short depth circuits that make best use of coherence window

Variational Quantum Eigensolver (VQE)

$$H = \sum_{\alpha} h_{\alpha} \sigma(\alpha)$$

Map problem onto Paulis



Prepare guess state $|\psi_G(\vec{\theta})\rangle$

Measure its energy

$$E(\vec{\theta}) = \sum_{\alpha} h_{\alpha} \langle \psi_G(\vec{\theta}) | \sigma_{\alpha} | \psi_G(\vec{\theta}) \rangle$$

$E(\vec{\theta})$

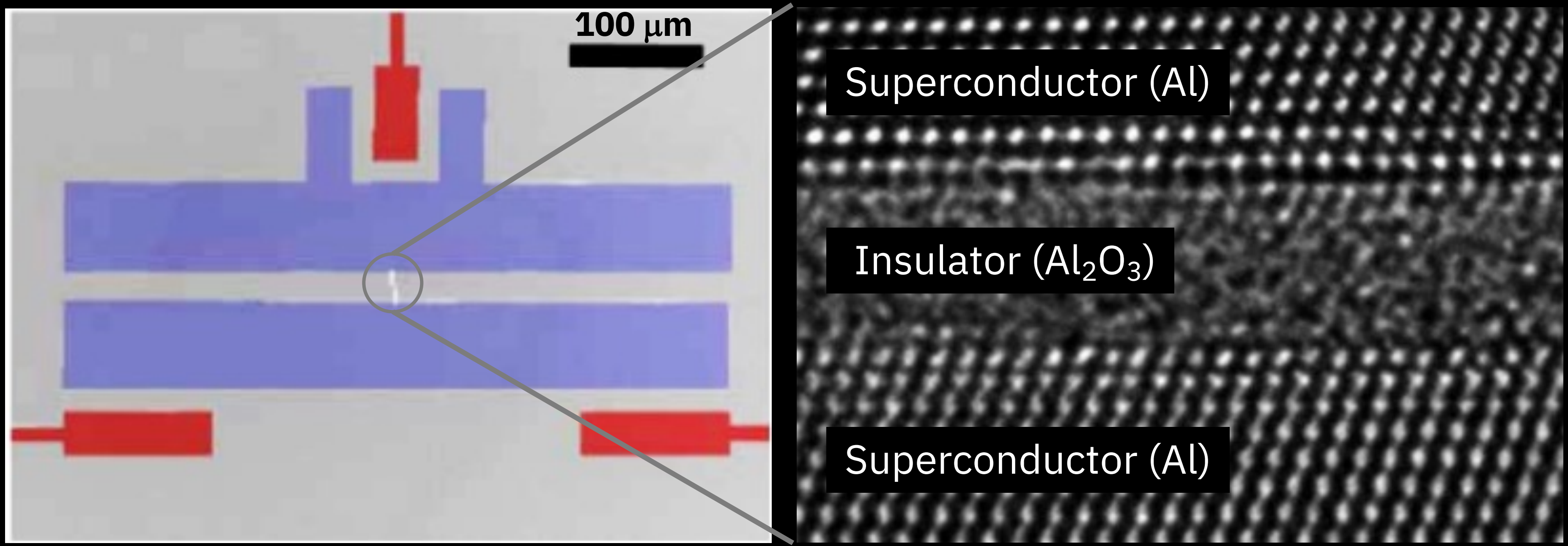
$\vec{\theta}$

Use classical optimizer

Nat. Commun 5, 4213 (2014)
Nature **549**, 242-246 (2017)

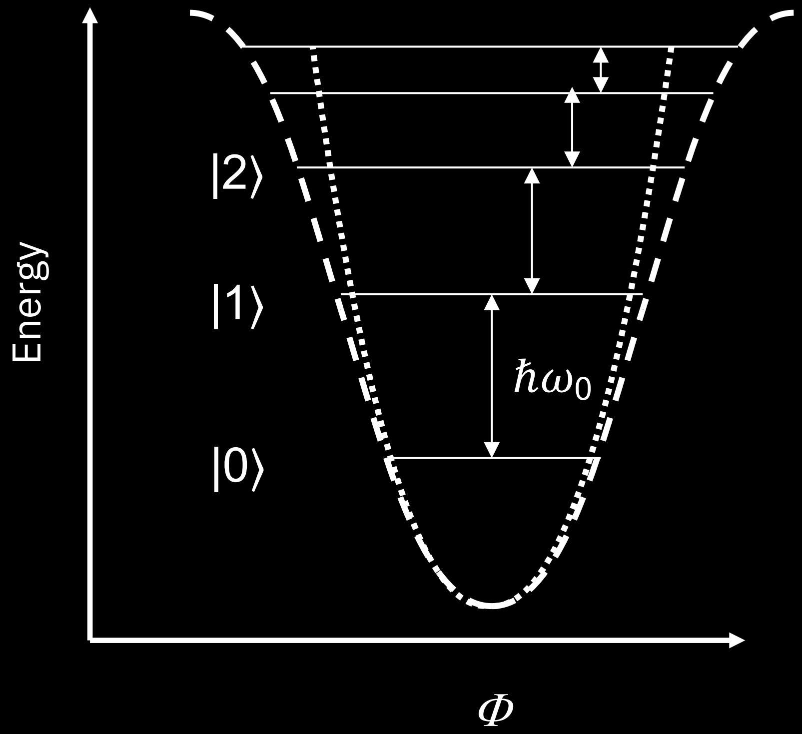
Quantum Hardware recap ..

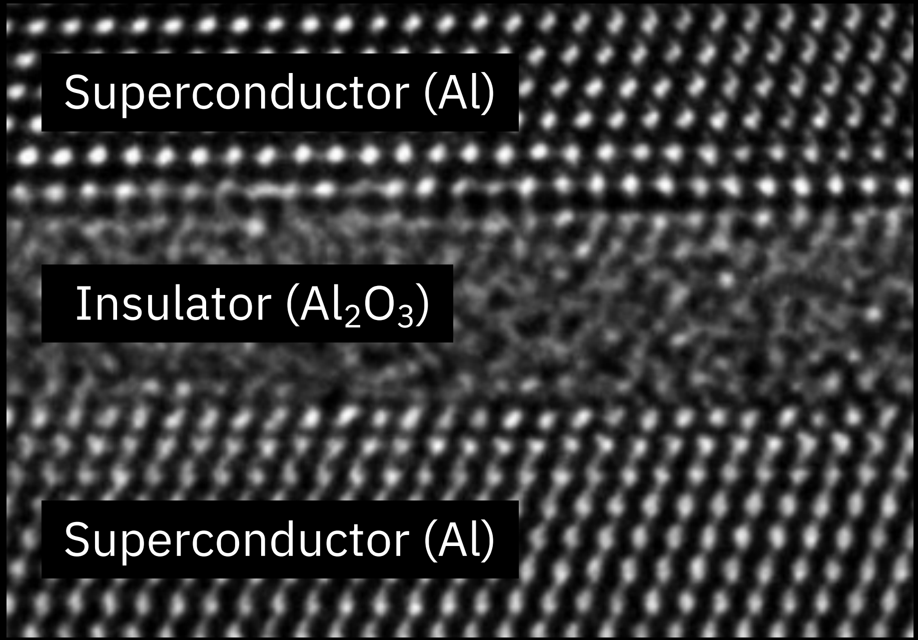
Artificial atom: Transmon



JAP, 125(16), 165301, 2019

Artificial atom: Transmon





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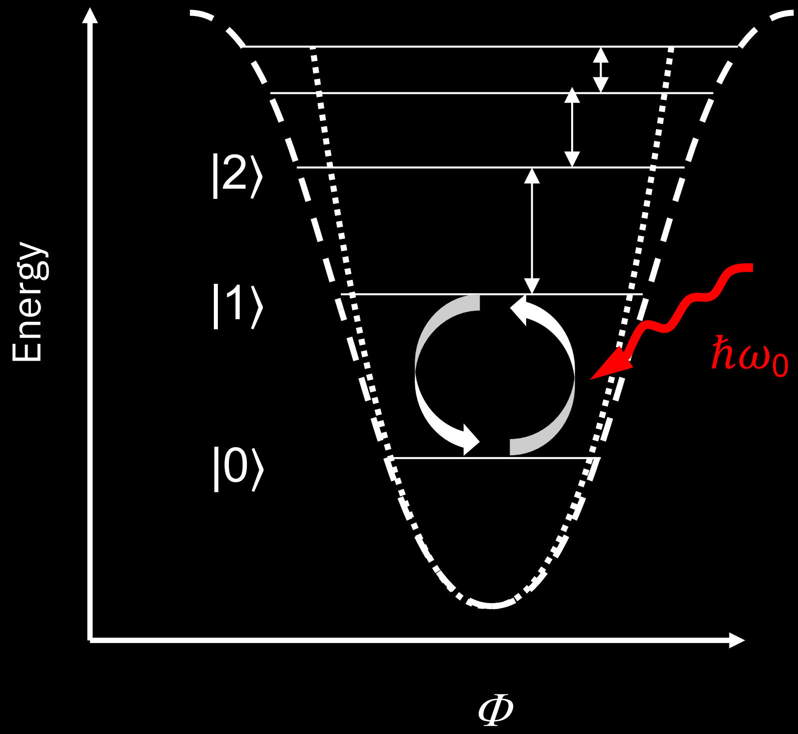
Single qubit control: Rabi Oscillations



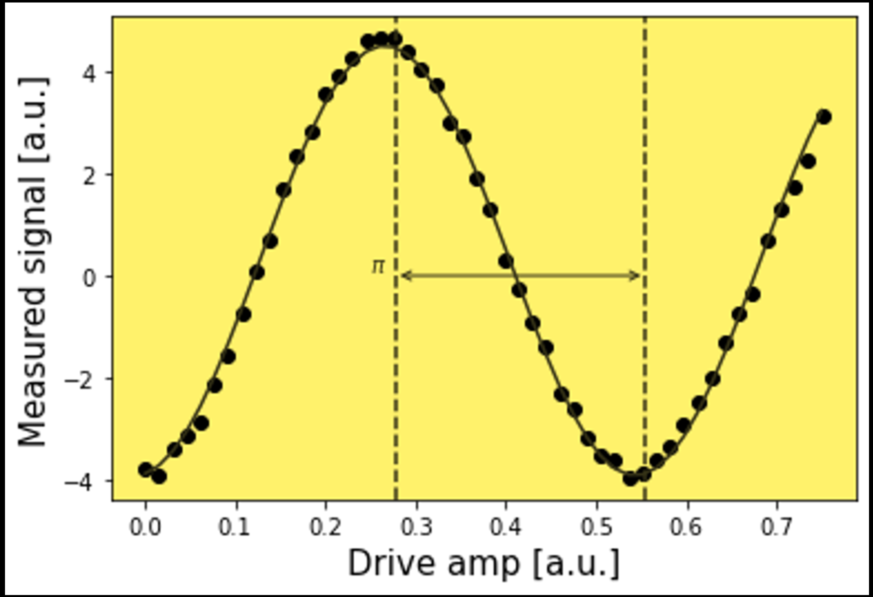


Image: QISKIT textbook

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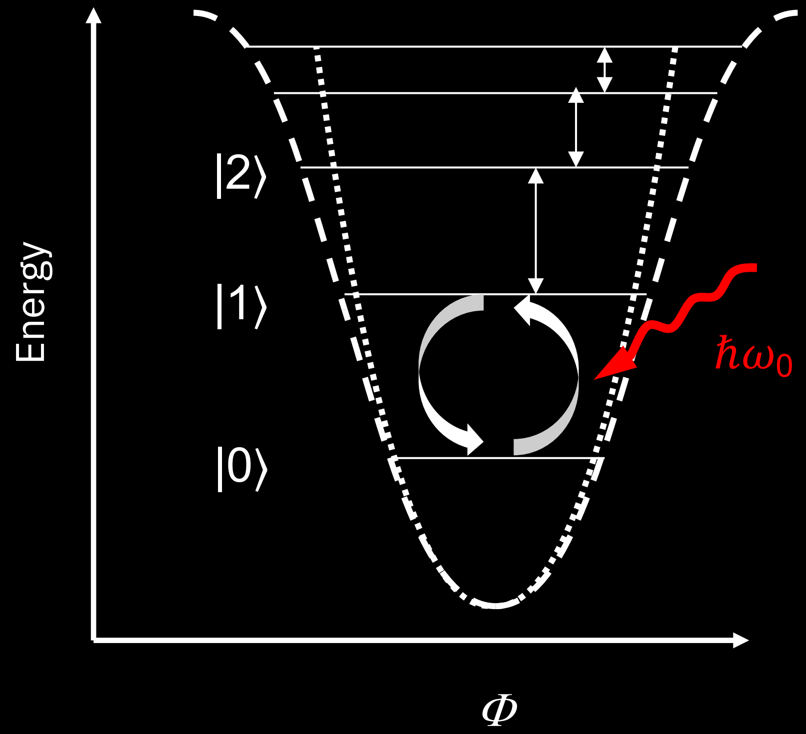

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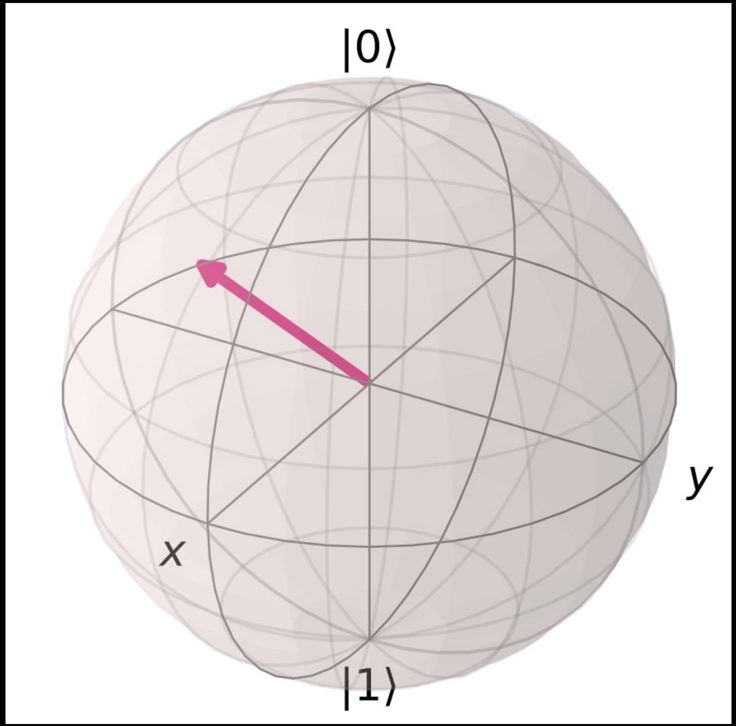


- Amplitude/duration of pulse controls angle of rotation.
- Phase of pulse controls axis of rotation

Two-qubit entangling gates

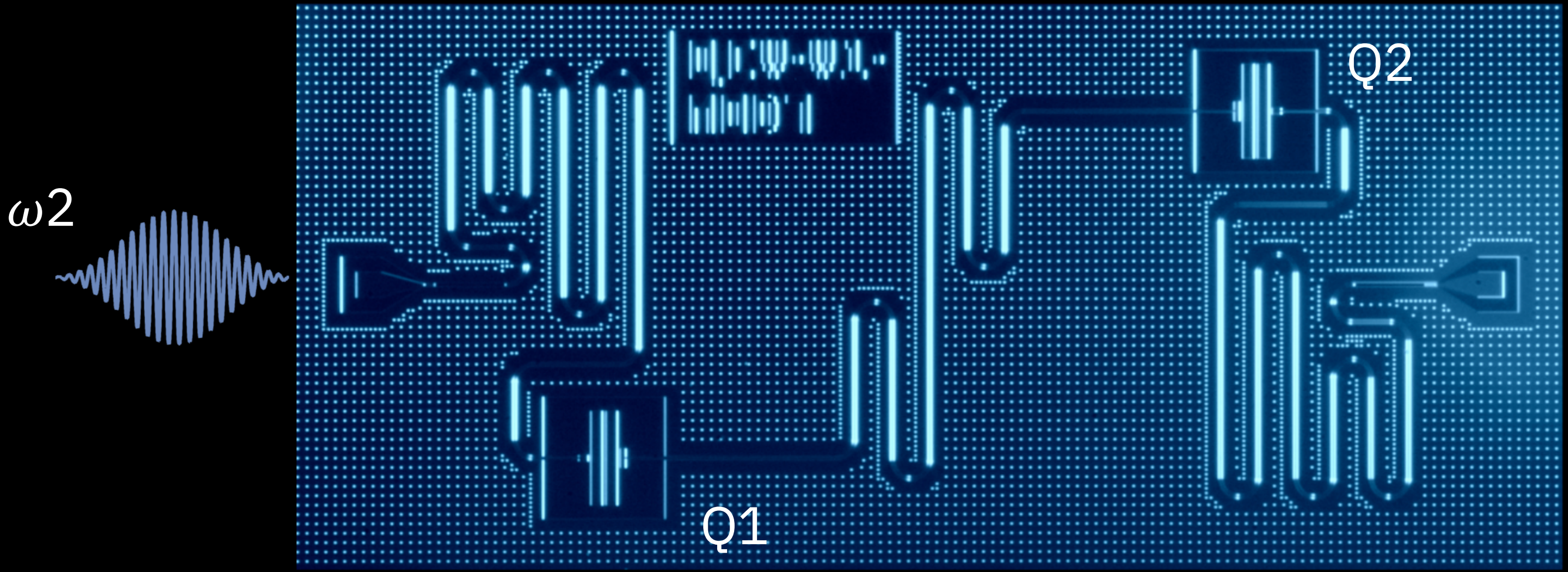
Apply operations on two qubit product states to create an entangled state, i.e. one that cannot be factored into its individual qubit components.

Entanglement generated by *conditional* rotations i.e rotations of a qubit (target) dependent on the state of the other (control).

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

$$U_{\text{CNOT}}|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A|0\rangle_B + |1\rangle_A|1\rangle_B\right) \neq (\ldots)_A(\ldots)_B$$

Two-qubit entangling gates: Cross resonance

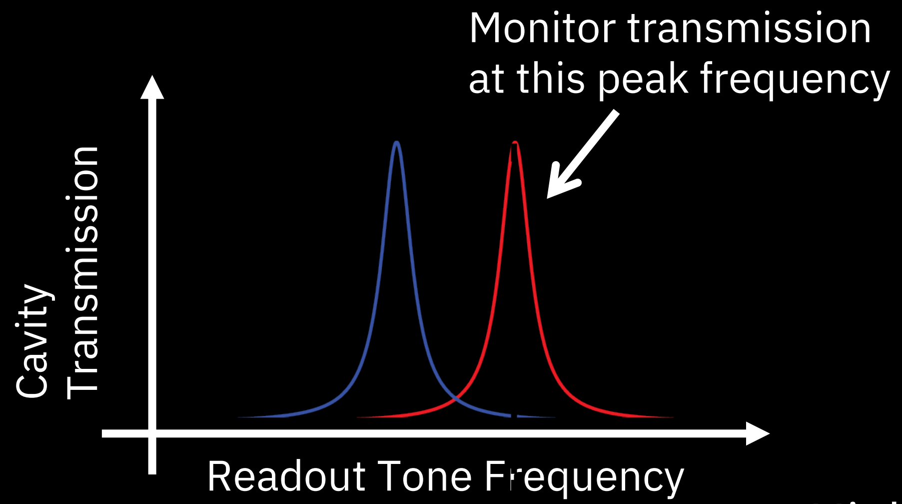


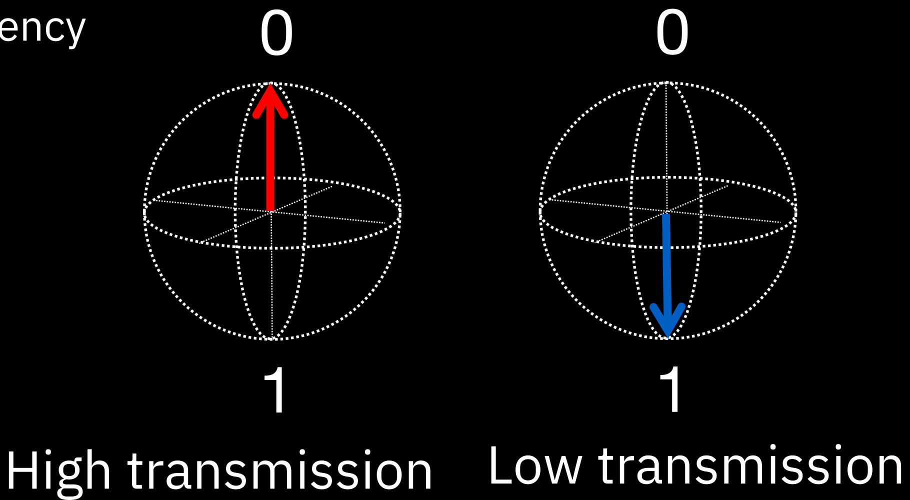
Can generate a CNOT with only microwave pulses

Dispersive readout

$$H = \frac{\hbar\omega_{01}'}{2}\hat{\sigma}_z + \hbar(\omega_r' + \chi\hat{\sigma}_z)\hat{a}^\dagger\hat{a}$$

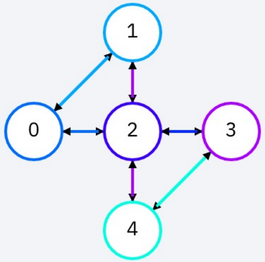
Qubit State dependent resonator frequency





Superconducting quantum processor: ibmq_5_yorktown

◯ Qubits ⇅ Connectivity



Single-qubit U2 error rate

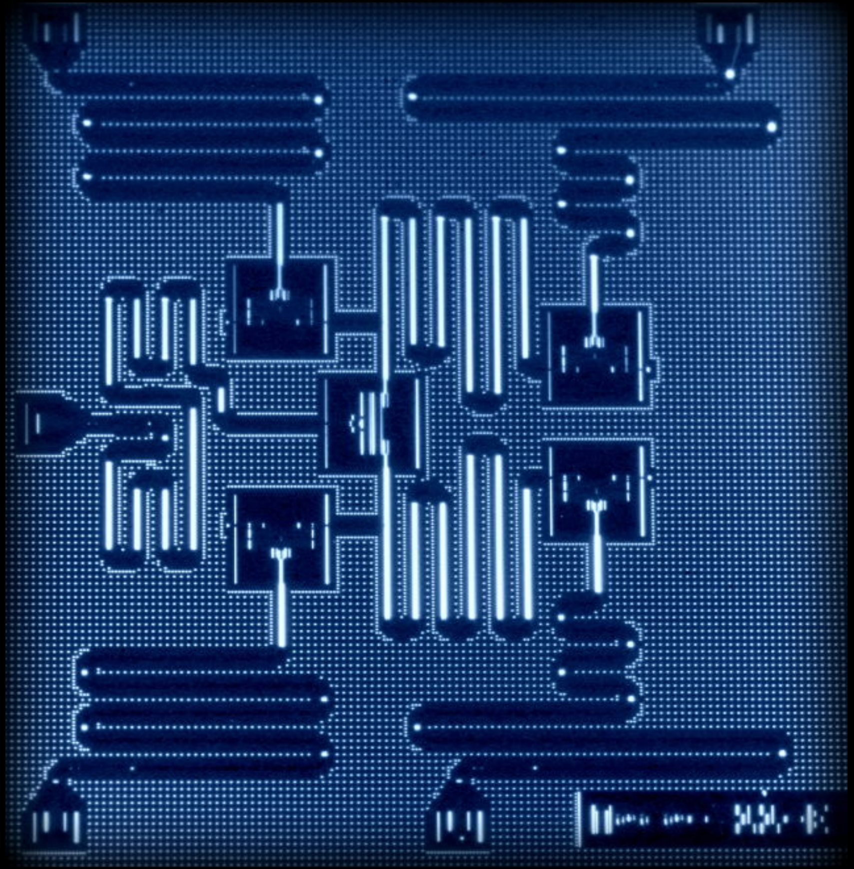
4.169e-4 — 9.786e-4

CNOT error rate

1.245e-2 — 1.713e-2

Download Calibrations

Qubits 5	Online since Jan 24, 2017
Basis gates u1, u2, u3, cx, id	Last calibration update Jun 30, 2020 4:58 AM
Maximum shots 8192	Maximum experiments 75



Device characterization

Qubit	T1 (µs)	T2 (µs)	Frequency (GHz)	Readout error	Single-qubit U2 error rate	CNOT error rate
Q0	64.2	74.54	5.286	2.45E-02	6.49E-04	cx0_1: 1.380e-2, cx0_2: 1.430e-2
Q1	77.35	83.17	5.238	1.75E-02	5.72E-04	cx1_0: 1.380e-2, cx1_2: 1.713e-2
Q2	50.9	41.91	5.031	2.75E-02	8.32E-04	cx2_0: 1.430e-2, cx2_1: 1.713e-2, cx2_3: 1.470e-2, cx2_4: 1.708e-2
Q3	60.04	47.72	5.296	3.35E-02	9.79E-04	cx3_2: 1.470e-2, cx3_4: 1.245e-2
Q4	57.19	64.79	5.084	1.45E-02	4.17E-04	cx4_2: 1.708e-2, cx4_3: 1.245e-2

Q: Which 2 qubits would you choose for a H_2 simulation?

Back to chemistry

The Electronic Structure Problem

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Interacting fermionic problems: A core challenge in modern computational physics and HPC

$$H_{\mathrm{e}} = -\sum_{i=1}^{N} \frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + \sum_{j>i} \frac{1}{r_{ij}}$$

$$H|\psi_G\rangle = E_G|\psi_G\rangle$$

Variational Quantum Eigensolver (VQE)

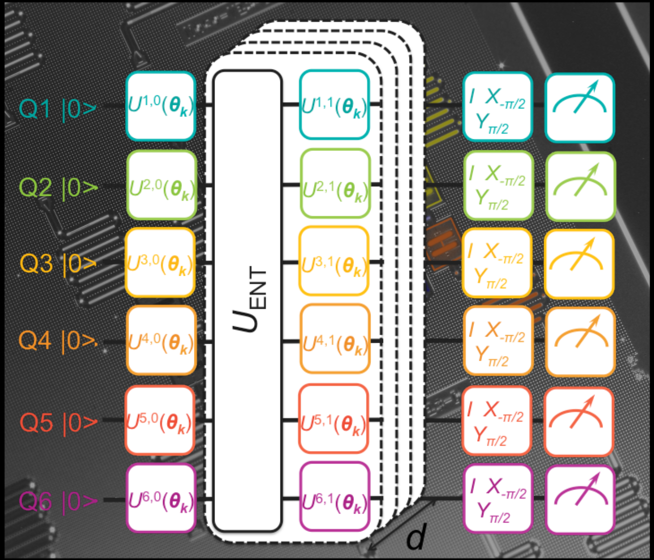
Variational principle: the energy of any trial wave-function is greater than or equal to the exact ground state energy

$$\frac{\langle \Psi(\vec{\theta}) | H | \Psi(\vec{\theta}) \rangle}{\langle \Psi(\vec{\theta}) | \Psi(\vec{\theta}) \rangle} \geq E_G$$

Variational Quantum Eigensolver (VQE)

$$H = \sum_{\alpha} h_{\alpha} \sigma(\alpha)$$

Map problem onto Paulis



Prepare guess state $|\psi_G(\vec{\theta})\rangle$

Measure its energy

$$E(\vec{\theta}) = \sum_{\alpha} h_{\alpha} \langle \psi_G(\vec{\theta}) | \sigma_{\alpha} | \psi_G(\vec{\theta}) \rangle$$

$E(\vec{\theta})$

$\vec{\theta}$

Use classical optimizer

Nat. Commun 5, 4213 (2014)
Nature **549**, 242-246 (2017)

The problem and its qubit representation

$$H_{\mathrm{e}} = -\sum_{i,j} \frac{1}{2} \langle i| \nabla_i^2 |j\rangle a_i^\dagger a_j + \sum_{i,j} \langle i| \frac{Z_A}{r_{iA}} |j\rangle a_i^\dagger a_j + \sum_{i,j,k,m} \langle i,j| \frac{1}{r_{ij}} |k,m\rangle a_i^\dagger a_j^\dagger a_k a_m$$

$$\{a_i^\dagger, a_j\} = \delta_{ij}$$

$$a_j \to \left(\prod_{i=1}^{j-1} \sigma_i^z \right) \sigma_j^+$$

$$a_i^\dagger \to \left(\prod_{i=1}^{j-1} \sigma_i^z \right) \sigma_j^-$$

In general, problem of *M* electrons in *N* spin orbitals (*M*<*N*) mapped onto *N* qubit- Hamiltonian with $O(N^4)$ Pauli strings

Jordan Wigner, Brayvi-Kitaev, Parity mapping ...

$$H = \sum_\alpha h_\alpha \sigma(\alpha)$$

$$\sigma_{\mathbf{A}} \in \pm\{I, \sigma^x, \sigma^y, \sigma^z\}^{\otimes M}$$

Mapping fermions to qubits

Pauli string

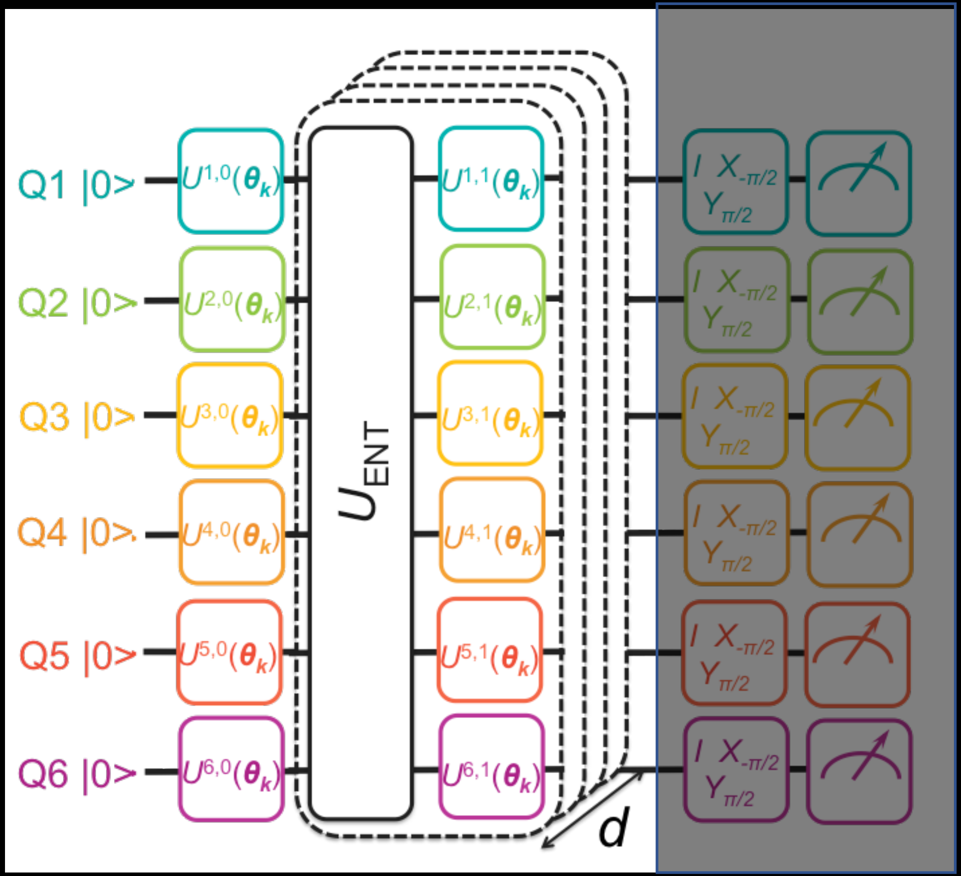
$$H = h_1 IXIY + h_2 XZZX + h_3 XZYZ$$

Number of non-identity single qubit Pauli operators : weight of the Pauli string

Larger weight Pauli strings are increasingly sensitive to measurement error

Choice of fermion-qubit mapping important: Each fermionic operator maps to O(N) qubits for JW, O(log N) for BK

Trial State Preparation

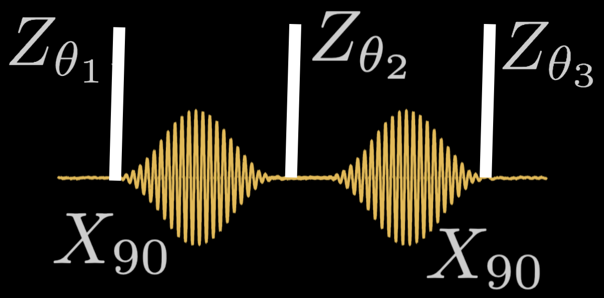


- Unitary Coupled Cluster ansatz : Offers physical intuition, focuses ground state search in ”good” space
- However, translates to very expensive gate count
- Alternative approach: Keeping hardware limitations in mind, do what hardware can do best!

A. Kandala, A. Mezzacapo, et al, Nature **549**, 242-246 (2017)

Trial state preparation: Arbitrary single qubit rotation

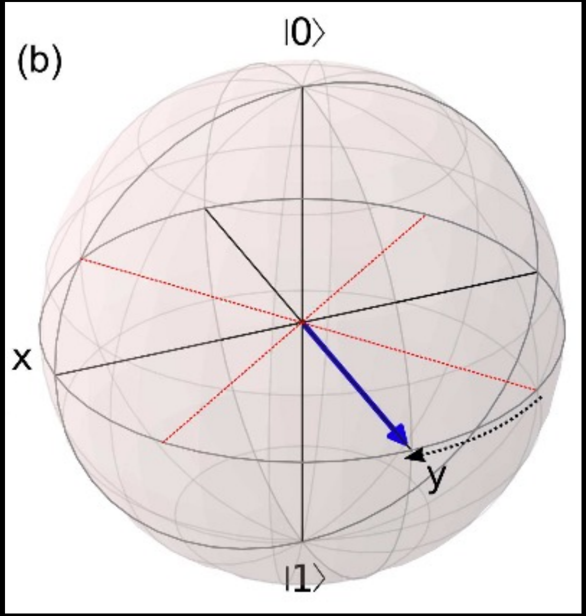
$$U(\vec{\theta}) = Z_{\theta_1} X_{90} Z_{\theta_1} X_{90} Z_{\theta_1}$$



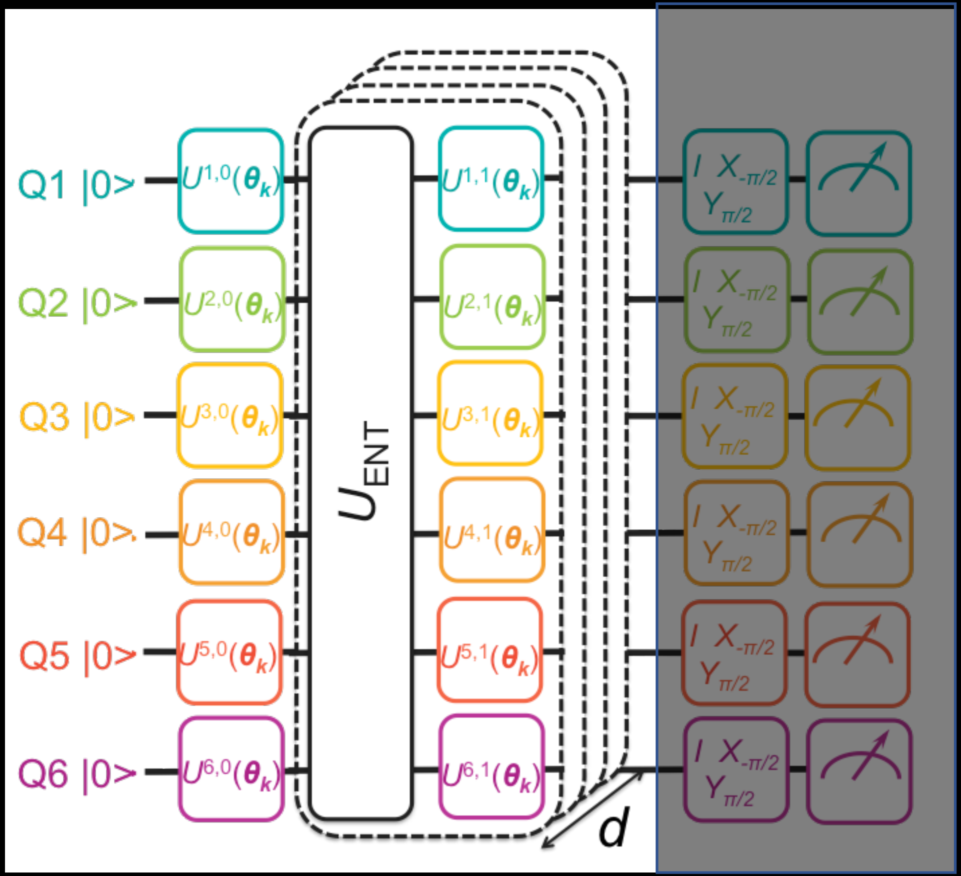
Variational parameters:

- Pulse envelope
- Pulse length
- Amplitude
- Phase

Software implemented Z-gates
(Perfect, zero time)



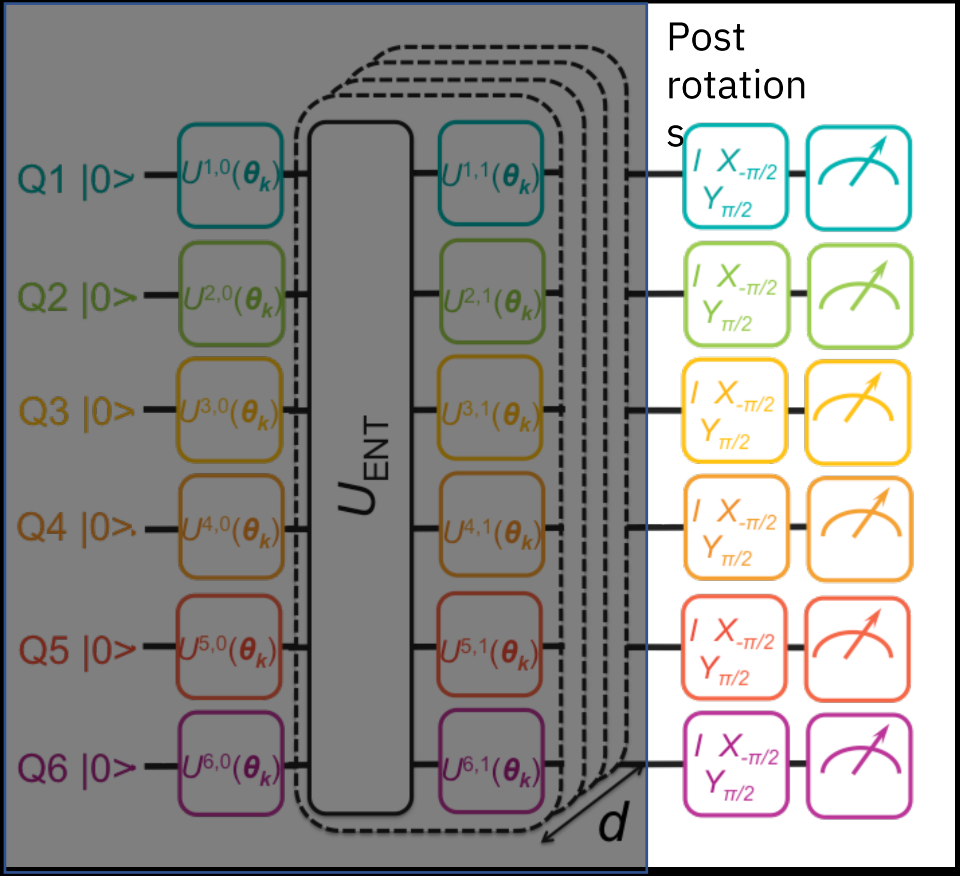
Trial State Preparation



- Sequence of interleaved arbitrary single qubit rotations and naturally available entangling gates
- Depth set by available quantum coherence (incoherent errors)
- $N(3d+2)$ variational parameters
- This structure offers some robustness to coherent errors

A. Kandala, A. Mezzacapo, et al, Nature **549**, 242-246 (2017)

Energy measurement : Measuring expectation values



Energy measurement : Measuring expectation values

$$H = 3\, Z_1 Z_2 + 4\, I_1 Z_2$$

$$\underline{|\psi\rangle} = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

$$\langle\psi|H|\psi\rangle = \underbrace{3\,\langle\psi|Z_1 Z_2|\psi\rangle}_{} + 4\,\langle\psi|I_1 Z_2|\psi\rangle$$

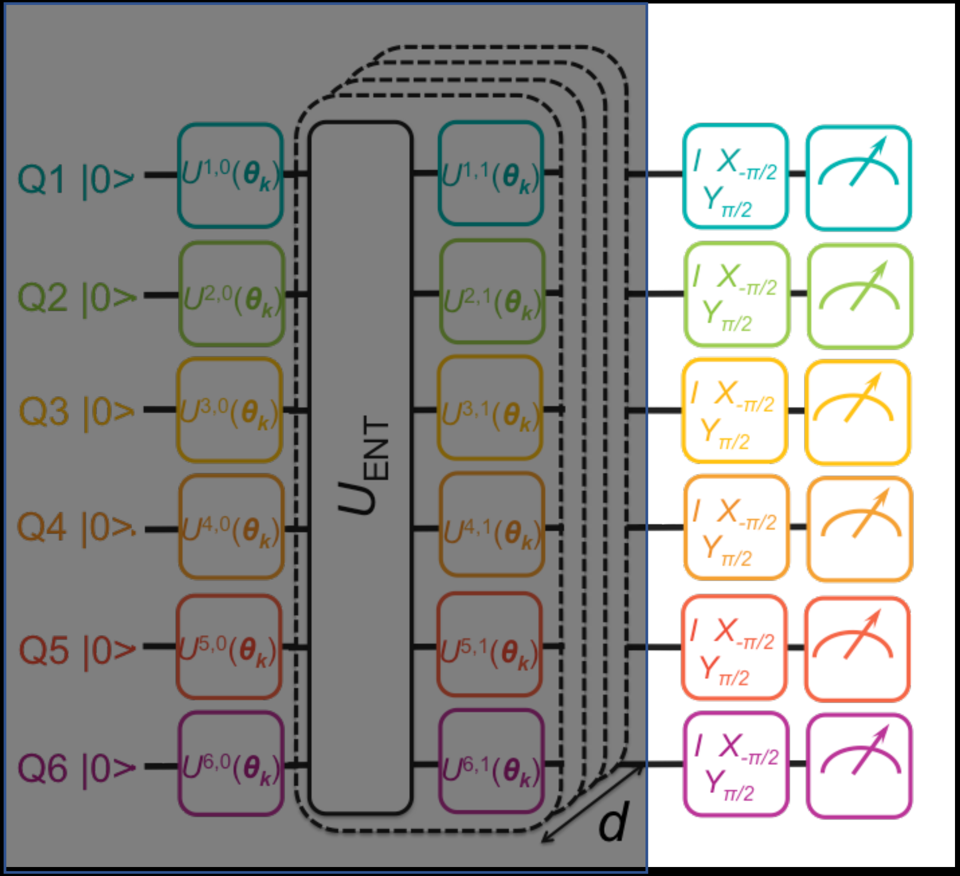
$$Z_1 Z_2|\psi\rangle = \alpha|00\rangle - \beta|01\rangle - \gamma|10\rangle + \delta|11\rangle$$

$$\boxed{\begin{aligned} Z|0\rangle &= +1|0\rangle \\ Z|1\rangle &= -1|1\rangle \end{aligned}}$$

$$\langle\psi|H|\psi\rangle = \alpha^2 - \beta^2 - \gamma^2 + \delta^2$$

$$= \underline{\underline{P_{00}}} - \underline{\underline{P_{01}}} - \underline{\underline{P_{10}}} + \underline{\underline{P_{11}}}$$

Energy measurement: Measurement Basis



Energy measurement: Measurement Basis

$$H = 3Z_1X_2 + 4I_1Z_2$$

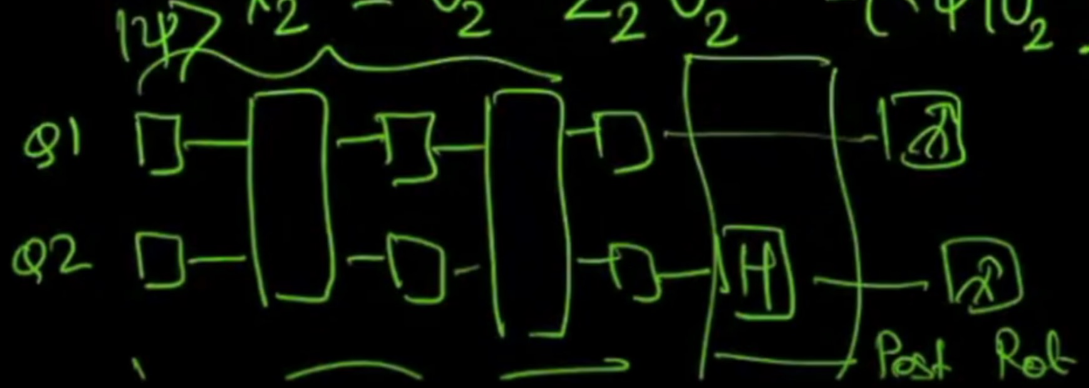
$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

$$\langle\psi|Z_1X_2|\psi\rangle = \langle\psi|Z_1(U_2^\dagger Z_2 U_2|\psi\rangle$$

$$X_2 = U_2^\dagger Z_2 U_2$$

$$= (\langle\psi|U_2^\dagger)\, Z_1Z_2\, (U_2|\psi\rangle)$$

$$X = HZH$$



Energy measurement: Pauli Grouping

$$H = 3 Z_1 Z_2 + 4 I_1 Z_2 \quad \Big| \quad H = 2X + IZ$$

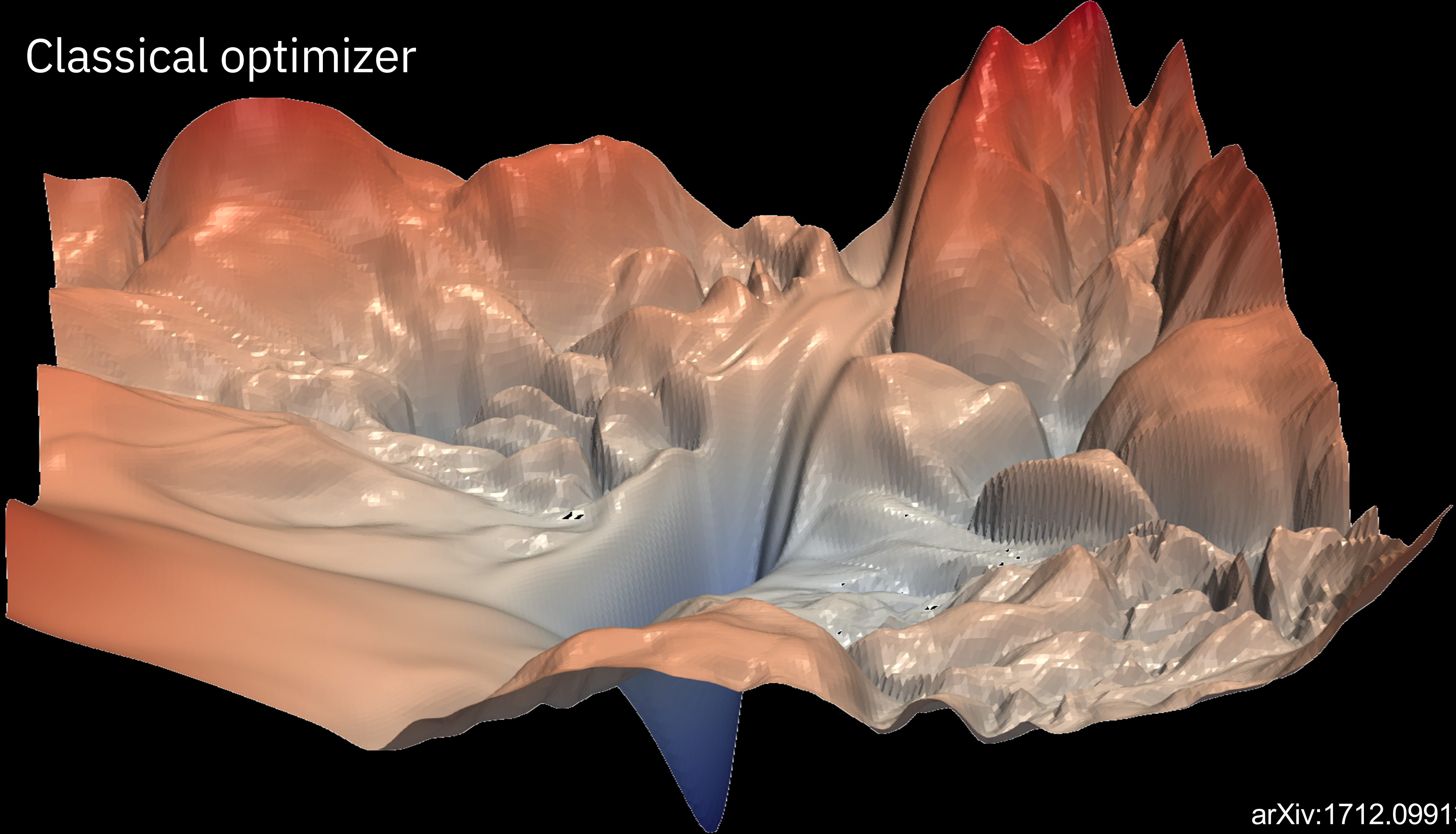
$$\langle \psi | \cancel{H}\, I_1 Z_2 | \psi \rangle$$

$$I_1 Z_2 \left(\alpha |00\rangle + \beta |01\rangle + \gamma |10\rangle + \delta |11\rangle \right)$$

$$\left(\alpha |00\rangle - \beta |01\rangle + \gamma |10\rangle - \delta |11\rangle \right)$$

$$\langle I_1 Z_2 \rangle = \alpha^2 - \beta^2 + \gamma^2 - \delta^2$$

Classical optimizer

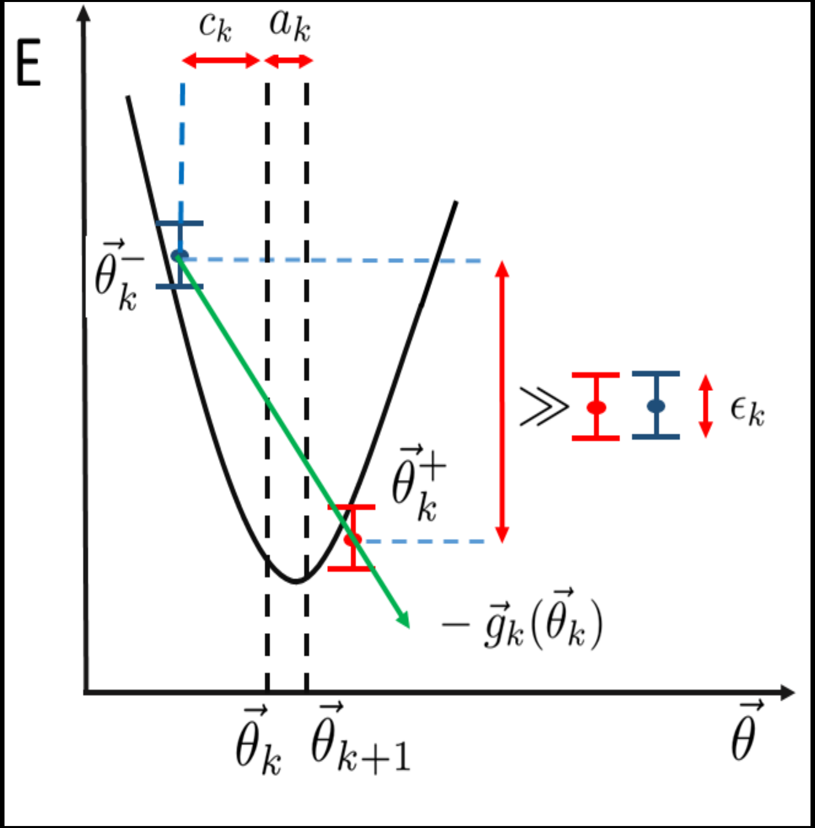


arXiv:1712.09913

Classical optimizer: Simultaneous Perturbation Stochastic Approximation (SPSA)

Need to reduce of calls to Quantum computer

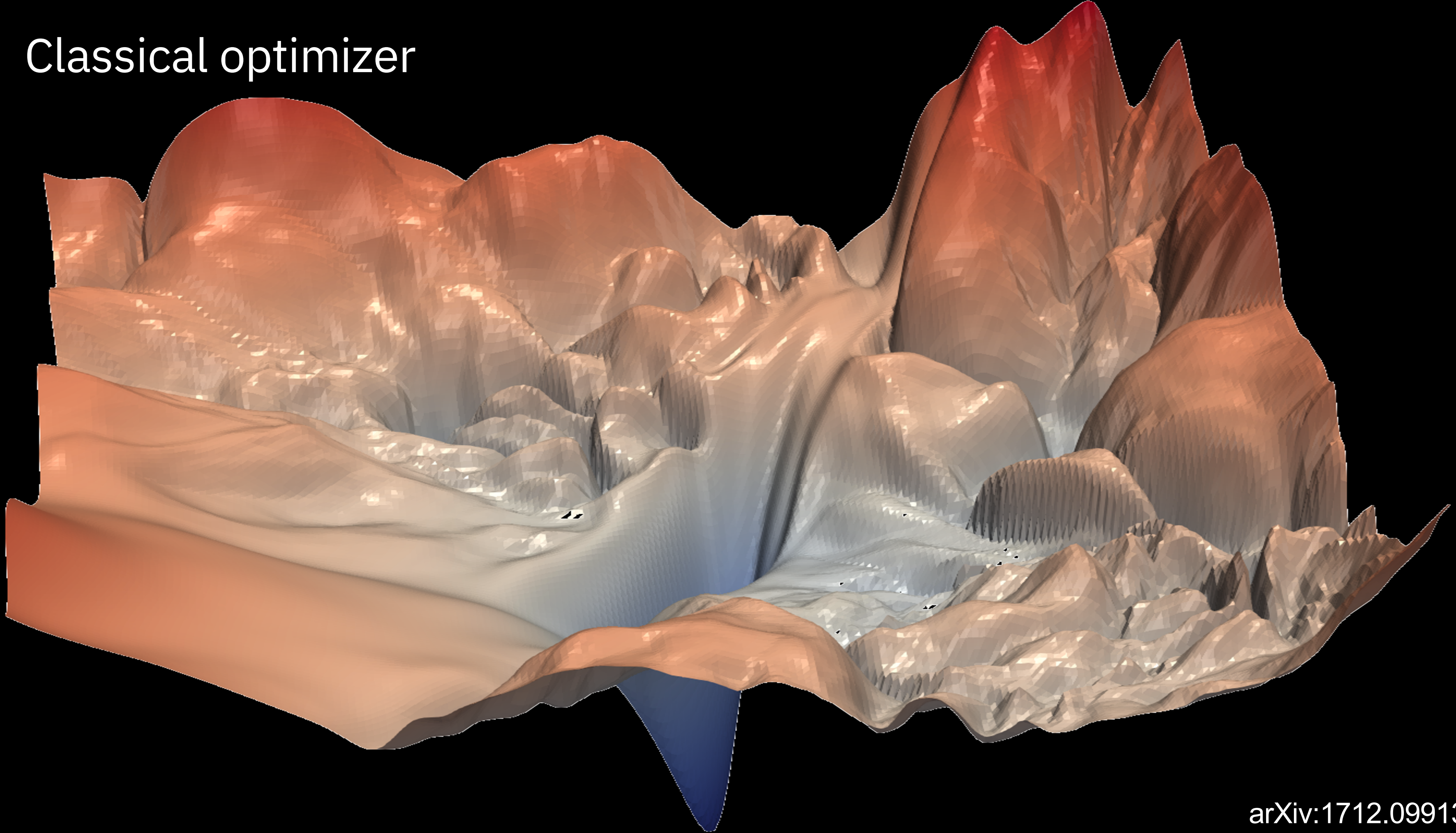
Gradient approx.: Regardless of dimension of optimization problem, utilizes only **two** measurements per iteration



[1] J. C. Spall, Multivariate stochastic approximation using a simultaneous perturbation gradient approximation, IEEE Transactions on Automatic Control 37, 332 (1992)

A. Kandala, A. Mezzacapo, et al, Nature **549**, 242-246 (2017)

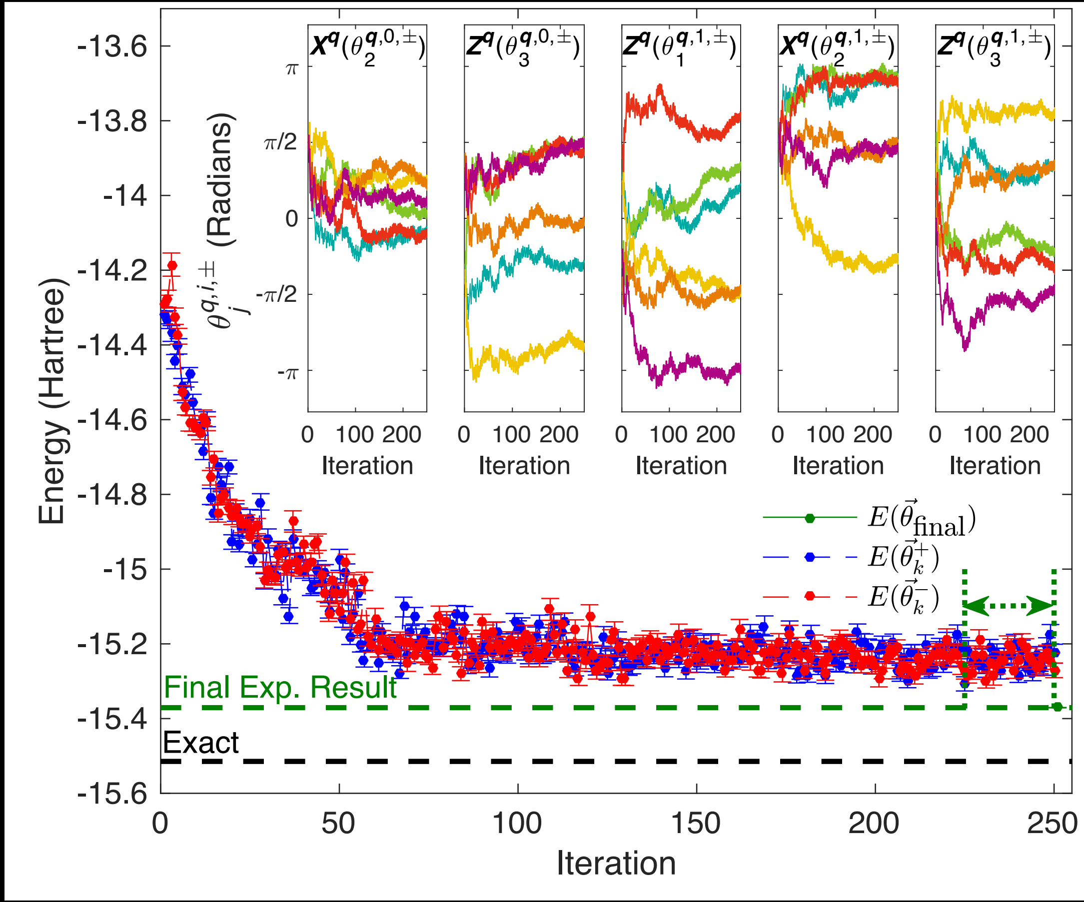
Classical optimizer

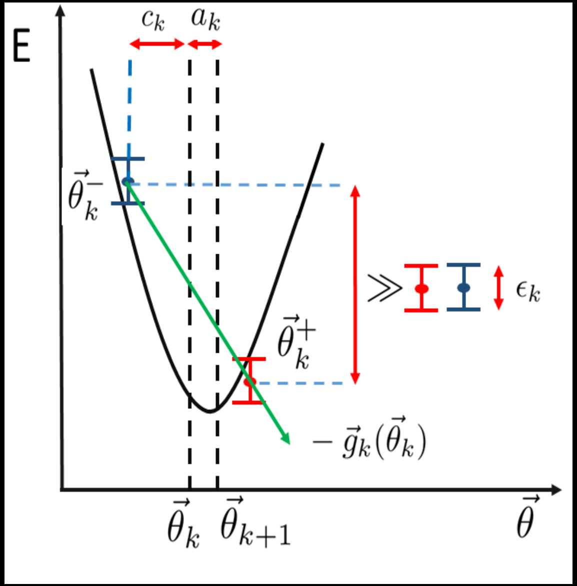


arXiv:1712.09913

Putting it all together ..

Experimental optimization of a 6 Qubit Hamiltonian





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Application to quantum chemistry : H_2

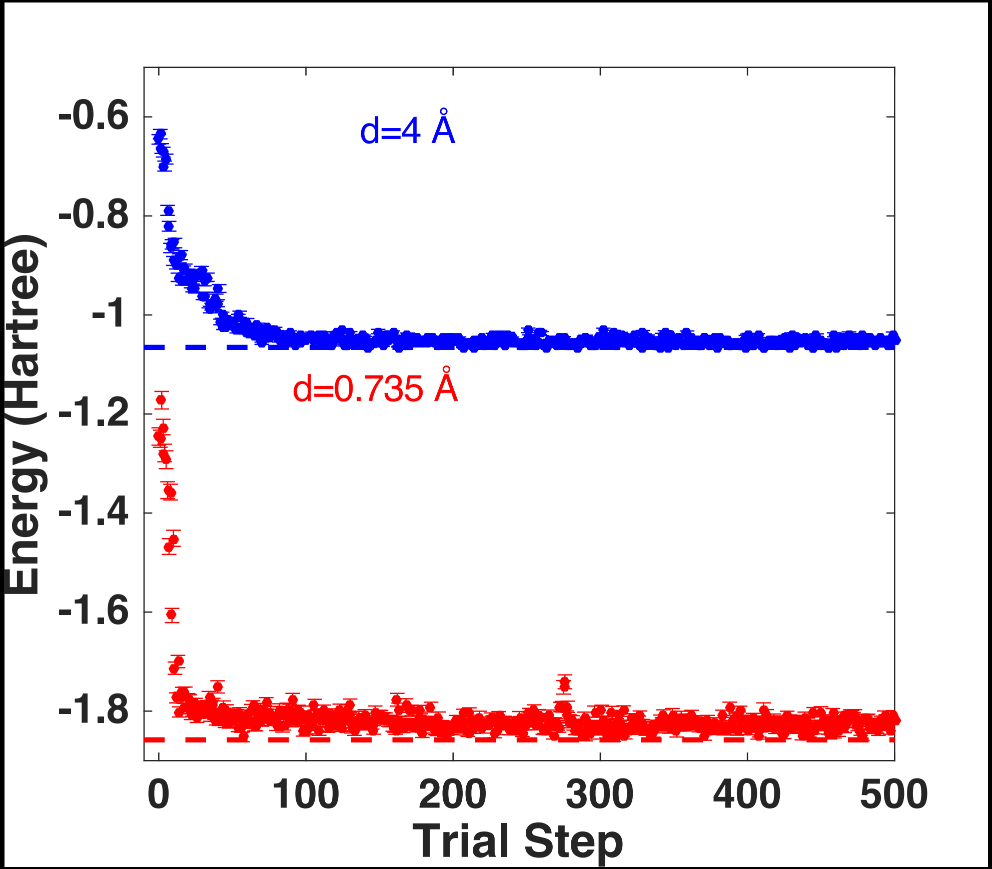
H_A: $1s^1$ H_B: $1s^1$
4 spin orbitals mapped to 2 qubits

Equilibrium d = 0.735 Å

H = (-1.05237)II+(0.39735)ZI+(0.39735)IZ+
(0.11279)ZZ+(0.18093)XX

Dissociation d = 4 Å

H = (-0.70461)II+(0.00012)ZI+(0.00012)IZ+
(1.6673e-10)ZZ+(0.33438)XX



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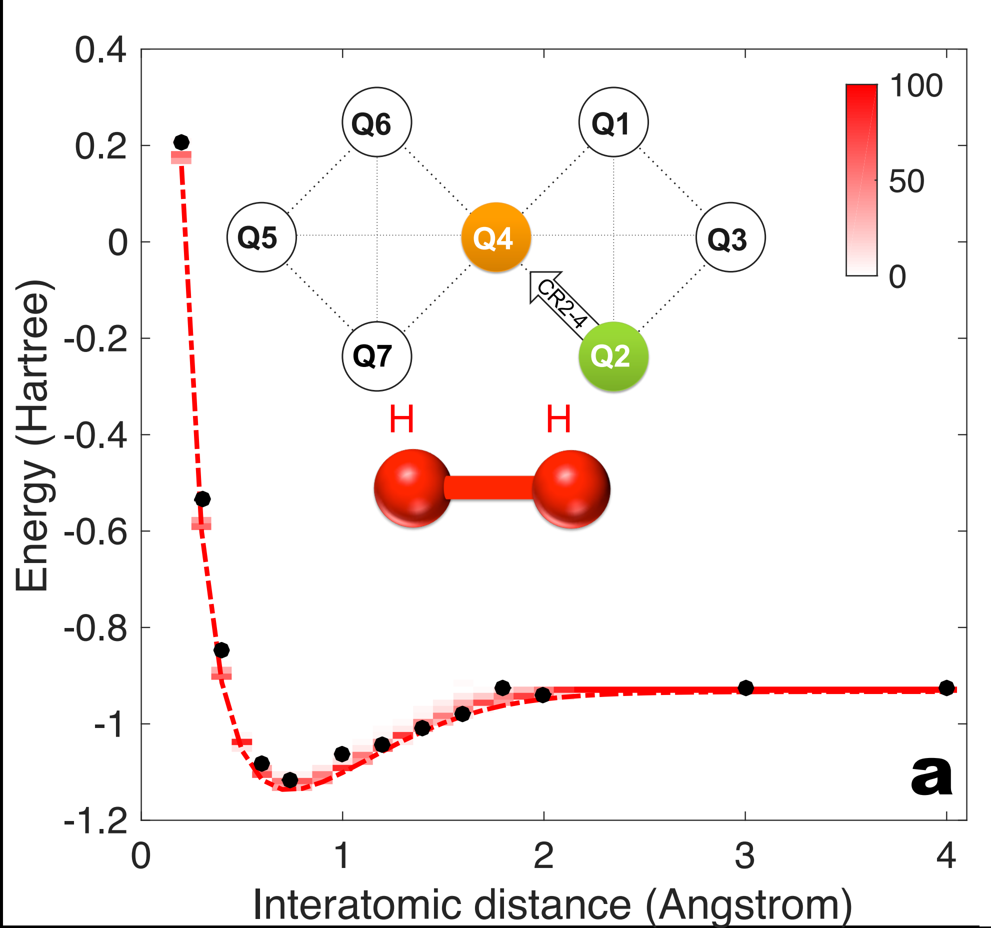

Application to quantum chemistry : Going beyond period 1 ....

II	-1.05237
ZI	0.39735
IZ	0.39735
ZZ	0.11279

XX	0.18093

H_2: 5 Pauli terms, 2 sets

ZZZZ	0.080333850925909334
IIII	-0.20665748323683217
ZIII	-0.096022179507889355
ZZII	-0.20612801807987652
IZII	0.36474560607027956
IIZI	0.096022179507889077
IIZZ	-0.20612801807987641
IIIZ	-0.36474560607027956
ZIZI	-0.14543788191435422
ZIZZ	0.056040328985617657
ZIIZ	0.11081066572357191
ZZZI	-0.056040328985617643
ZZIZ	0.063672720404946023
IZZI	0.11081066572357193
IZZZ	-0.063672720404946037
IZIZ	-0.095215796658694896

XZXX	0.0081947444613071196
XZIX	0.0012708408559466877

XZXZ	-0.0026669416291266101
XZII	-0.012585096432460004
XIII	0.012585096432460002
IIXZ	0.012585096432460008
IIXI	0.012585096432460006
XZXI	-0.0026669416291266101
XIXZ	0.0026669416291266101
XIXI	0.0026669416291266101
XZIZ	0.0072647375176923996
XIIZ	-0.0072647375176923996
IZXZ	0.0072647375176923988
IZXI	0.0072647375176923988

ZZXZ	0.00024654966581589 4
ZIXZ	-0.011962198277325331
ZIXI	-0.011962198277325331
ZZXI	0.00024654966581589 4

YYXX	-0.02892604472017965
YYIX	-0.0074989926703520624

XXXX	0.02892604472017965
XXII	-0.029639606309848882
IXII	0.0027917513494058743
IIXX	-0.029639606309848868
IIIX	0.0027917513494058743
XIXX	-0.0081947444613071196
XIIX	-0.0012708408559466877
XXXI	-0.0081947444613071196
XXIX	0.0074989926703520624
IXXI	-0.0012708408559466 88
IXXX	0.0074989926703520624
IXIX	0.0093271960584065342

ZZXX	-0.0028953260749665956
ZIXX	0.039154818592760203
ZZIX	-0.0097693536789154 93
IZXX	-0.024279988585959 71
IZIX	-0.0080251584900907554

XXYY	-0.02892604472017965
IXYY	-0.0074989926703520624

ZXZX	-0.0093271960584065342
ZXII	0.0027917513494058743
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ZIZX	-0.016781393784256322
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IXZX	-0.0093271960584065342

XZZZ	-0.00024654966581589405
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XIZZ	0.00024654966581589405

YYZZ	0.0028953260749665956
YYZI	0.039154818592760 21
YYIZ	-0.024279988585959714

XZYY	-0.0081947444613071196
XIYY	0.0081947444613071196

XZZX	-0.0012708408559466877
XIZX	0.0012708408559466877
IZZX	0.0080251584900907554

XXZZ	-0.0028953260749665956
XXZI	-0.039154818592760 21
XXIZ	0.024279988585959714
IXZZ	-0.0097693536789154965
IXIZ	0.0080251584900907554

YYXZ	0.0081947444613071196
YYXI	0.0081947444613071196

YYYY	0.02892604472017965
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IIYY	0.029639606309848868

ZZYY	0.0028953260749665956
ZIYY	-0.039154818592760203
IZYY	0.024279988585959 71

XXZX	-0.0074989926703520624

YYZX	0.0074989926703520624

ZZZX	0.0097693536789154 93

ZXXZ	-0.0012708408559466 88
ZXXI	-0.0012708408559466 88
ZXIZ	0.0080251584900907554

ZXXX	0.0074989926703520624

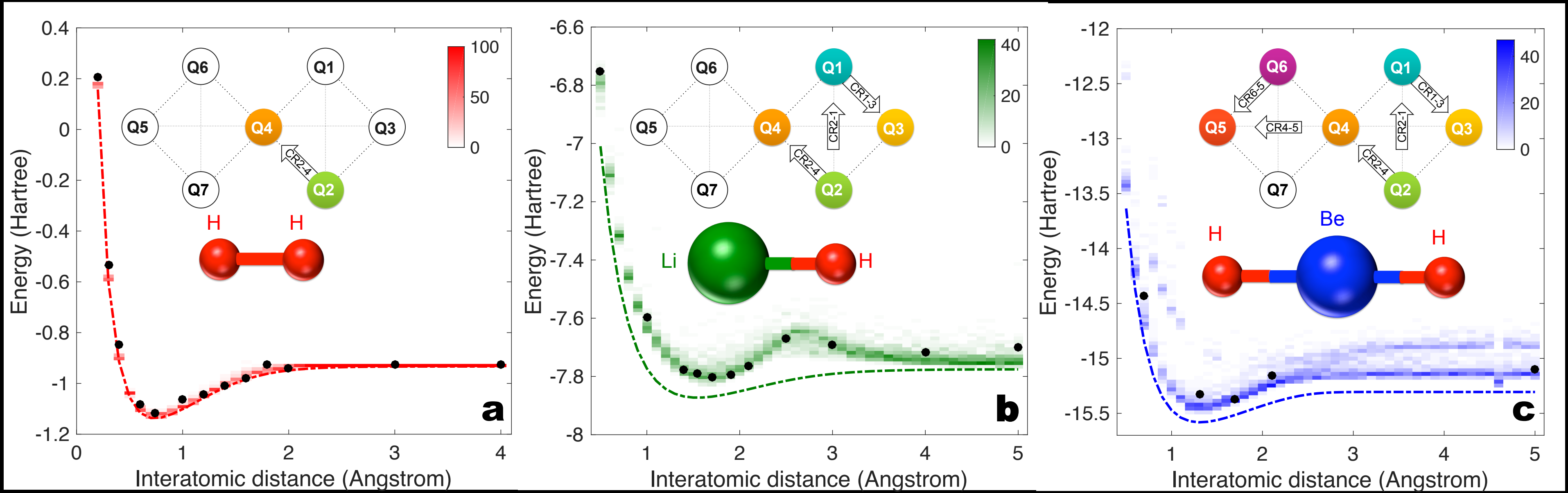
ZXYY	-0.0074989926703520624

XXXZ	-0.0081947444613071196
IXXZ	-0.0012708408559466 88

ZZYY	0.0028953260749665956
ZIYY	-0.039154818592760203
IZYY	0.024279988585959 71

LiH: 100 Pauli terms, 25 sets

VQE for quantum chemistry



H_2: 2 qubits
5 pauli terms, 2 sets

LiH: 4 qubits
100 pauli terms, 25 sets

BeH_2: 6 qubits
165 pauli terms, 44 sets

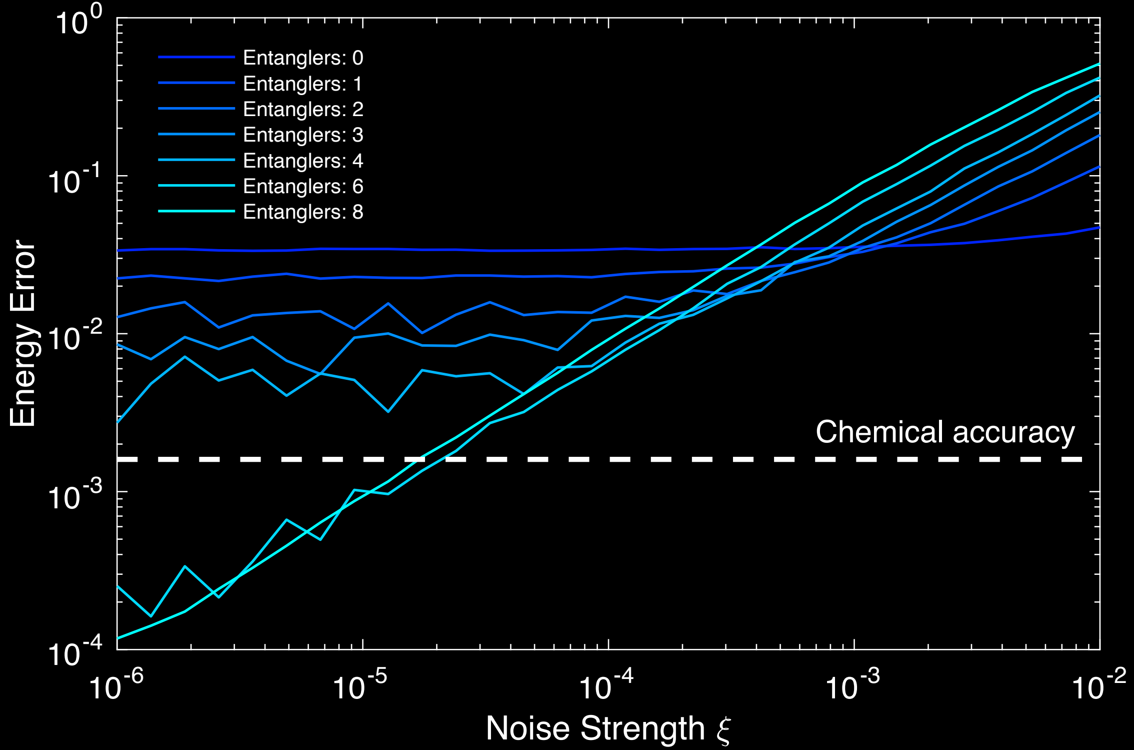
- Decoherence
- Sampling error
- Limited iterations

- Accuracy of the classical optimizer
- Insufficient depth

A. Kandala, A. Mezzacapo, et al, Nature **549**, 242-246 (2017)

Performance trade-off: Decoherence v/s Circuit depth

IBM **Quantum**



A. Kandala, A. Mezzacapo, et al, Nature **549**, 242-246 (2017)

Error mitigation

The longitude problem

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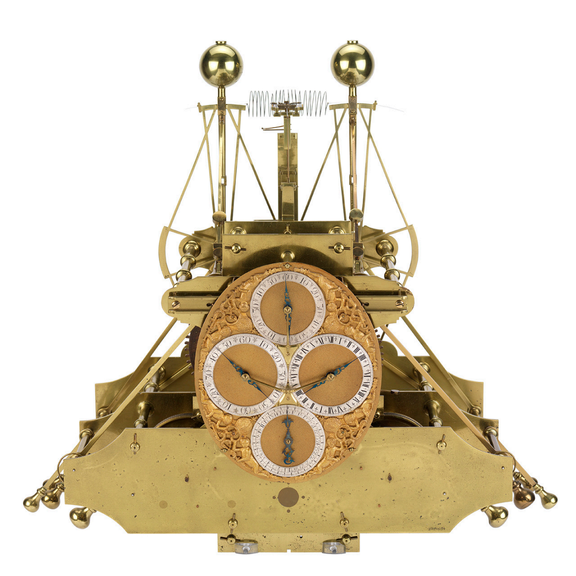
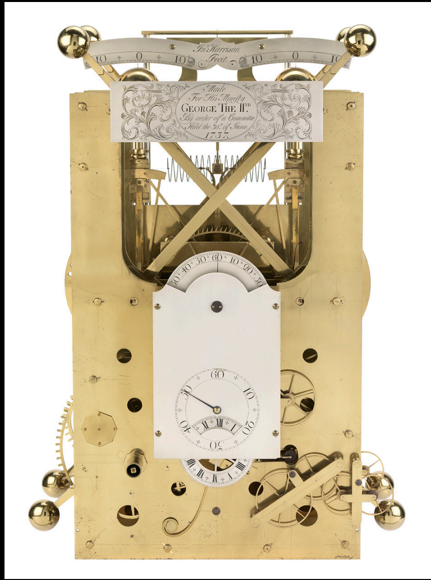
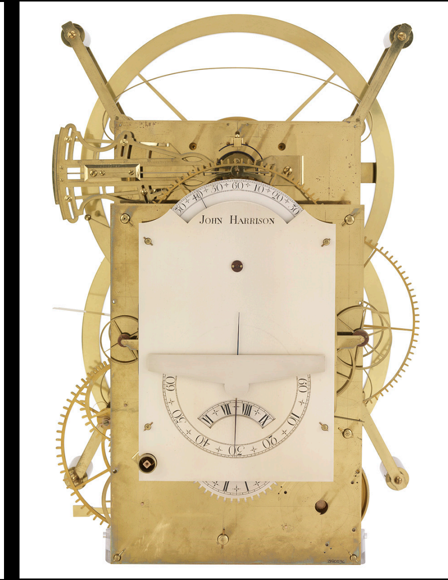


H1
1730-1735



H2
1737-1739



H3
1740-1759
Invention of
Bimetallic strip

H4
1755-1759

http://collections.rmg.co.uk

Zero-noise extrapolation

Expectation value of observable of interest:

$$E_K(\lambda) = E^* + \cancel{\sum_{k=1}^{n} a_k \lambda^k} + R_{n+1}(\lambda, \mathcal{L}, T)$$

Assume experimentalist has exquisite control over incoherent noise (T_1, T_2)

$$E_K(\lambda) = E^* + a_K \lambda + \mathcal{O}(\lambda^2)$$

$$E_K(c\lambda) = E^* + a_K c\lambda + \mathcal{O}(c^2\lambda^2)$$

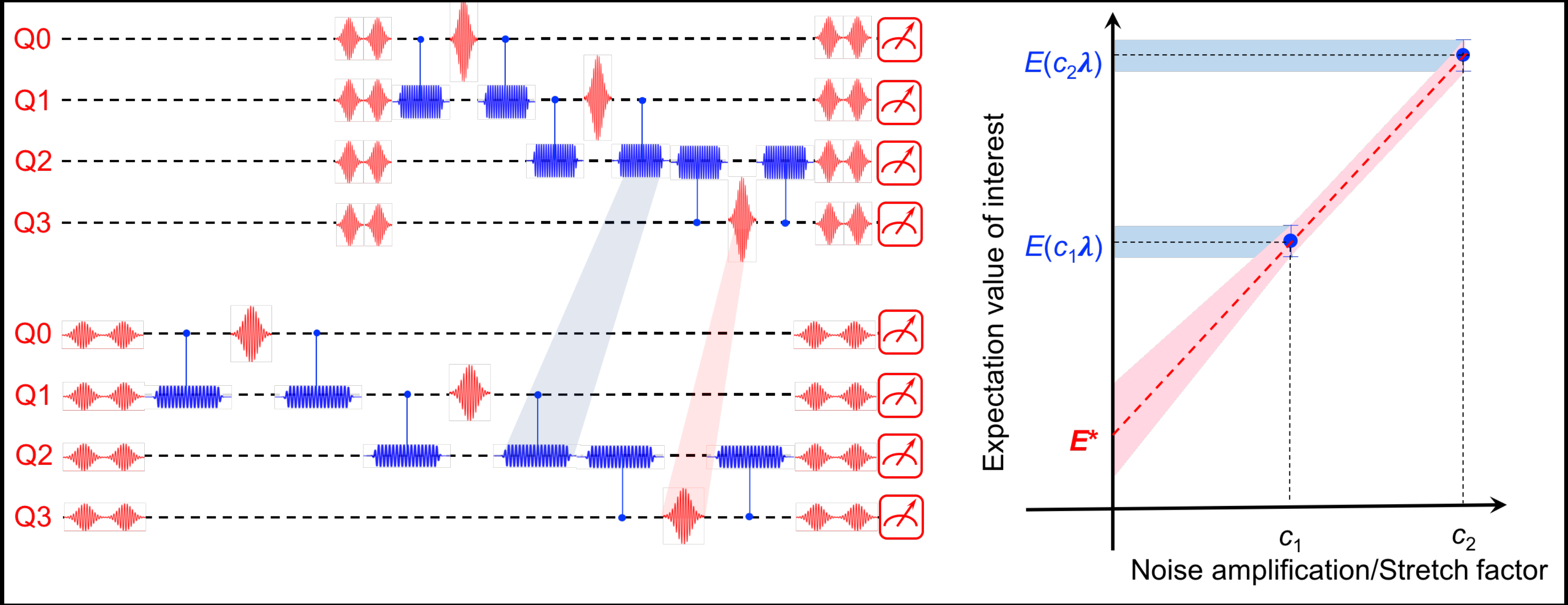
$$\hat{E}_K^2(\lambda) = \frac{cE_K(\lambda) - E_K(c\lambda)}{c-1} = E^* + \mathcal{O}(\lambda^2)$$

With *N* measurements, can reduce error in estimate to $\mathcal{O}(\lambda^N)$

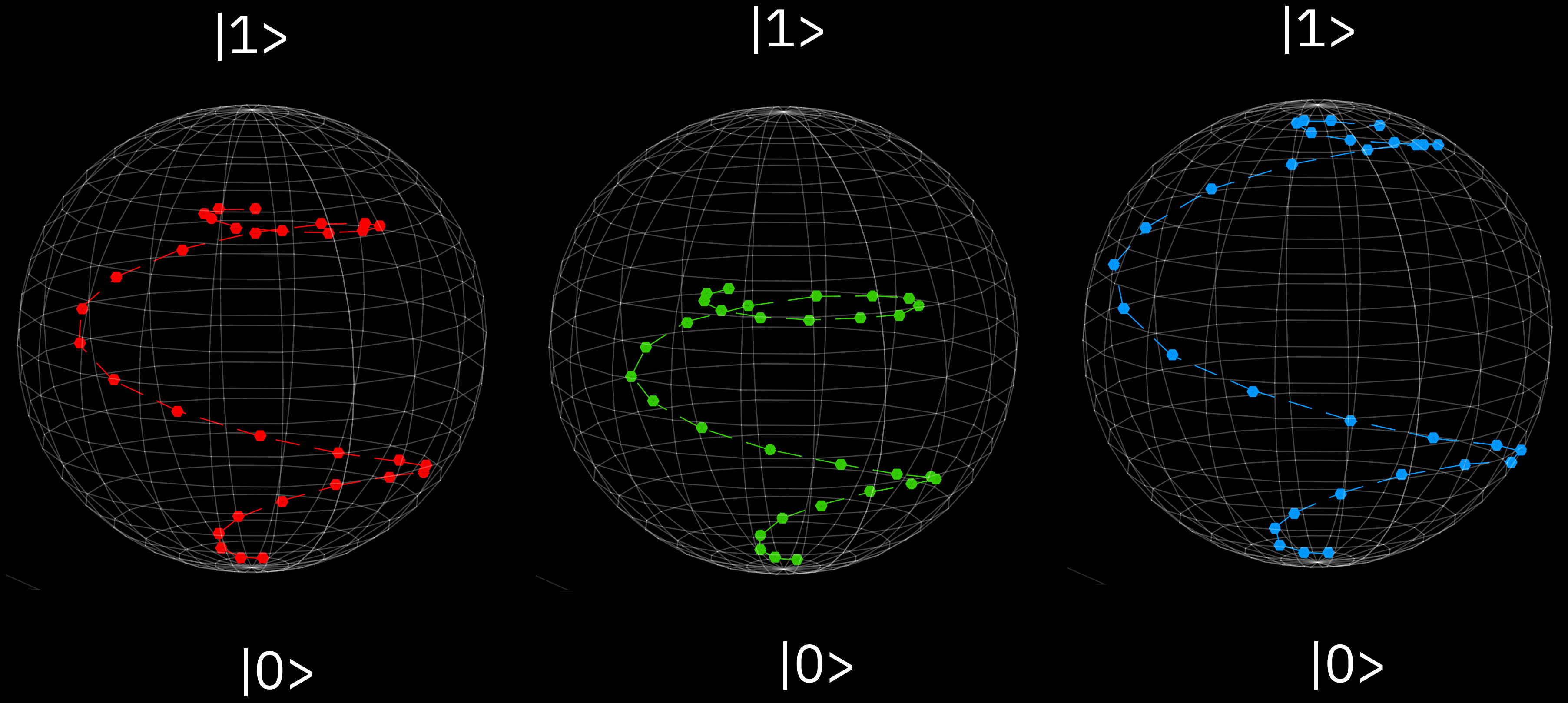
How does one measure $E(c_i\lambda)$??

When two wrong's make a right

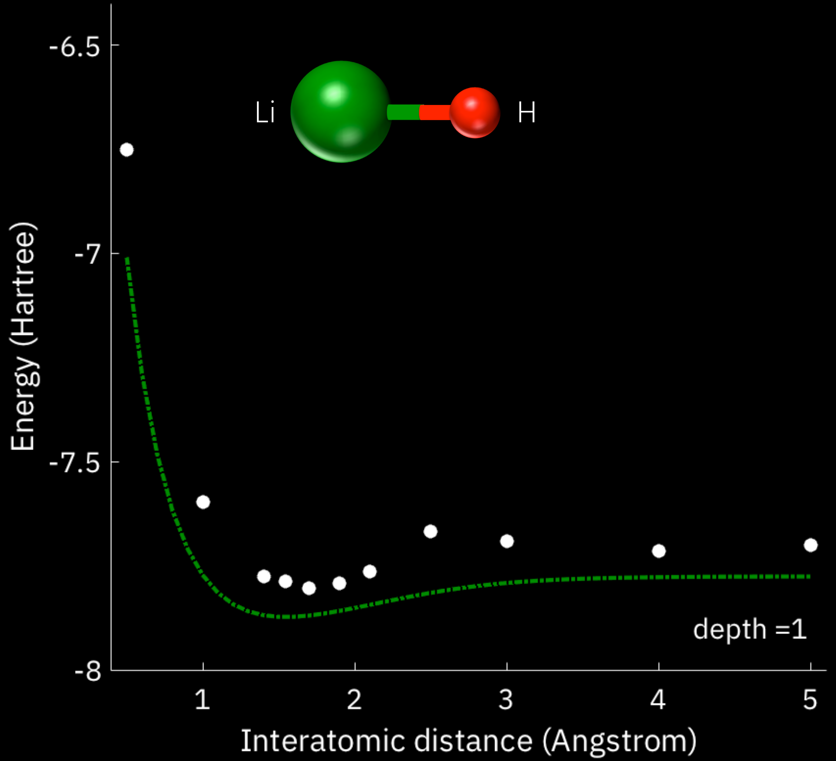
Amplifying noise strength equivalent to to rescaling dynamics under the assumption of time invariant noise.



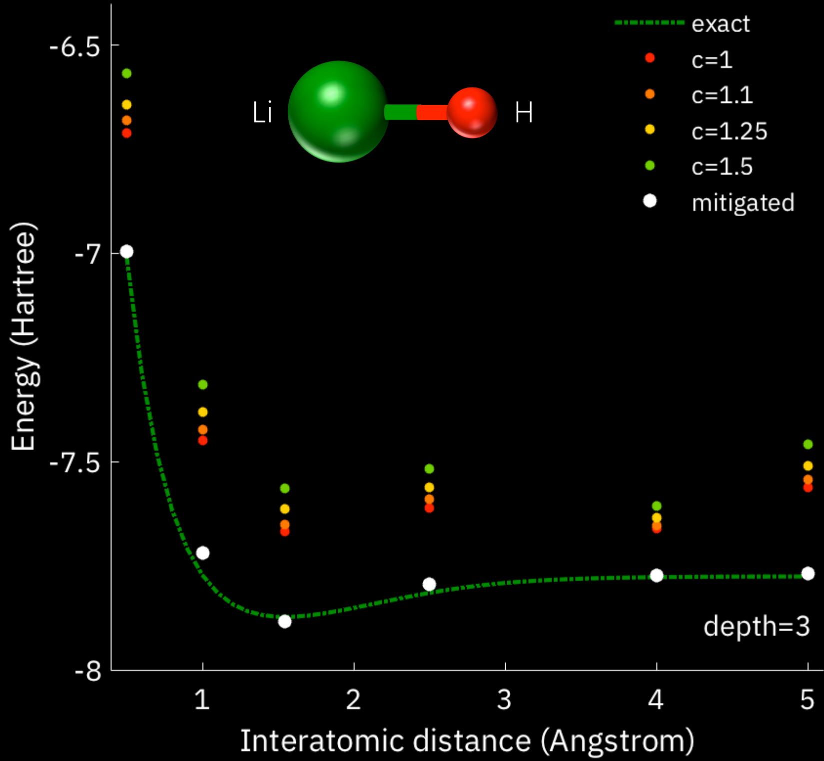
Error Mitigation: 1Q trajectory



Error Mitigation in molecular simulation: 4Q LiH

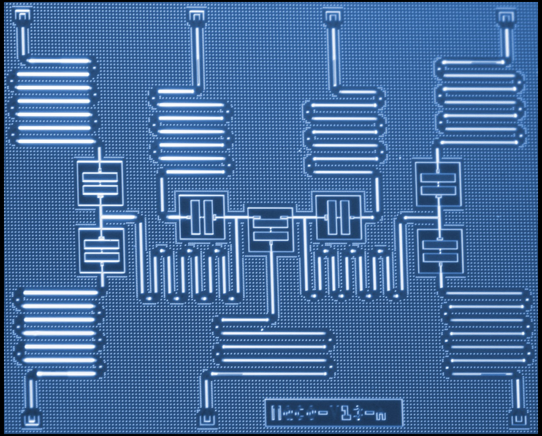


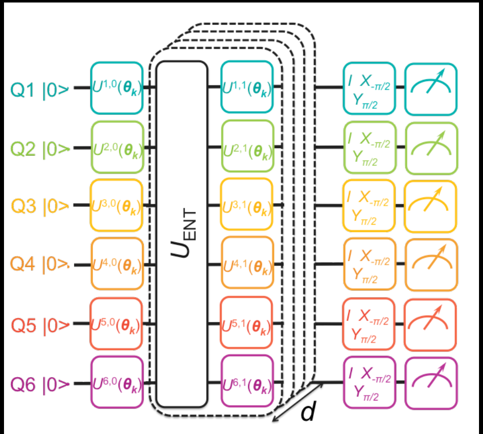
Kandala et al
Nature **549**, 242-246 (2017)

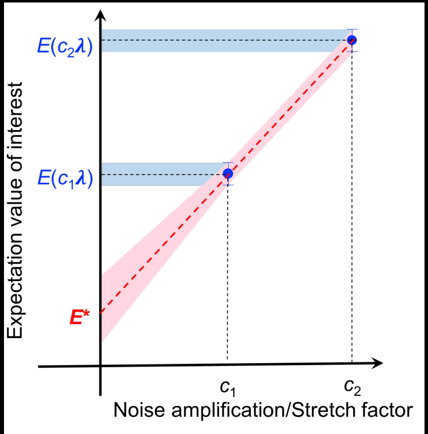


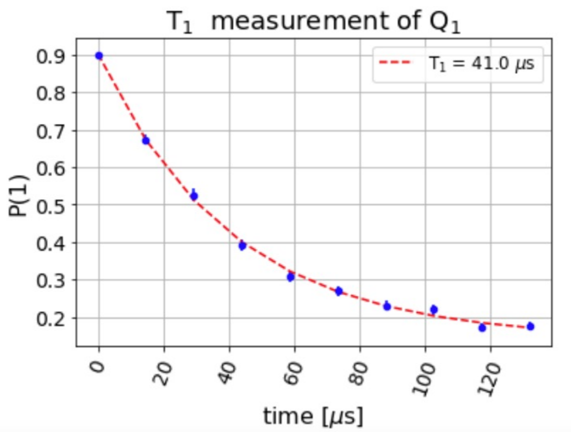
Kandala et al
Nature **567**, 491–495 (2019)

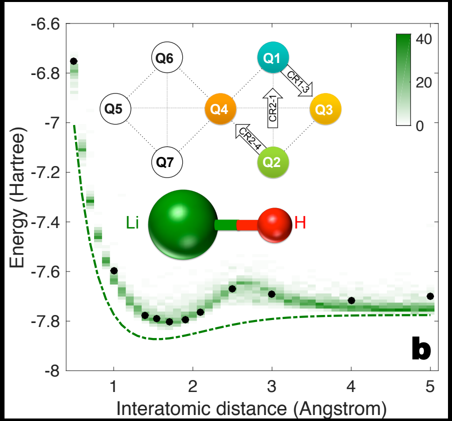
What we've covered today











Techniques go beyond just chemistry …

Qiskit Global Summer School

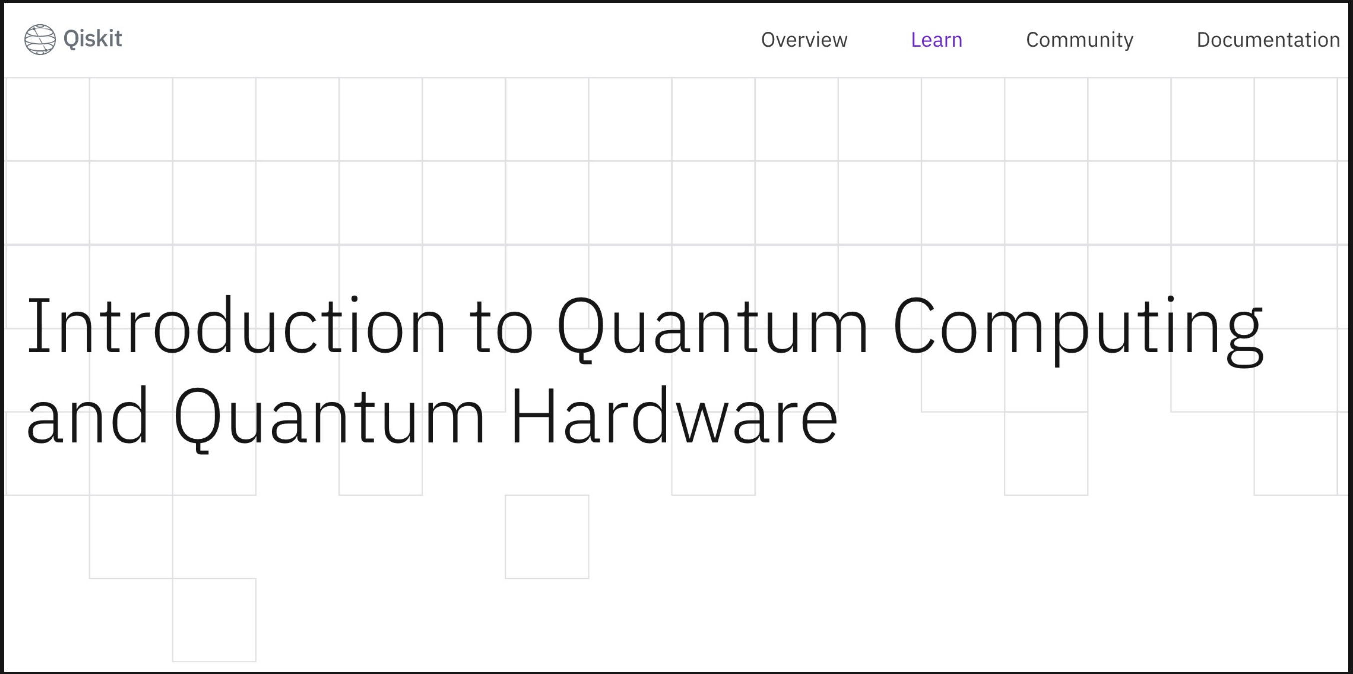
27 lectures

- From qubits to quantum chemistry applications.

Course materials

- Video recordings
- Lecture notes
- Hands-on labs

Course website



IBM Quantum Challenge