Simulating chemistry on a quantum computer II

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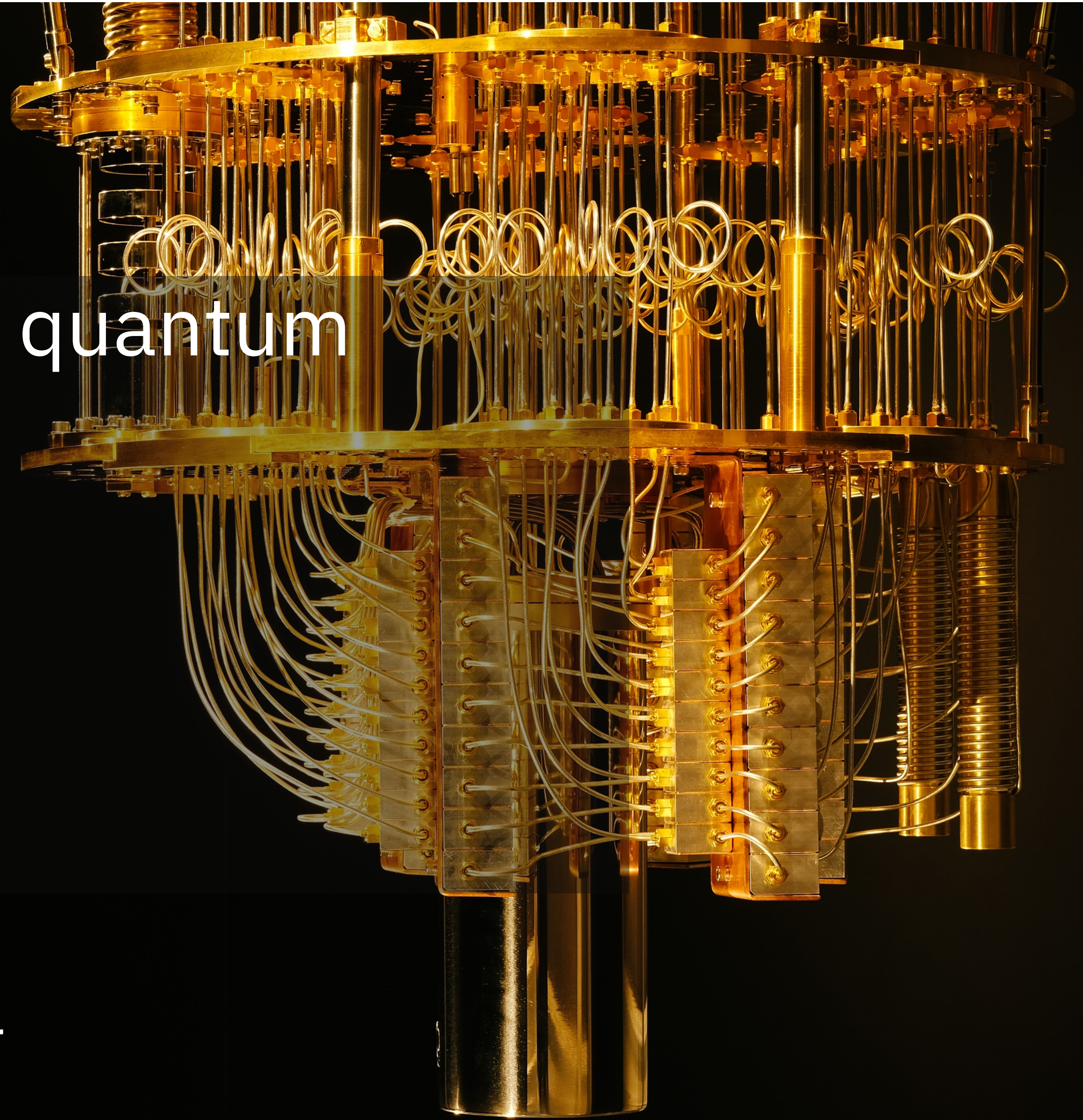
IBM Quantum

QISKIT Global Summer School
July 29, 2020



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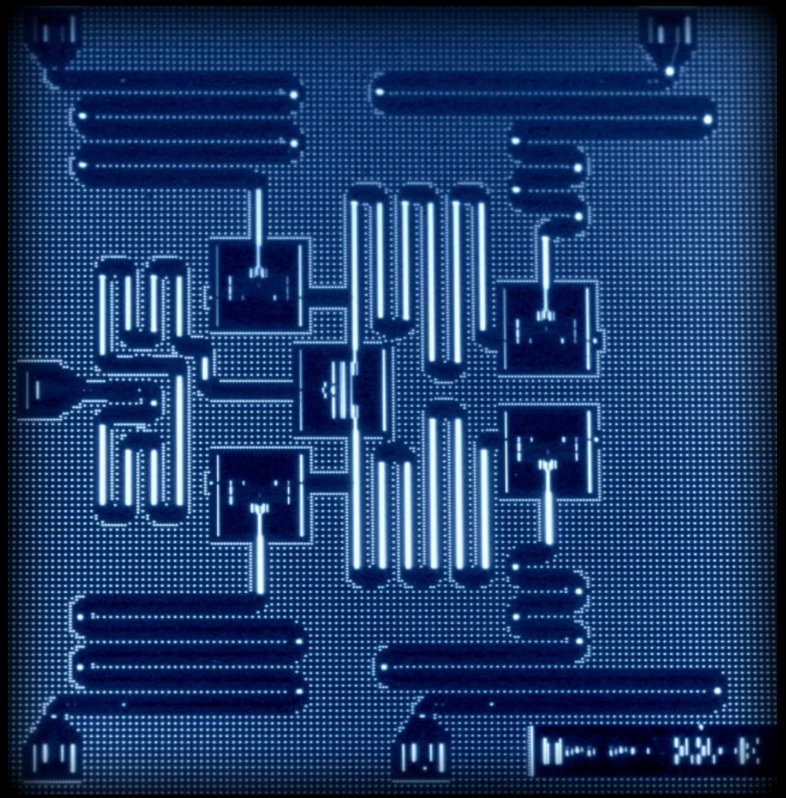
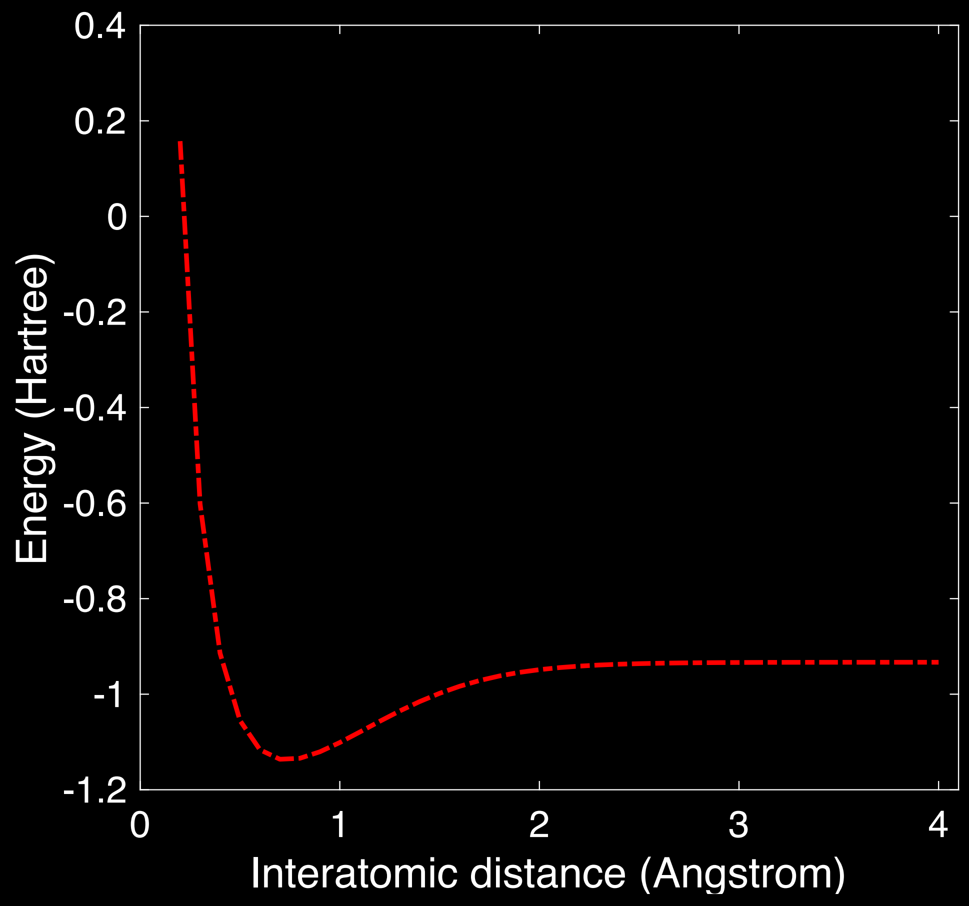
Motivations: Quantum hardware meets quantum algorithms





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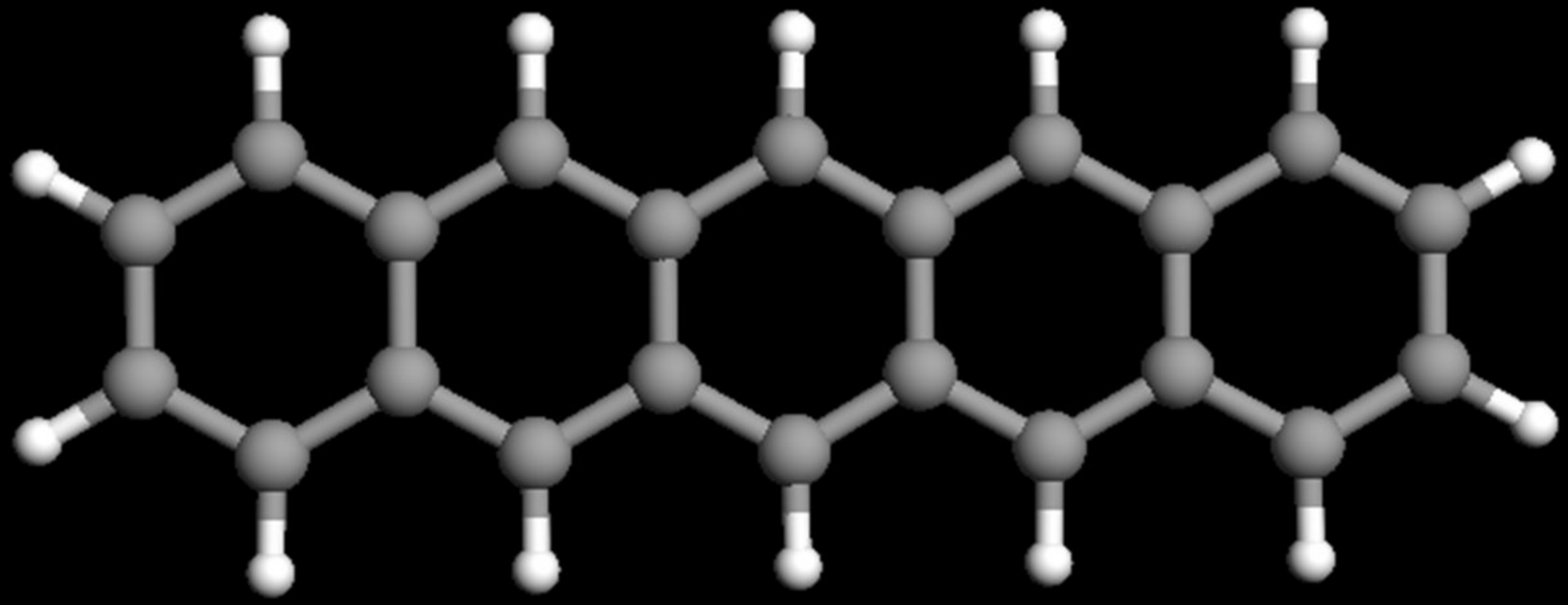
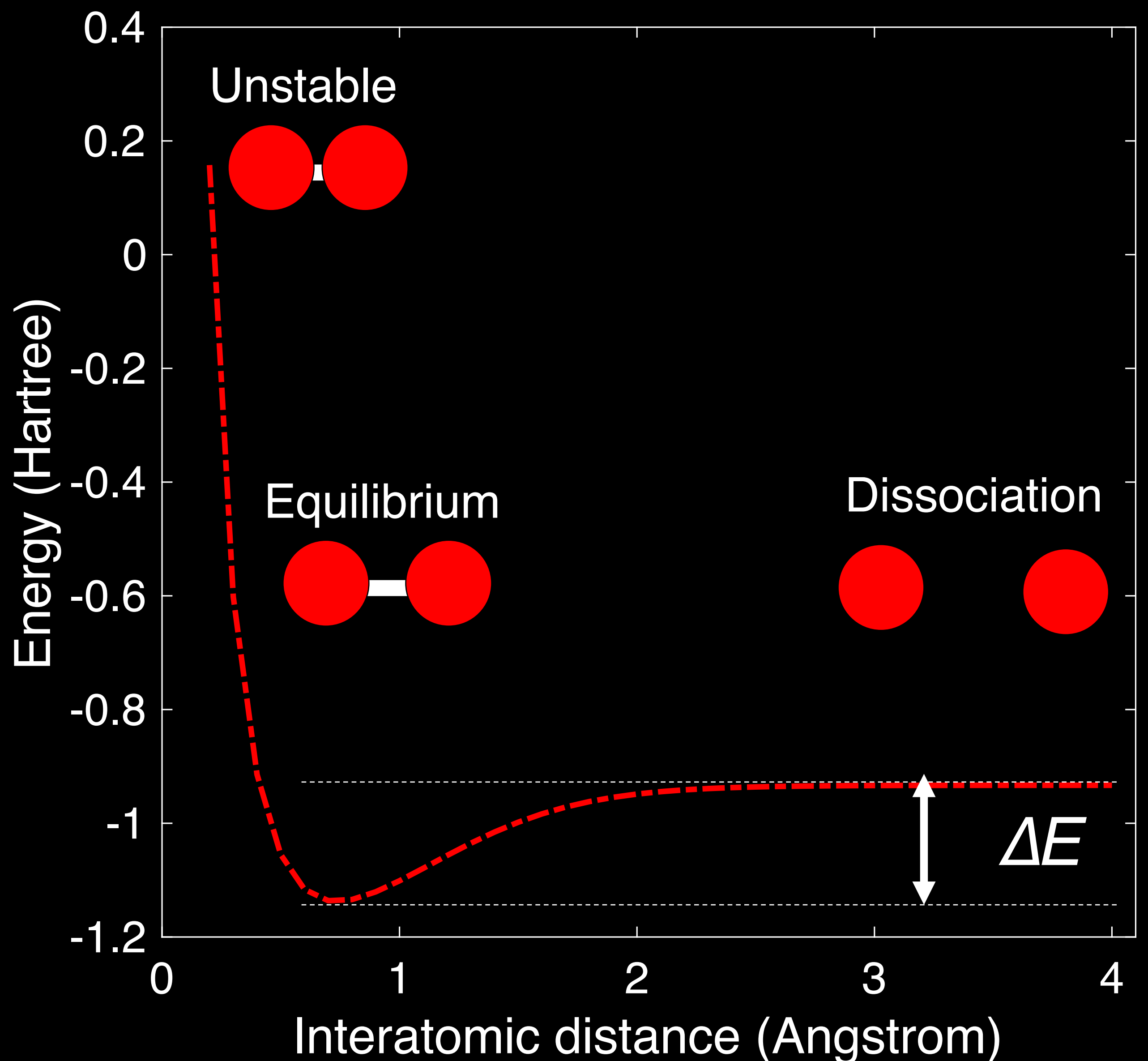


Potential energy curve of a molecule



Rate ∝ Exp($-\Delta E/kT$)

The Electronic Structure Problem

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

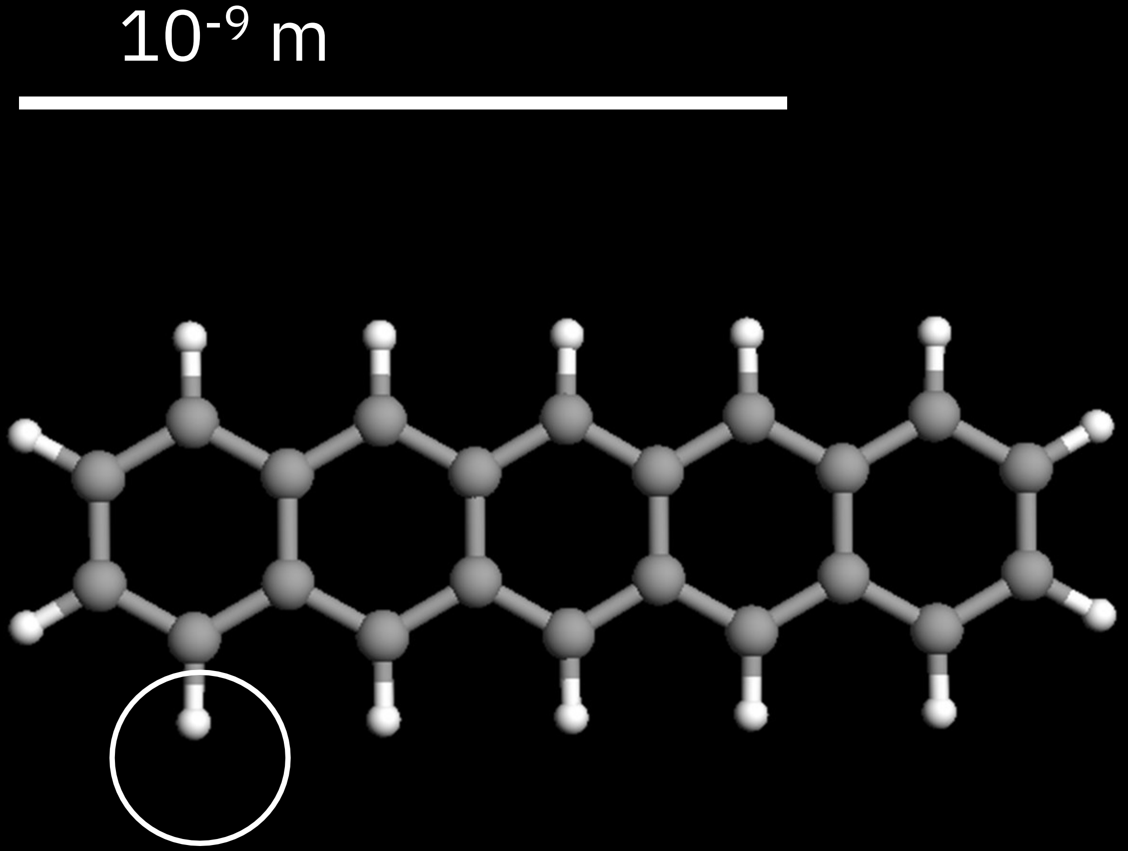
$$H_{\mathrm{e}} = -\sum_{i=1}^{N} \frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + \sum_{j>i} \frac{1}{r_{ij}}$$

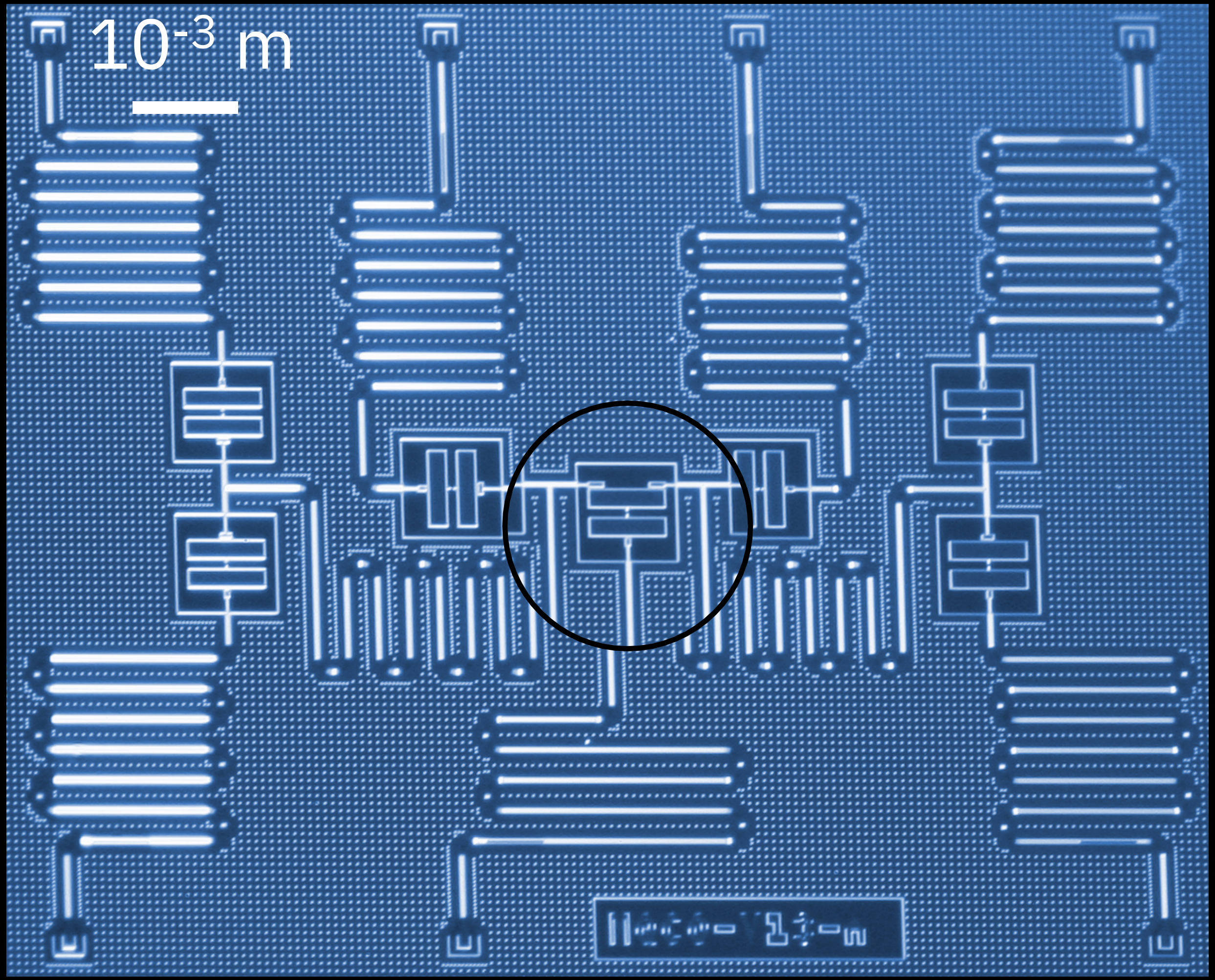
$$H|\psi_G\rangle = E_G|\psi_G\rangle$$

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

Natural atoms

Artificial Atoms





Classical

0

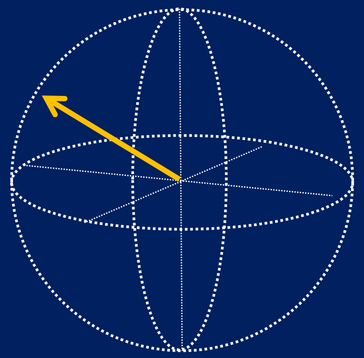
1

10110…1001

N bit number: 2^N possible states
Always in 1 of those states

Quantum

0



1

Quantum Bits (“Qubits”) can be in a superposition of 0 and 1

10110…1001
11010…1010
00100…1101
10110…1111

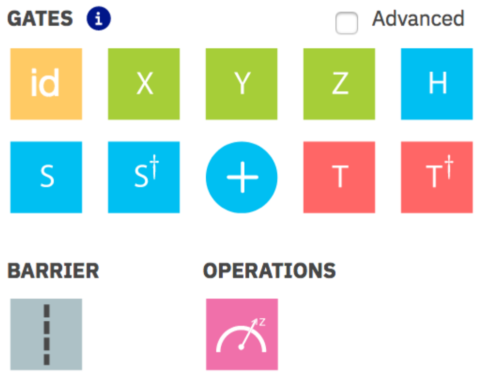
Can be in a superposition of all 2^N states

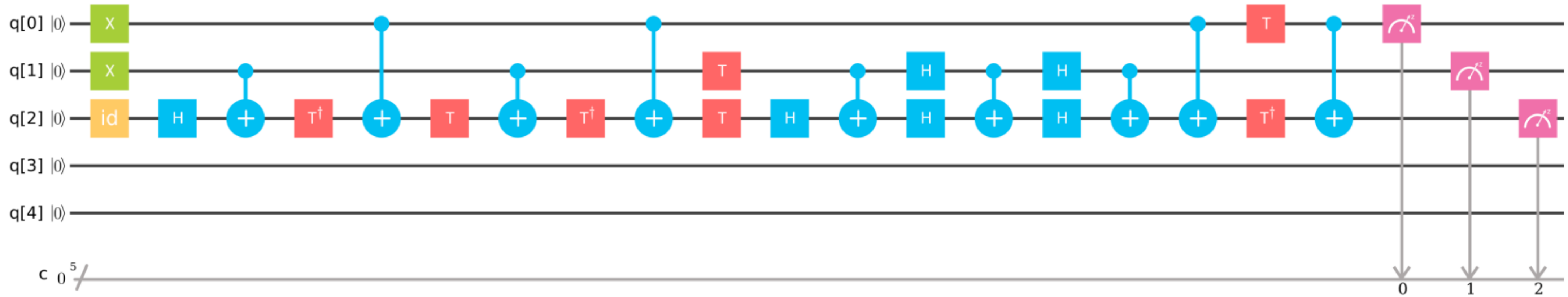
Quantum Circuits

Decompose unitary $U \in \mathbf{U}(2^N)$

$$|\psi\rangle = U|0\ldots 0\rangle$$

$$U = \mathrm{CNOT}_{0,2}\, T_0\, T_2^\dagger \ldots X_0\, X_1$$



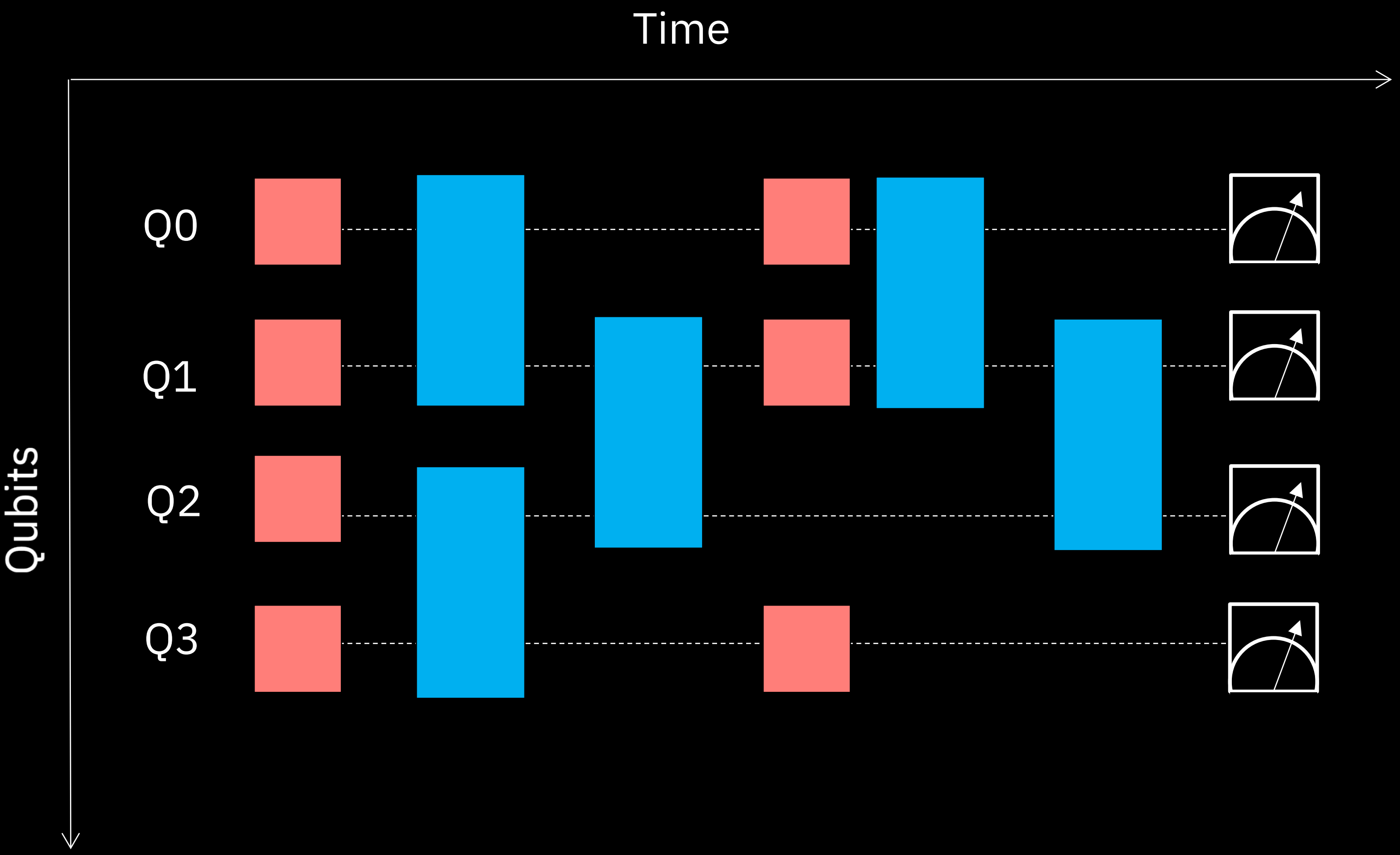


Universal gate set: CNOT (two-qubit gate) and single qubit rotations

David DiVincenzo, Two-Bit Gates are Universal for Quantum Computation, PRA 15, 1015 (1995)

Short depth circuits

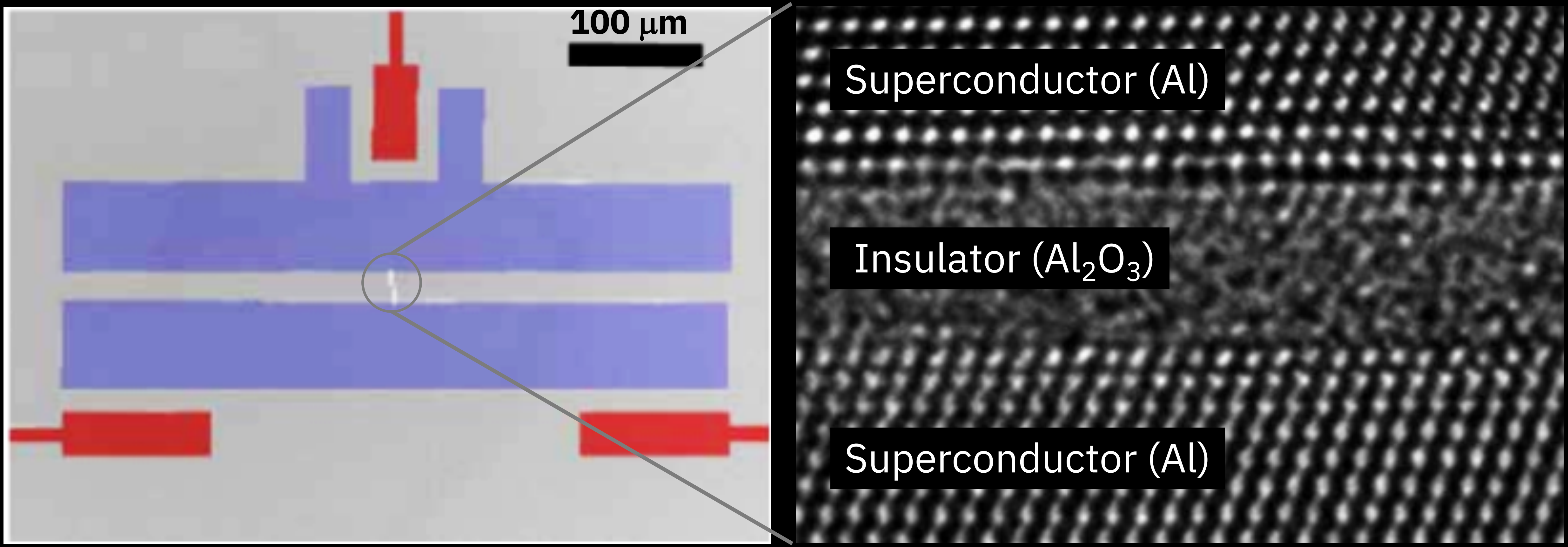
Approximate quantum computing with noisy quantum hardware



- 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

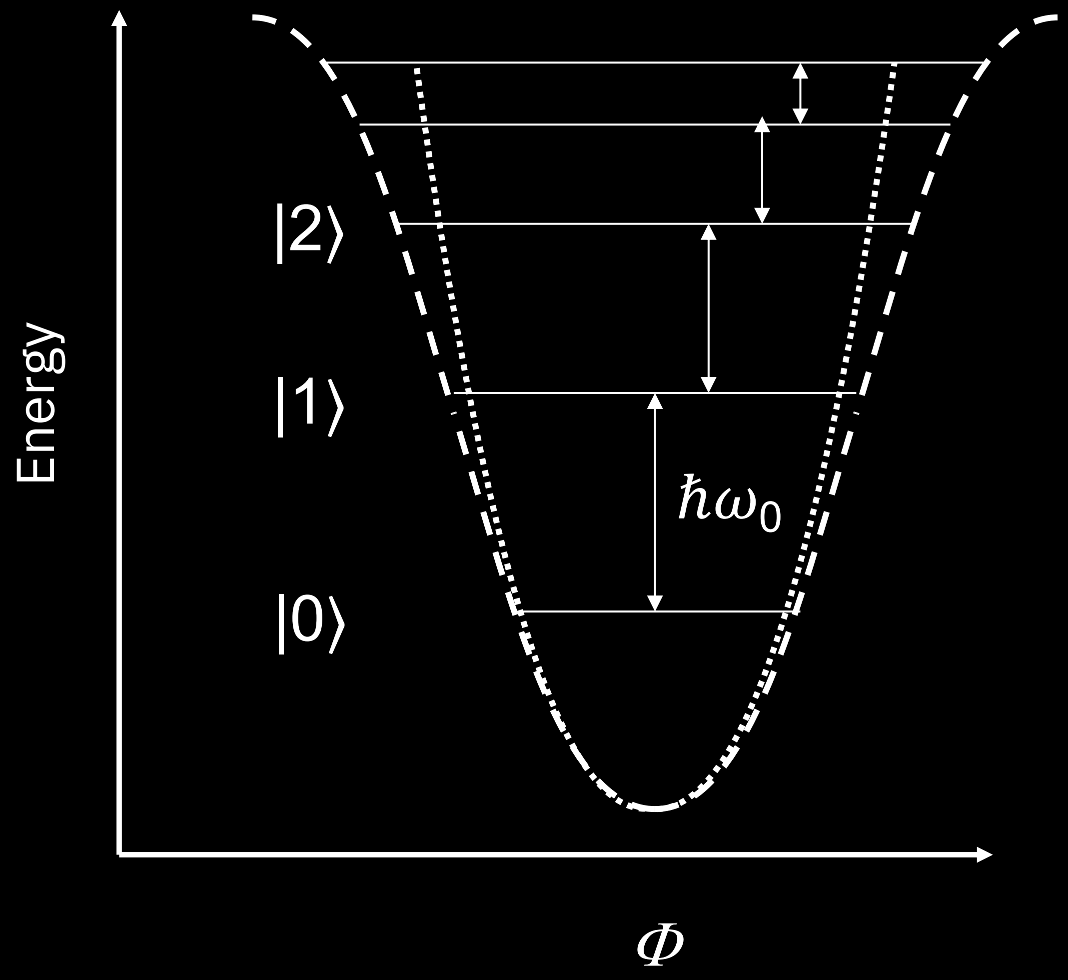
Quantum Hardware recap ..

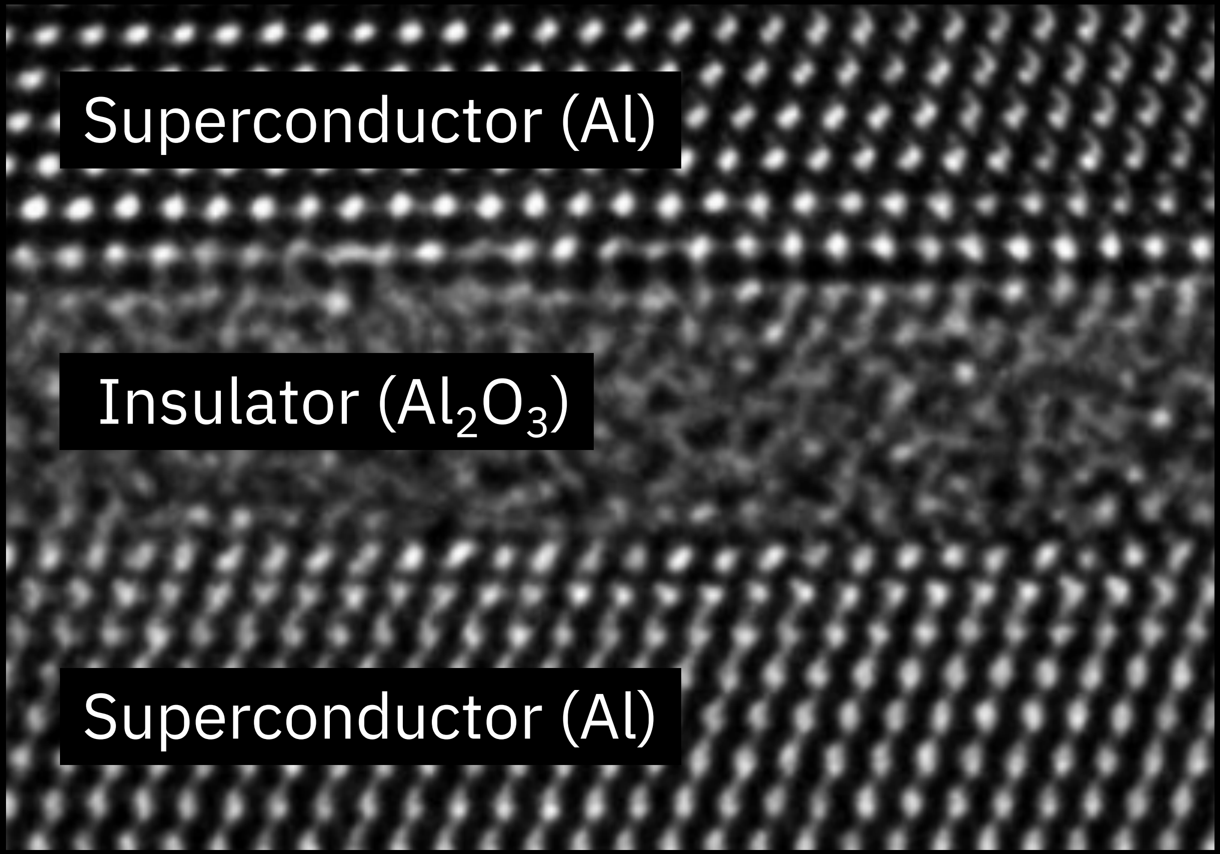
Artificial atom: Transmon



JAP, 125(16), 165301, 2019

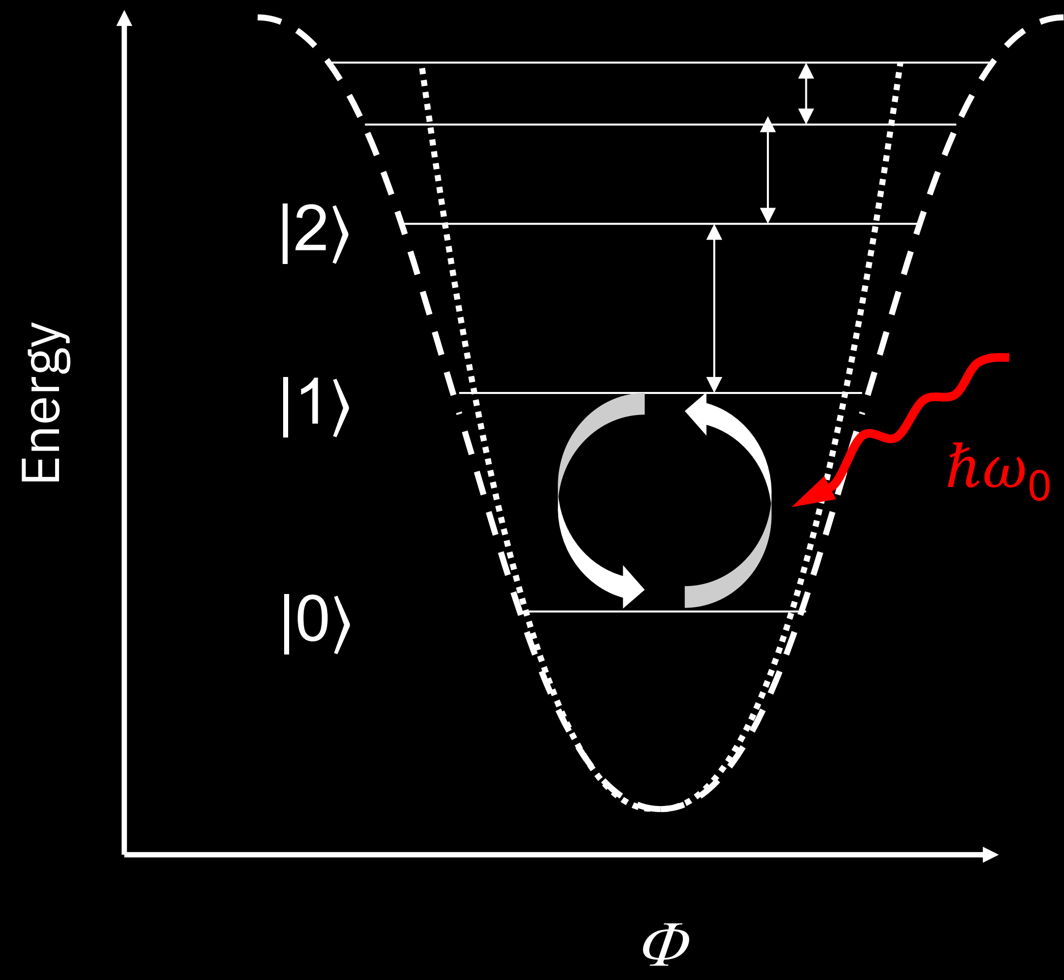
Artificial atom: Transmon





JAP, 125(16), 165301, 2019

Single qubit control: Rabi Oscillations



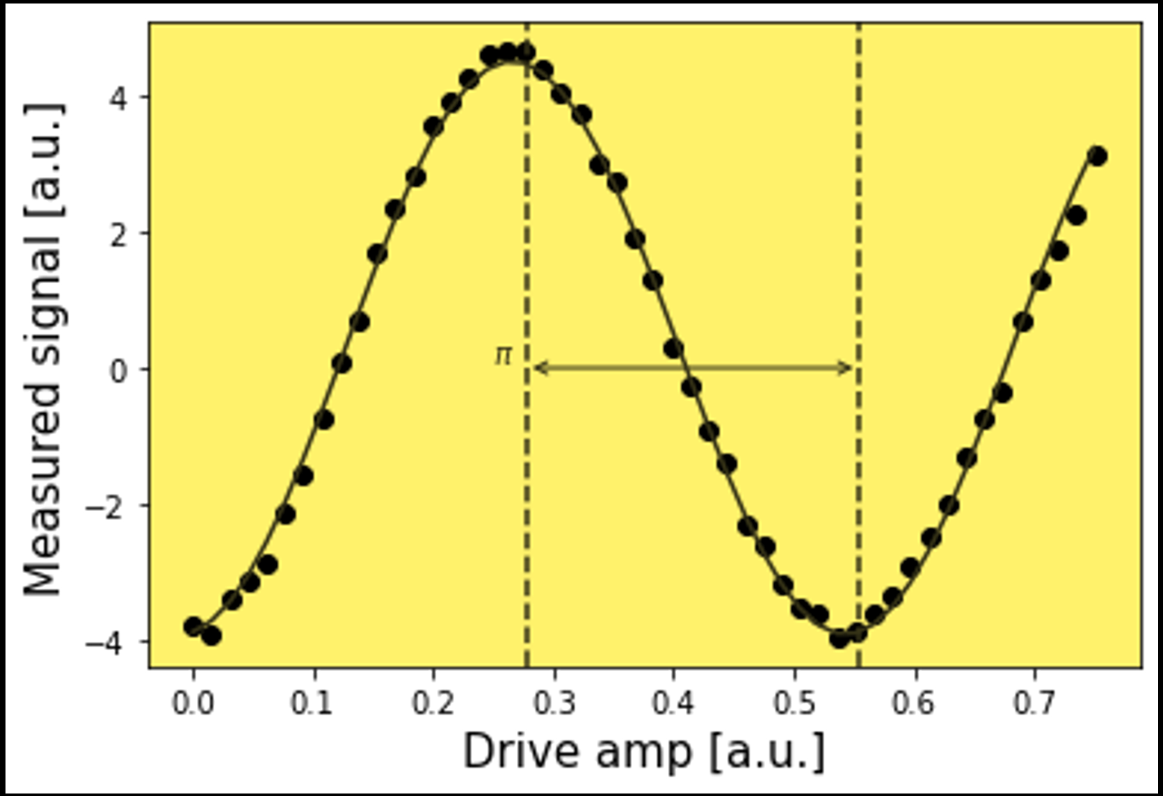


Image: QISKIT textbook

Single qubit control: Rabi Oscillations

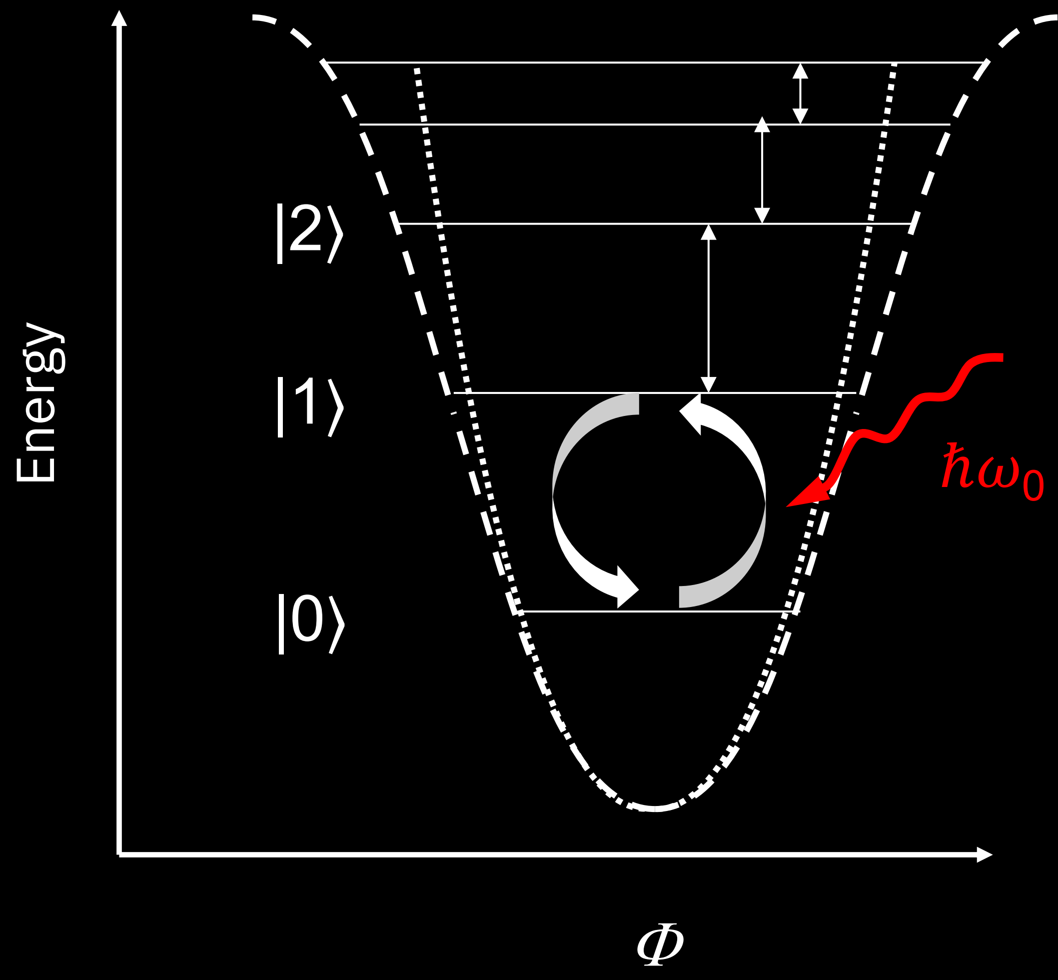
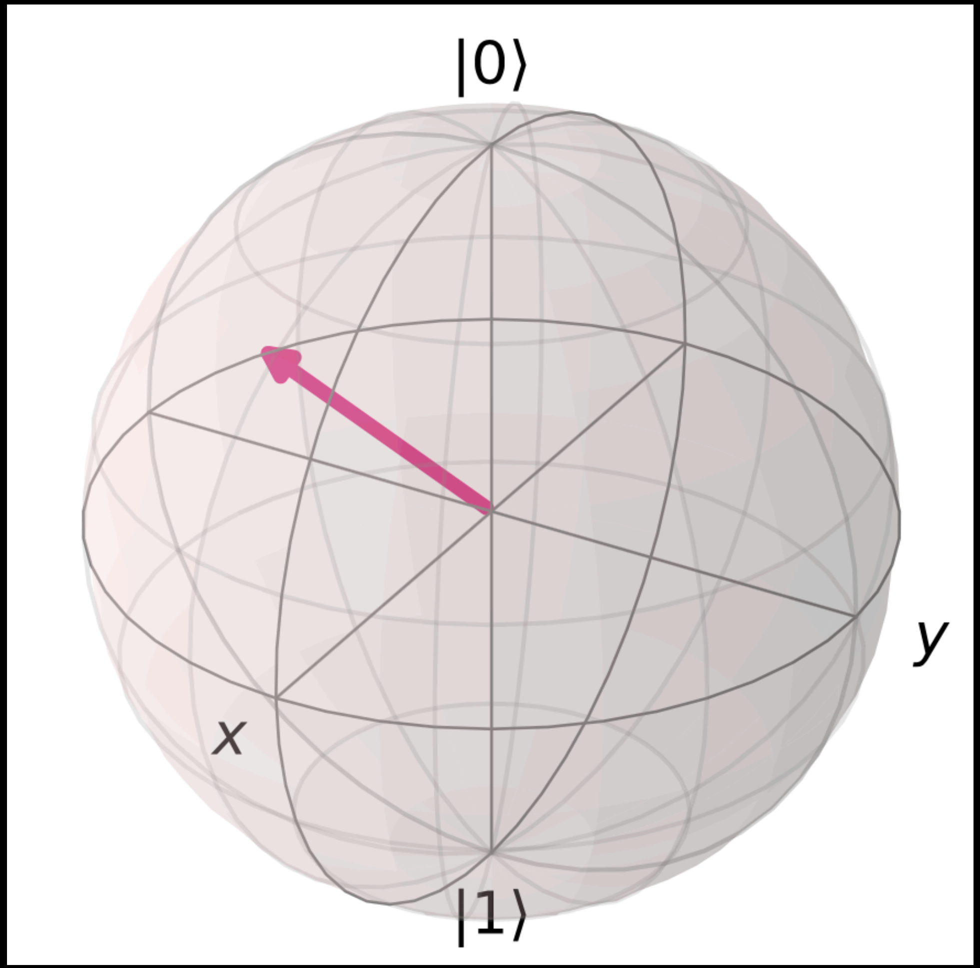


Image: QISKIT textbook



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

Two-qubit entangling gates

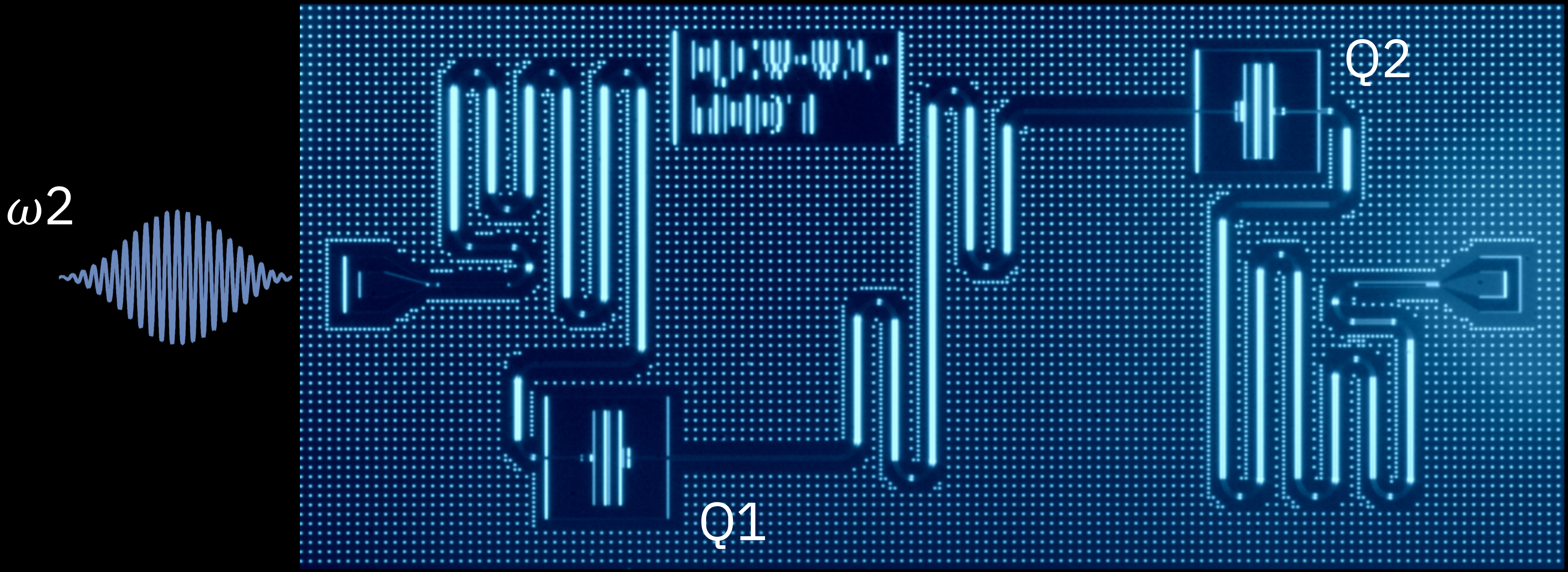
Apply operations on two qubit product states to create an entangled state, i.e. one that cannot be factored into its individual qubit components.

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



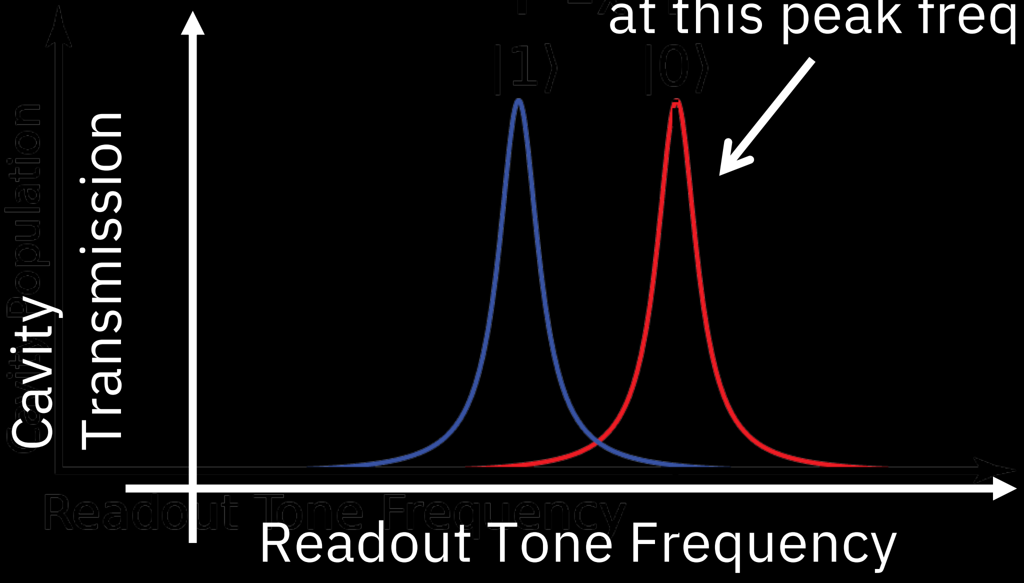
Can generate a CNOT with only microwave pulses

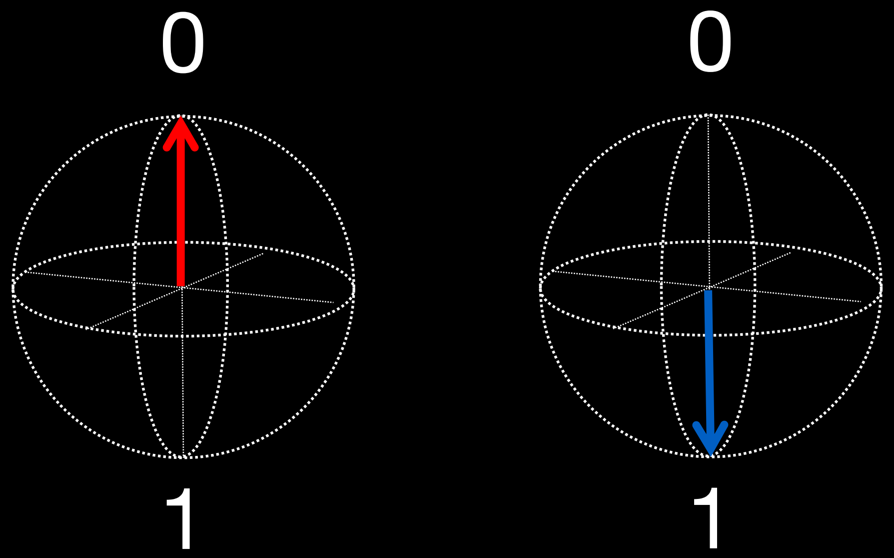
Dispersive readout

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

Qubit State dependent resonator frequency

Monitor transmission at this peak frequency





High transmission

Low transmission

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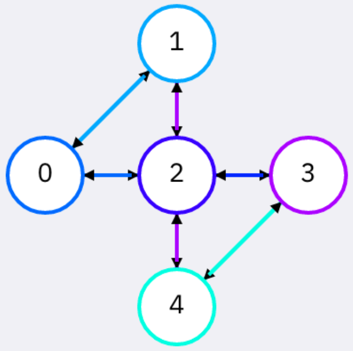
Superconducting quantum processor: ibmq_5_yorktown

○ Qubits ⇅ Connectivity



Single-qubit U2 error rate

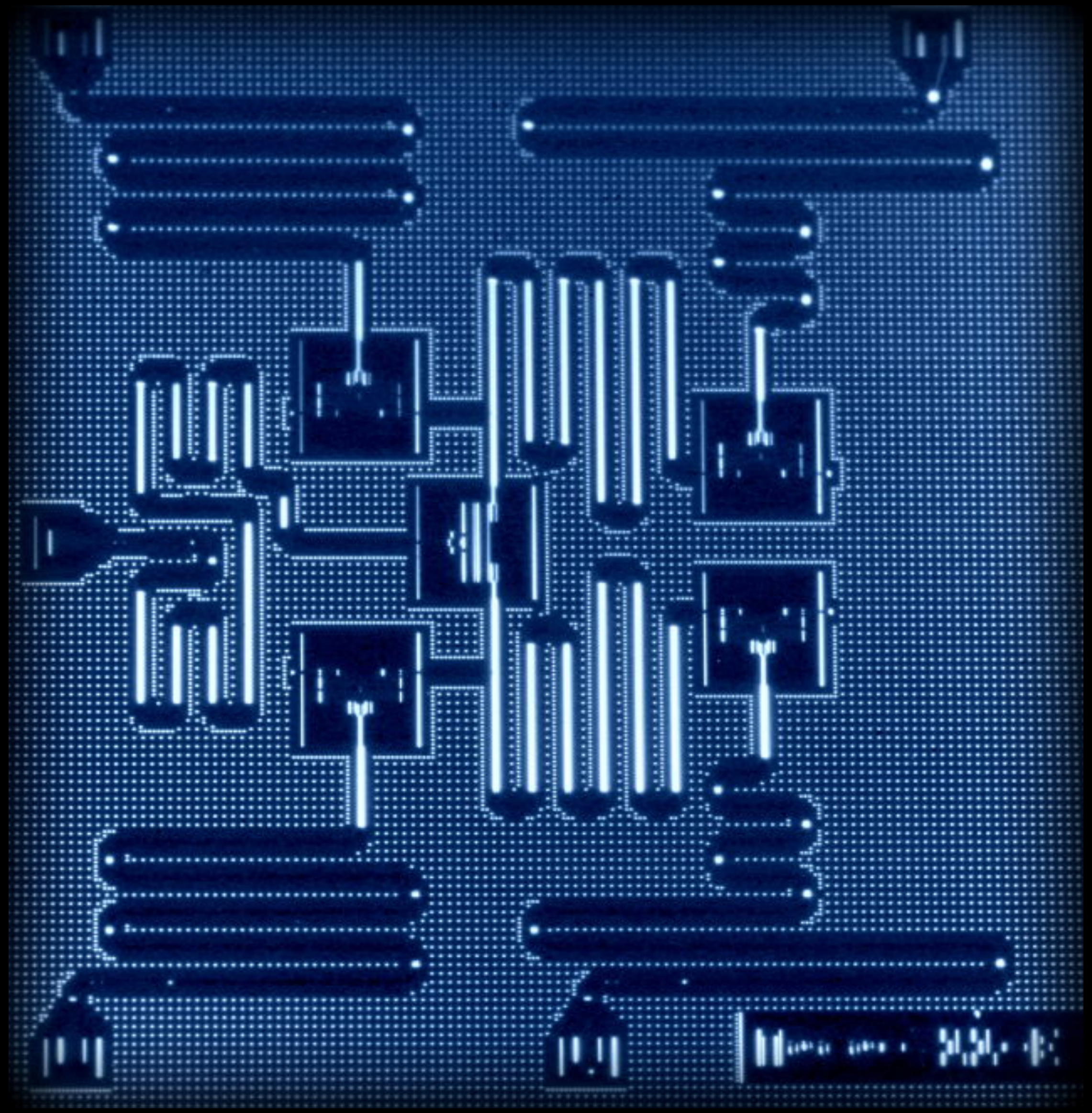
4.169e-4 9.786e-4

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?

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

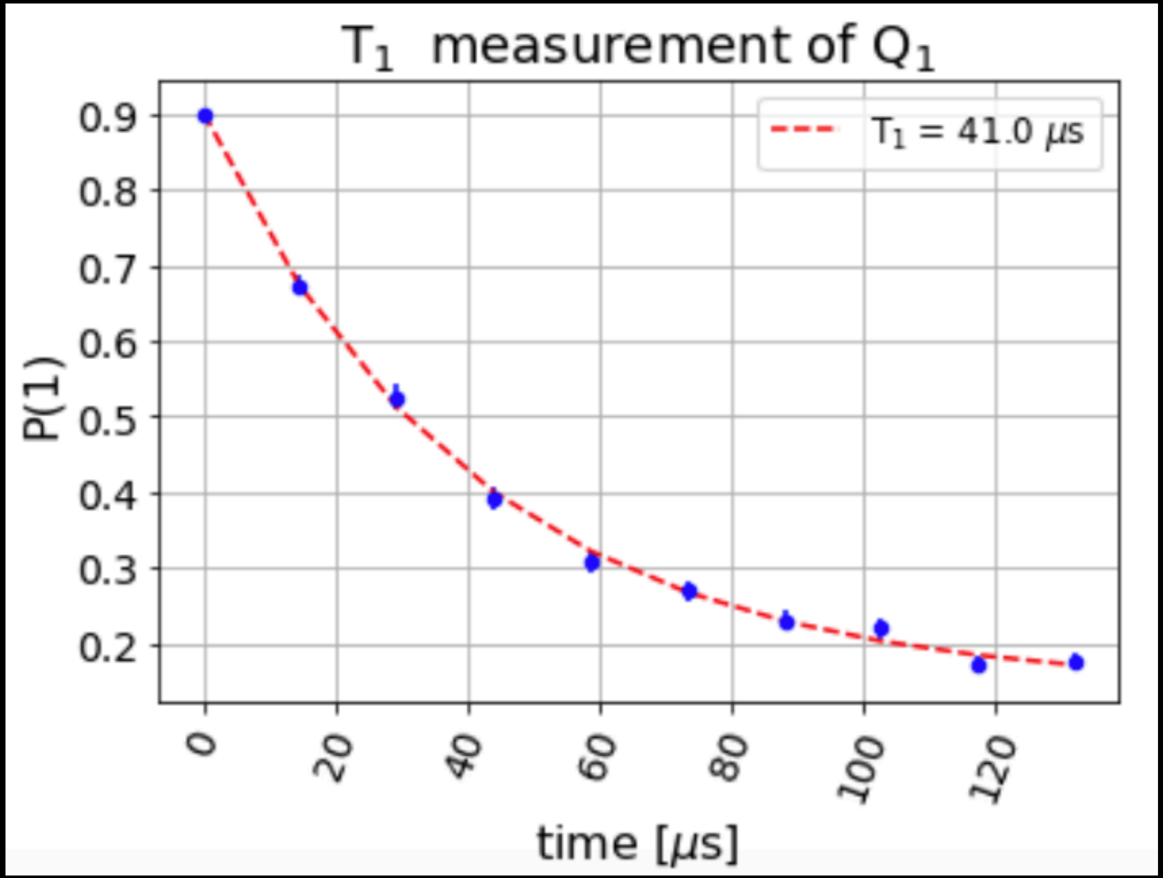
Hardware errors

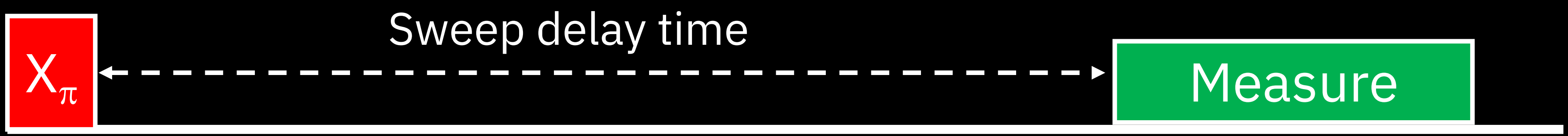
Errors

- Incoherent
- Leakage
- Coherent
- Measurement

Incoherent errors: Energy relaxation

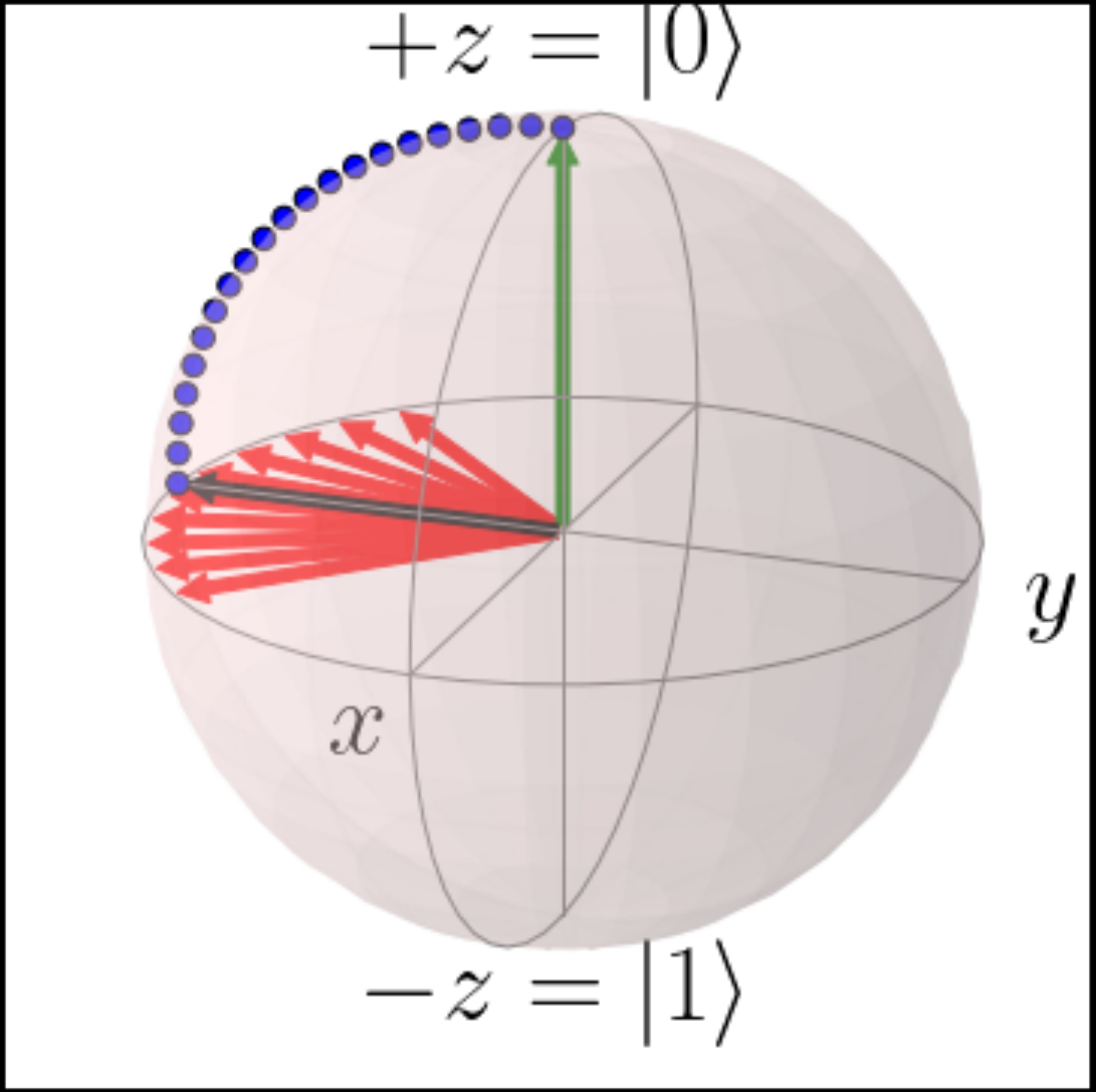
- Initialize qubit in |1> state and probe its decay to |0>
- How quickly does the qubit lose its energy?
- P(|1>) = exp{-t/T_1}

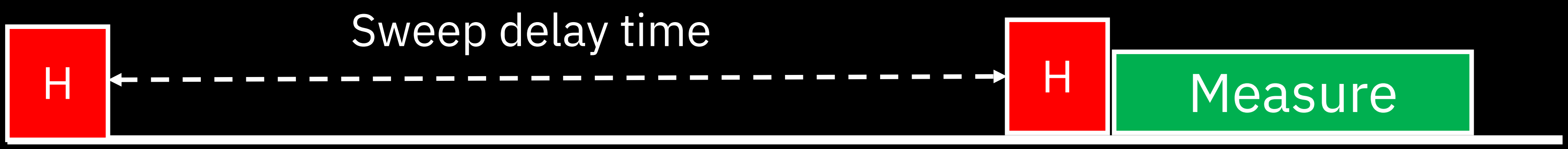




Incoherent errors: Dephasing

- Initialize qubit in superposition state
- How quickly does the qubit lose its phase coherence?
- Characteristic time: T_2





Coherence budget

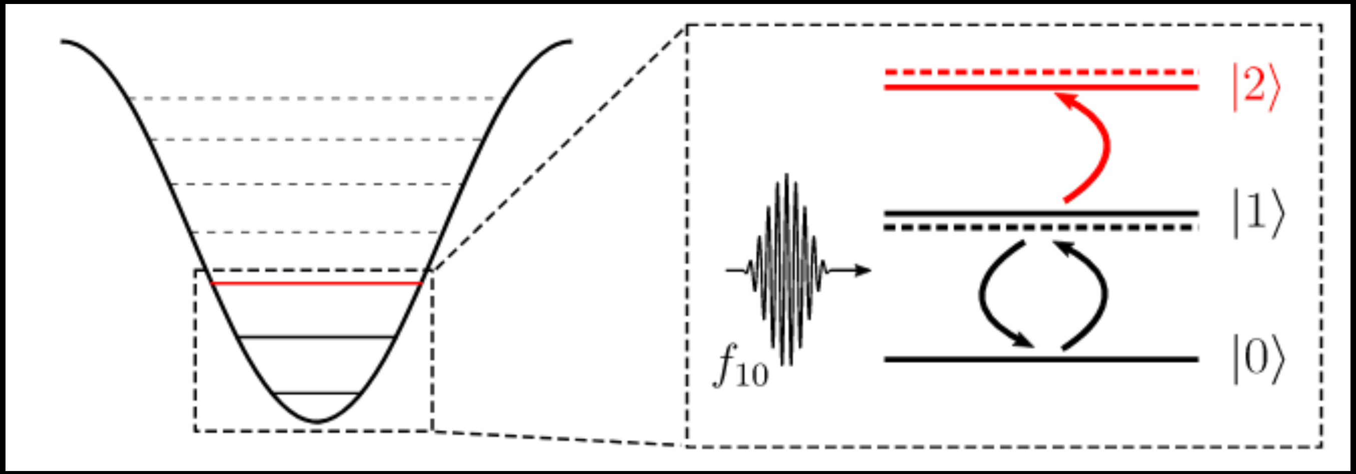
Single qubit gate time ~ 0.01×10^{-6} s

Two qubit gate time ~ 0.1×10^{-6} s

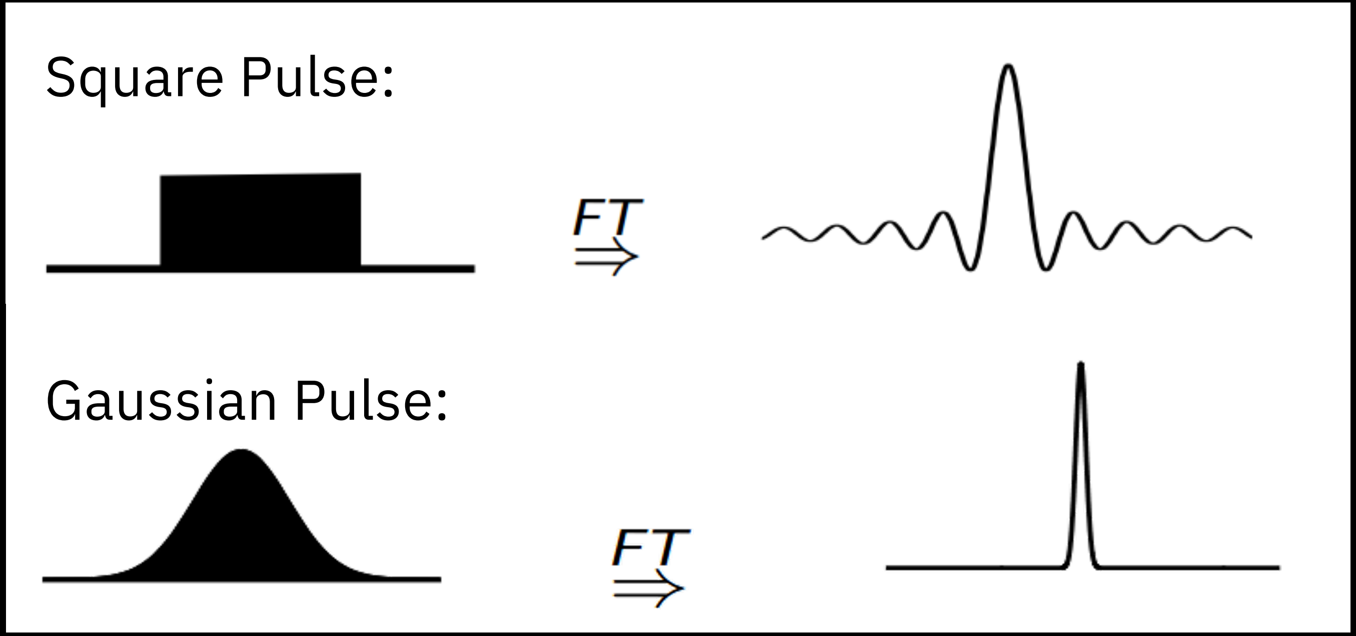
T_1 , T_2 ~ 100×10^{-6} s

Leakage errors

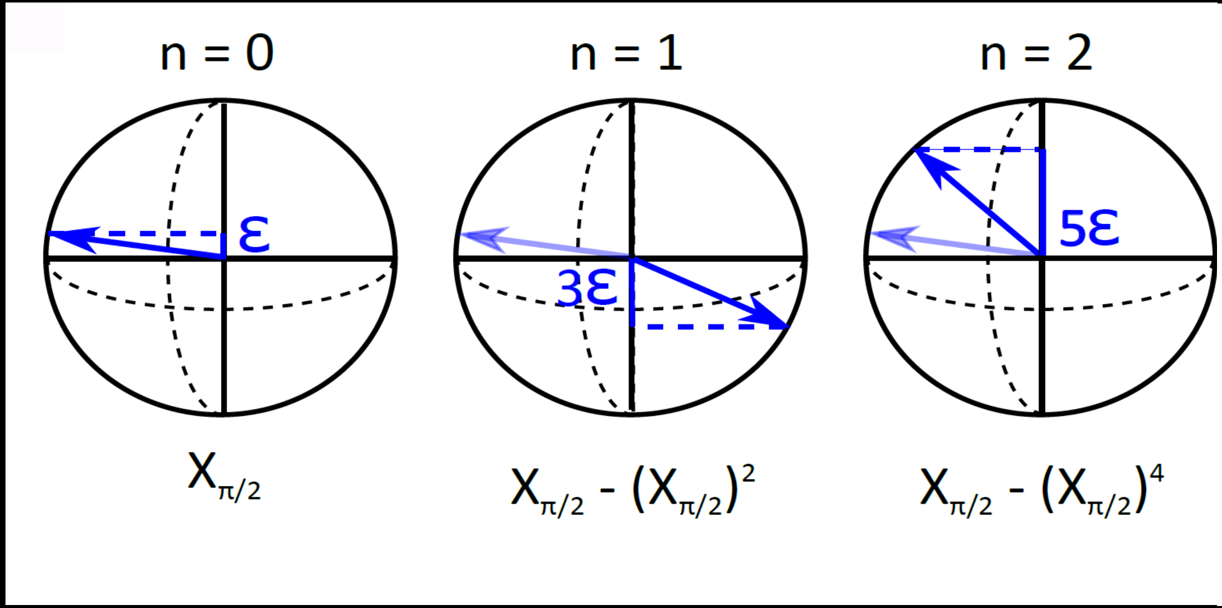
- Transmon qubits are weakly anharmonic ($\boldsymbol{\omega}_{01}$- $\boldsymbol{\omega}_{12}$ ~ 0.330 GHz). Not true two-level systems.
- Can place limits on gate speed
- **Leakage out of computational subspace**
- Pulse shaping is important

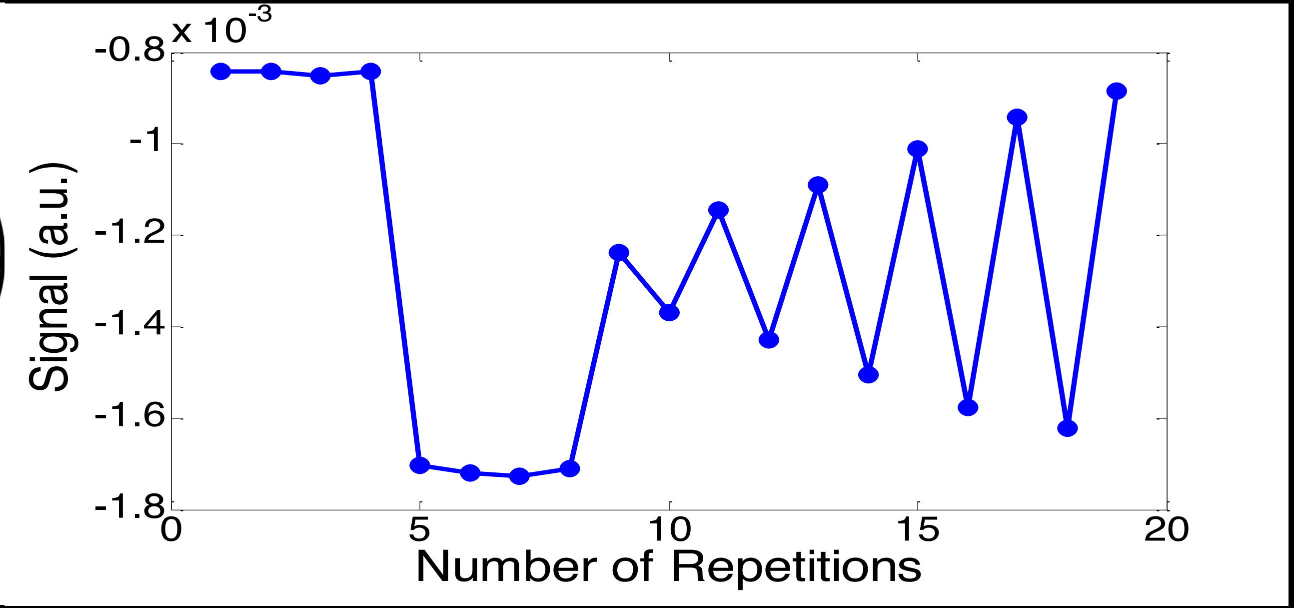


PRL 116,020501 (2016)

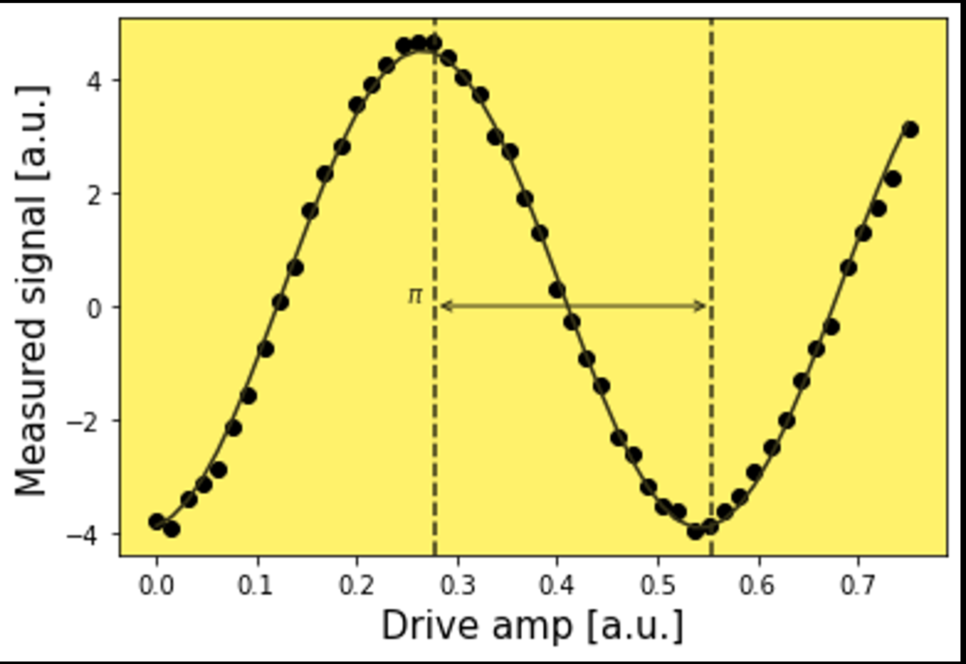


Coherent errors





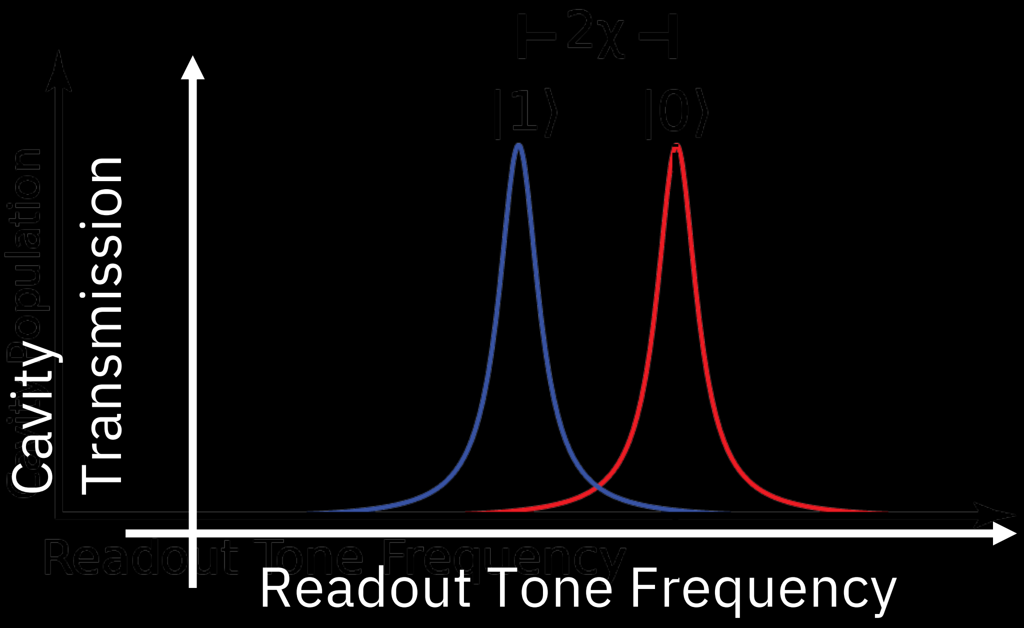
Example: Under/Over rotations



Measurement errors

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

Qubit State dependent resonator frequency



Monitor transmission
at this peak frequency

Example:

Prepare ‘0’
Measured {‘0’ : 99%   ‘1’: 1%}

Prepare ‘1’
Measured {‘0’ : 5%   ‘1’: 95%}

Measurement fidelity: 97%

Back to chemistry

The Electronic Structure Problem

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

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

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

The problem and its qubit representation

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

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

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

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

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 ...

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

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

Variational Quantum Eigensolver (VQE)

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

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

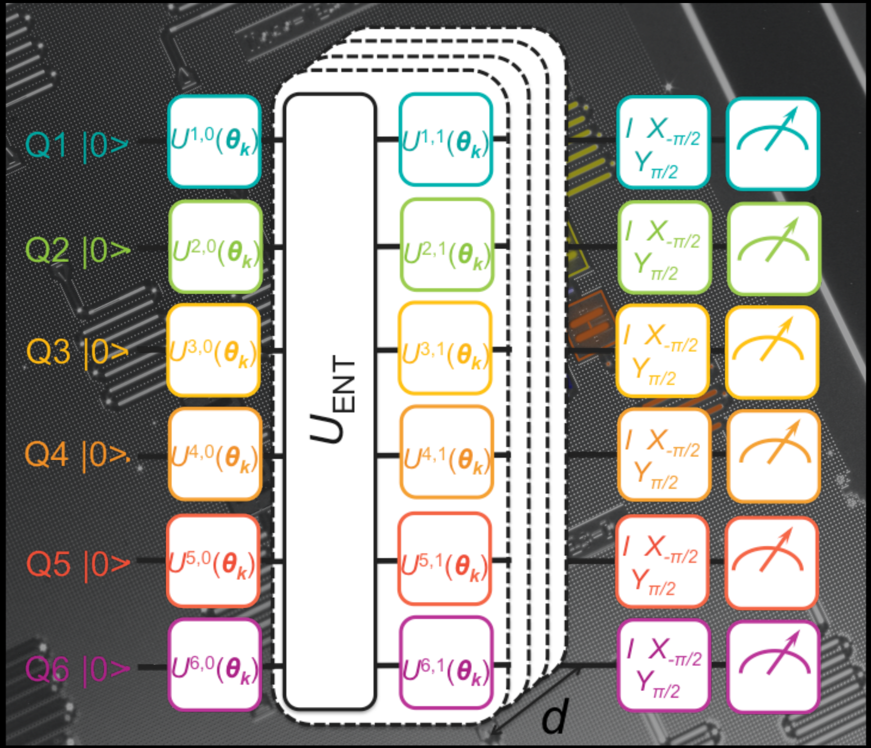
Variational principle

Variational principle

Variational Quantum Eigensolver (VQE)

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

Map problem onto Paulis



$E(\vec{\theta})$

$\vec{\theta}$

Use classical optimizer

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

Measure its energy

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

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

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

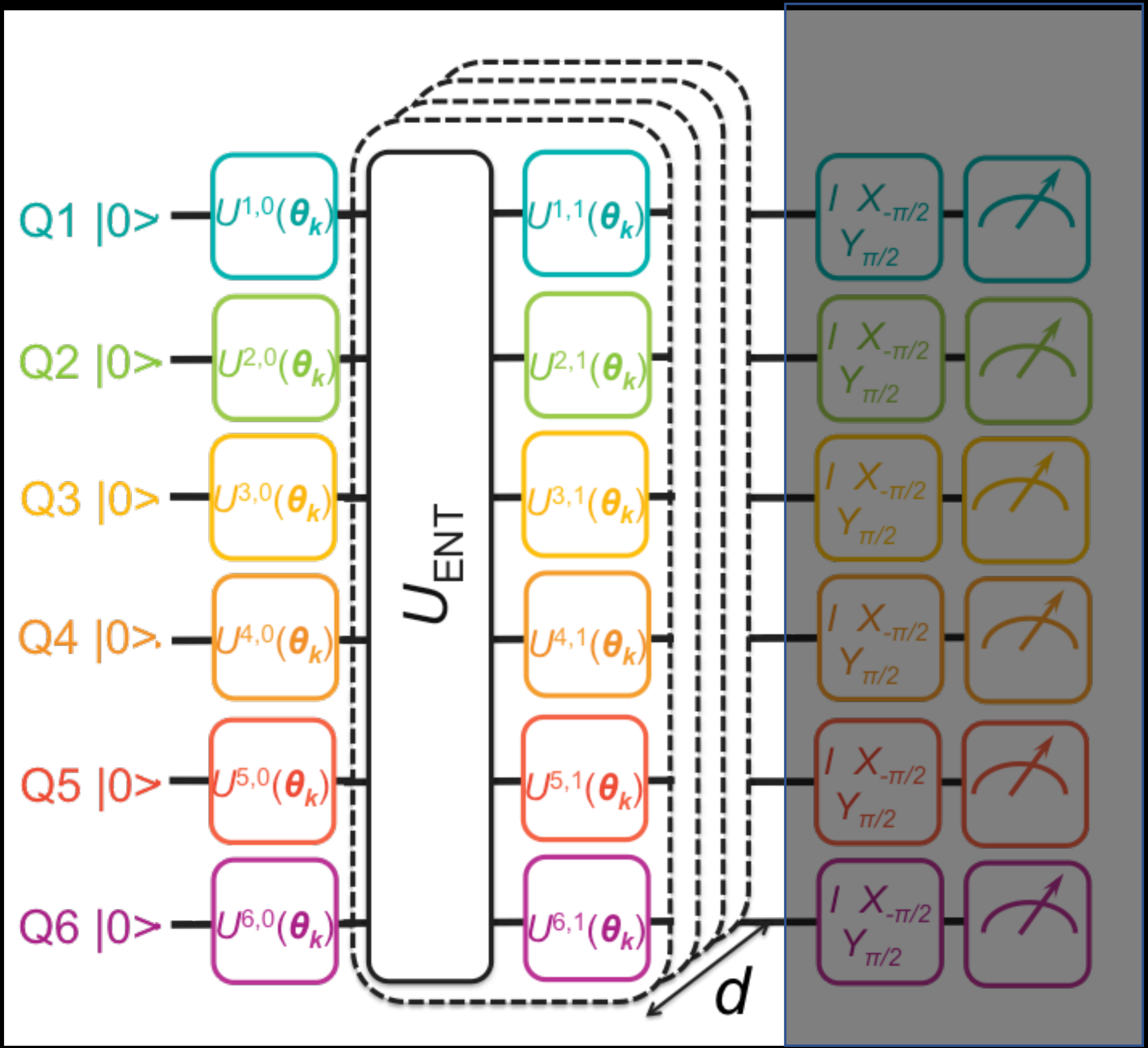
Choice of fermion-qubit mapping important: Each fermionic operator maps to O(N) qubits for JW, O(log N) for BK

Tapering of qubits

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

Tapering of qubits

Trial State Preparation



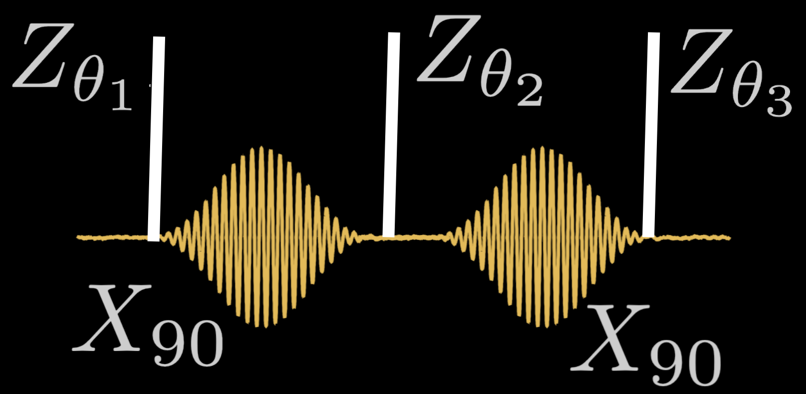
- Unitary Coupled Cluster ansatz : Offers physical intuition, focuses ground state search in ”good” space
- However, translates to very expensive gate count
- Alternative approach: Keeping hardware limitations in mind, do what hardware can do best!

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

Trial State Preparation

Trial state preparation: Arbitrary single qubit rotation

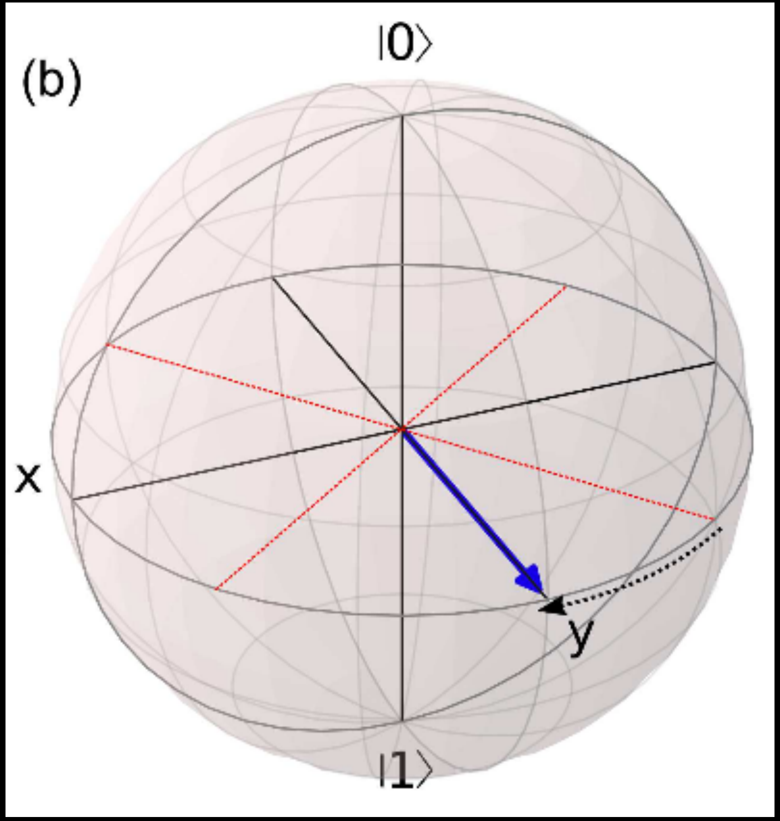
$$U(\vec{\theta}) = Z_{\theta_1} X_{90} Z_{\theta_1} X_{90} Z_{\theta_1}$$



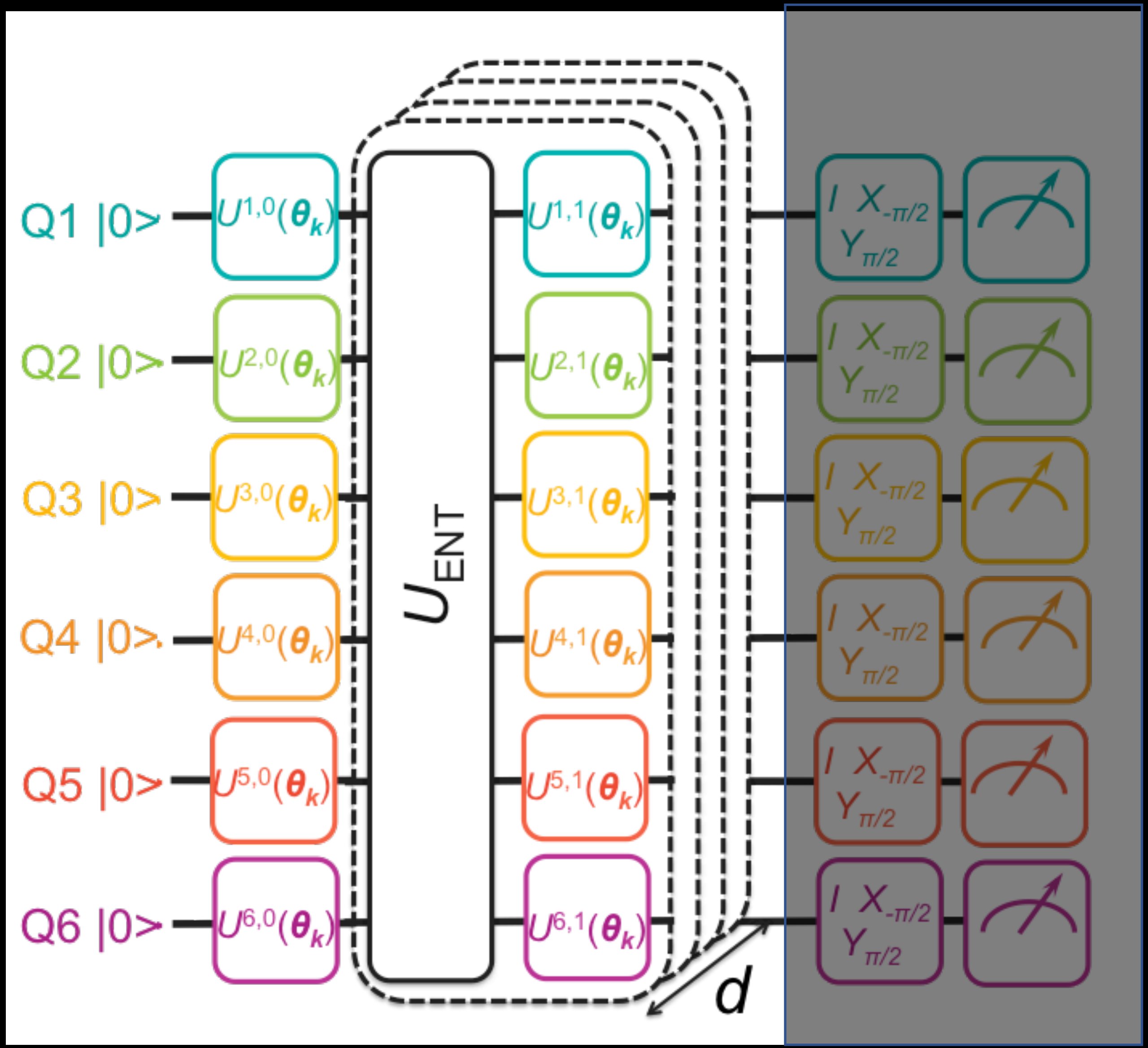
Variational parameters:

- Pulse envelope
- Pulse length
- Amplitude
- Phase

Software implemented Z-gates
(Perfect, zero time)



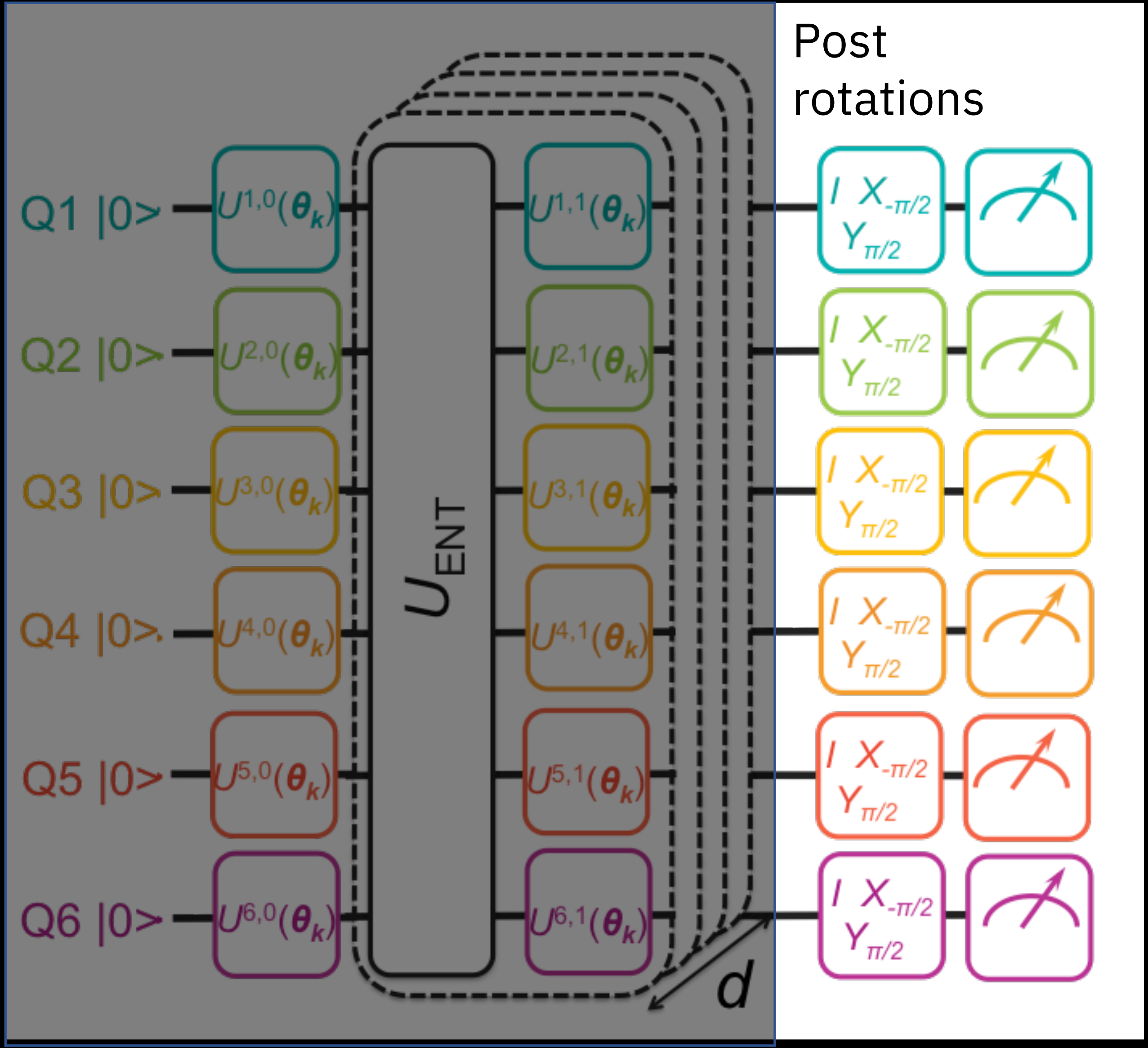
Trial State Preparation



- 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)

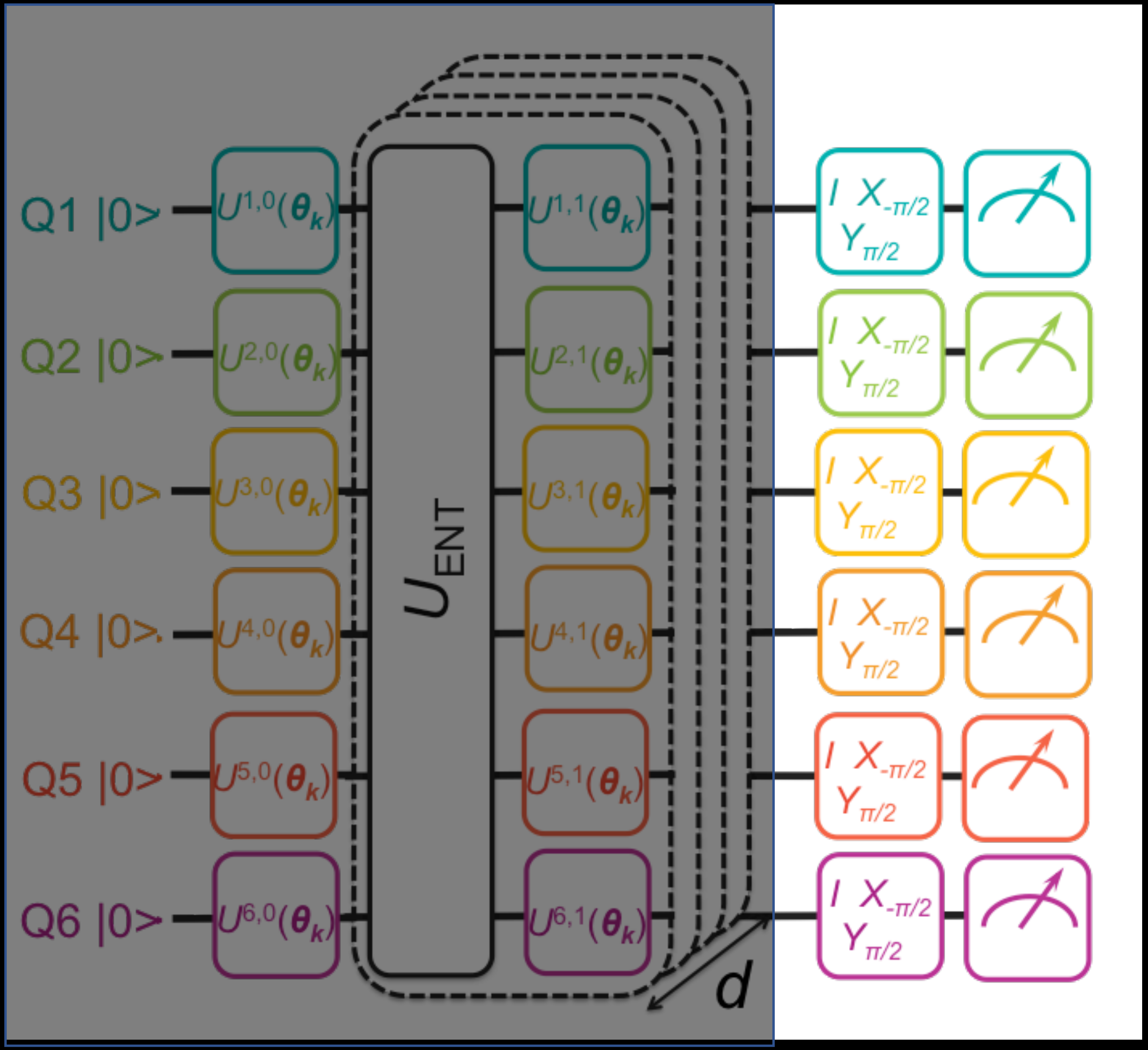
Energy measurement : Measuring expectation values



Energy measurement : Measuring expectation values

Energy measurement : Measuring expectation values

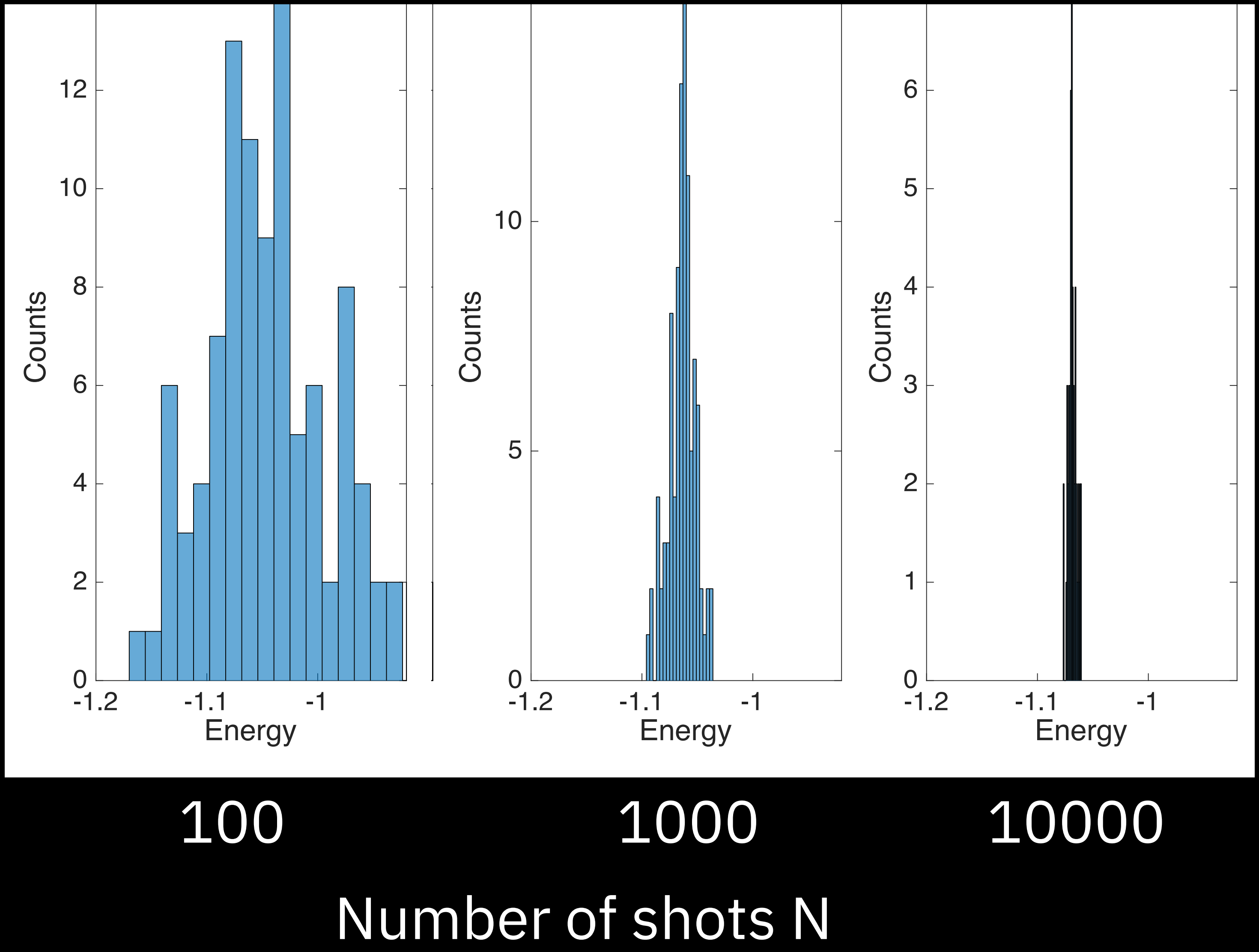
Energy measurement: Measurement Basis



Energy measurement: Measurement Basis

Energy measurement: Pauli Grouping

Energy measurement: Shot noise

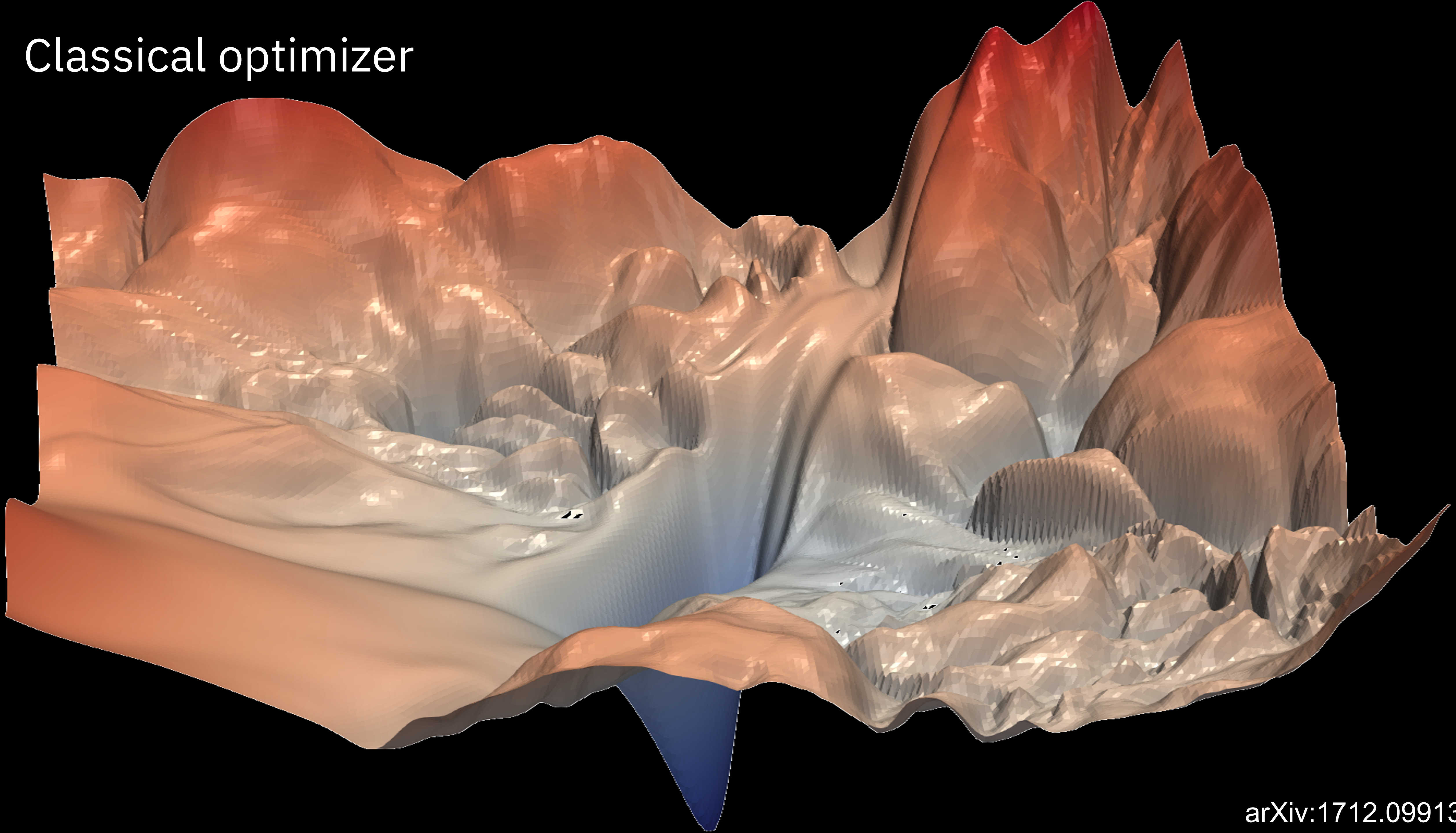


Even if ground state preparation is *perfect*, estimating <*O*> will still have error

$$\epsilon_{\langle O \rangle} = \sqrt{\frac{\langle O^2 \rangle - \langle O \rangle^2}{S}}$$

Can affect accuracy of classical optimizer

Classical optimizer

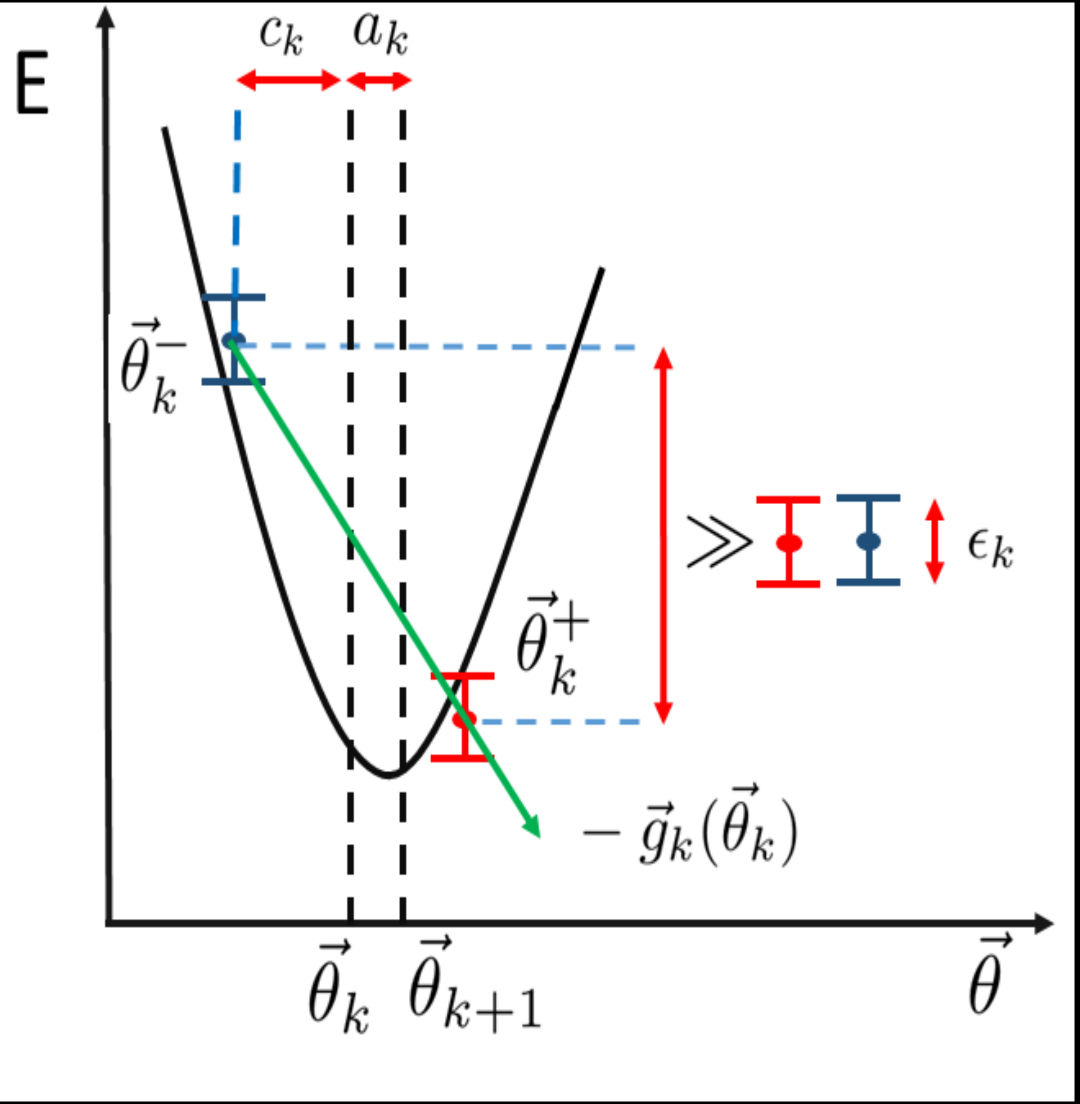


arXiv:1712.09913

Classical optimizer: Simultaneous Perturbation Stochastic Approximation (SPSA)

Need to reduce of calls to Quantum computer

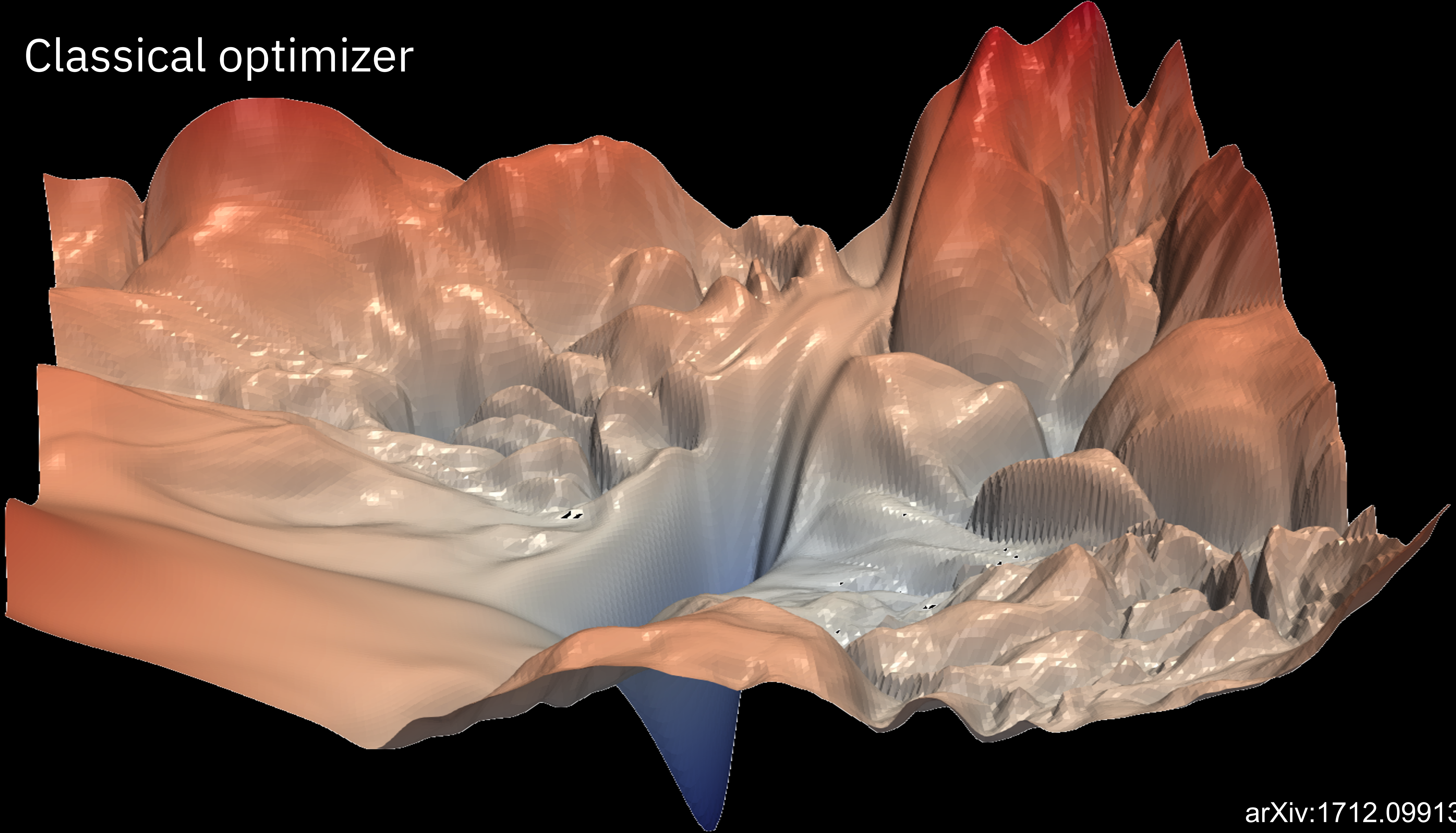
Gradient approx.: Regardless of dimension of optimization problem, utilizes only **two** measurements per iteration



[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)

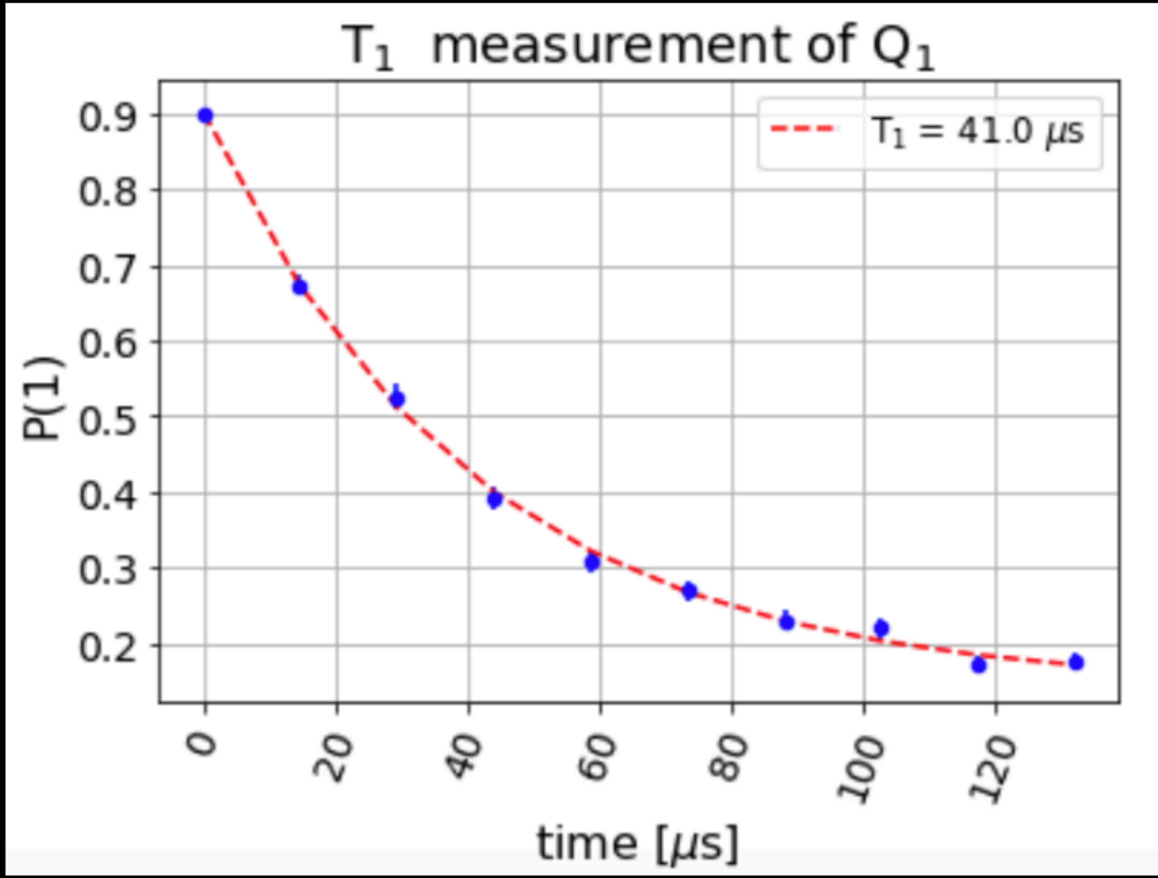
Classical optimizer



arXiv:1712.09913

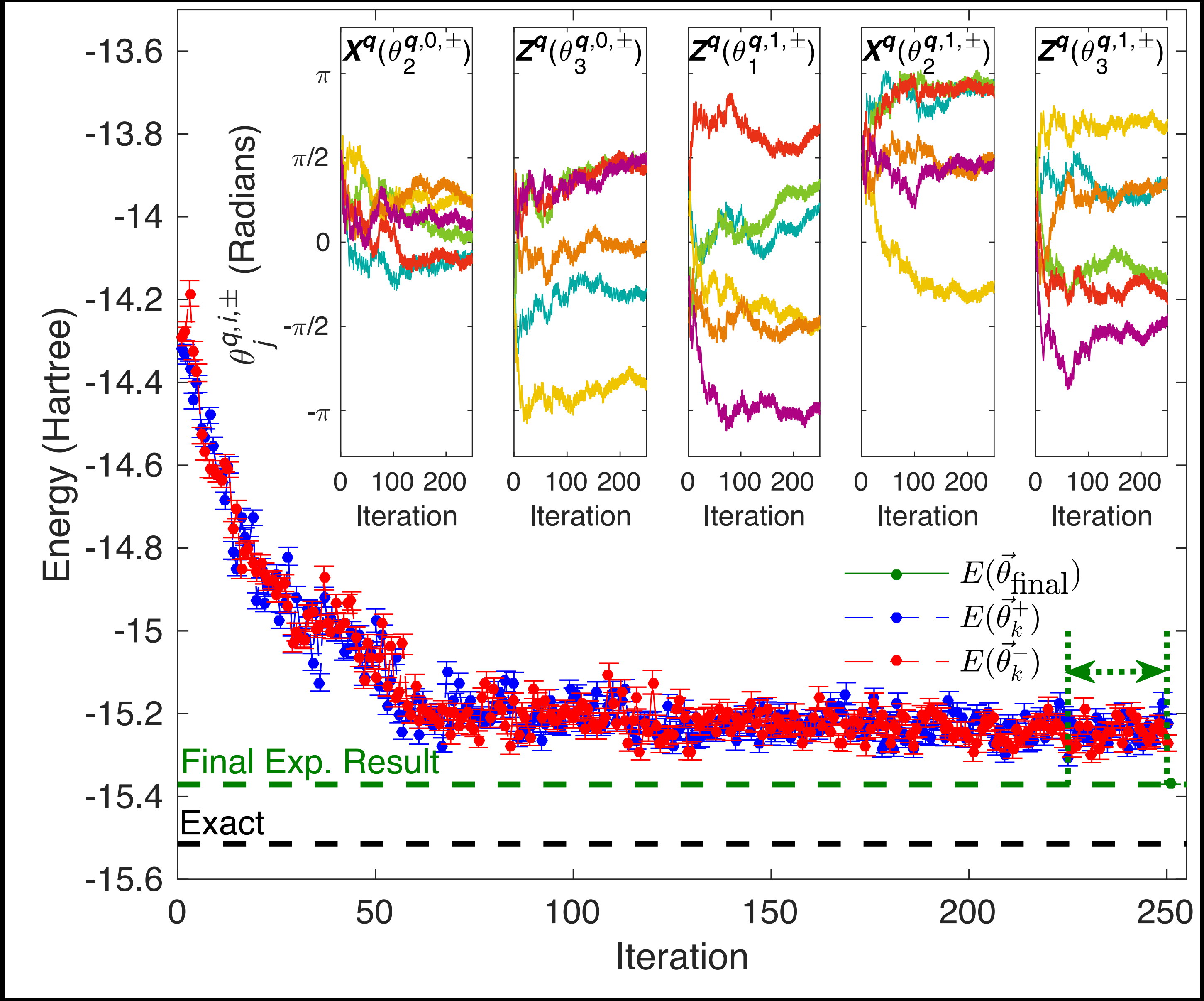
Run time overhead

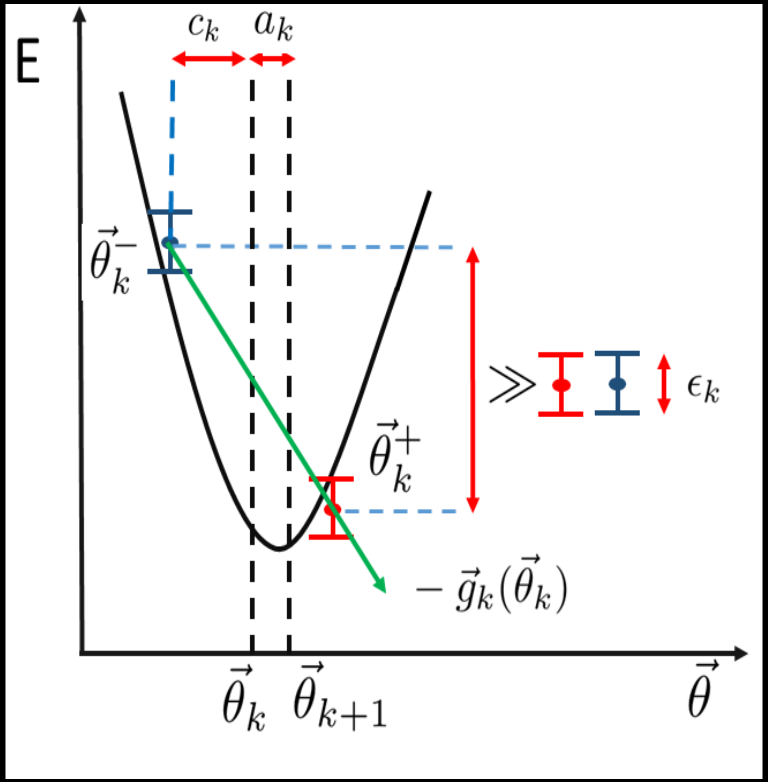
- Number of energy estimations per iteration
- Number of Pauli strings in the Hamiltonian
- Number of shots
- System initialization



Putting it all together ..

Experimental optimization of a 6 Qubit Hamiltonian





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

Application to quantum chemistry : H_2

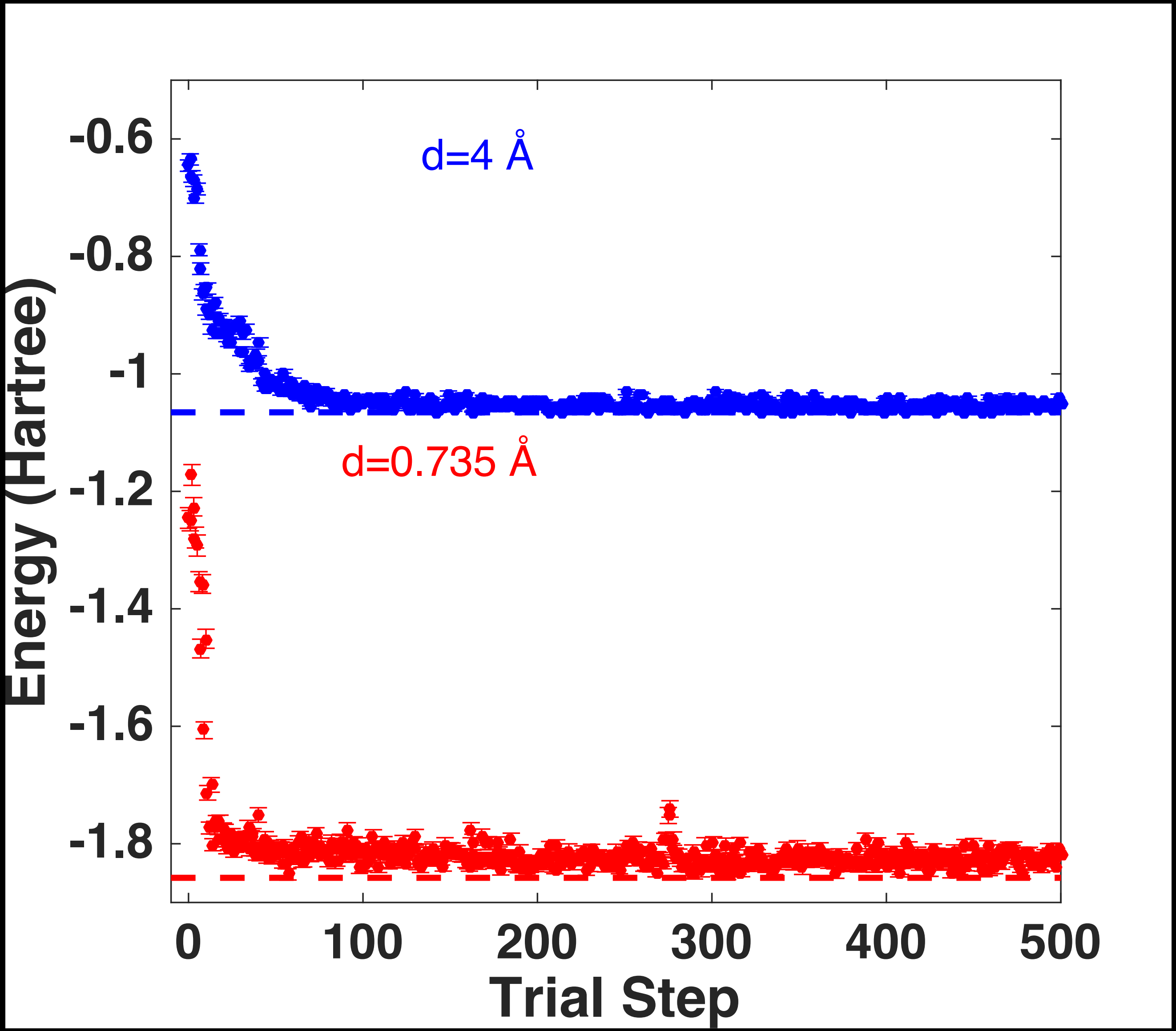
H_A: $1s^1$ H_B: $1s^1$
4 spin orbitals mapped to 2 qubits

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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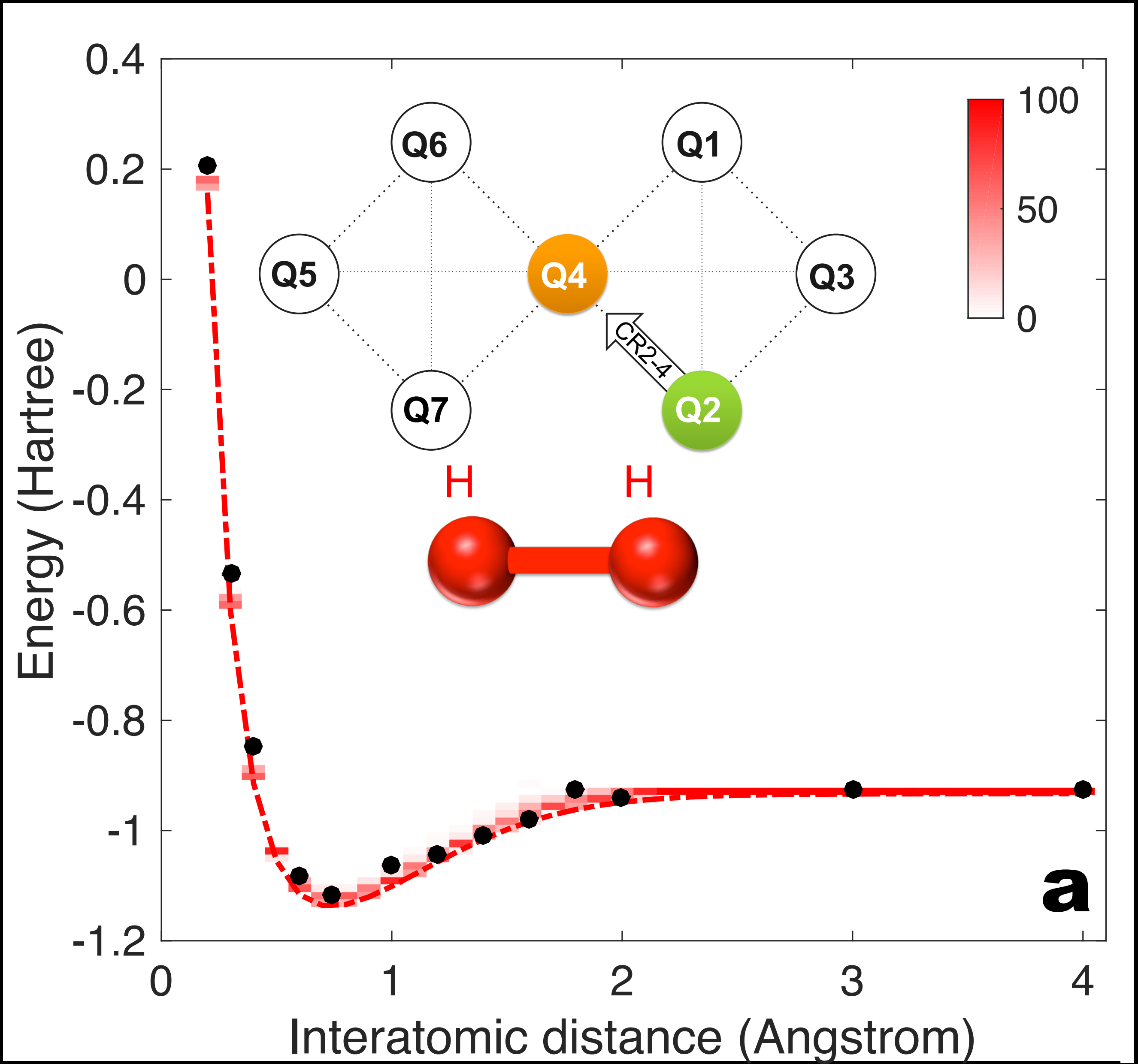

Application to quantum chemistry : Going beyond period 1 ....

II
-1.05237
ZI
0.39735
IZ
0.39735
ZZ
0.11279

XX
0.18093

H_2: 5 Pauli terms, 2 sets

ZZZZ
0.0803338509259093 34
IIII
-0.20665748323683217
ZIII
-0.09602217950788935 5
ZZII
-0.20612801807987652
IZII
0.36474560607027956
IIZI
0.09602217950788907 7
IIZZ
-0.20612801807987641
IIIZ
-0.36474560607027956
ZIZI
-0.14543788191435422
ZIZZ
0.05604032898561765 7
ZIIZ
0.11081066572357191
ZZZI
-0.05604032898561764 3
ZZIZ
0.06367272040494602 3
IZZI
0.11081066572357193
IZZZ
-0.06367272040494603 7
IZIZ
-0.09521579665869489 6

XZXX
0.00819474446130711 96
XZIX
0.00127084085594668 77

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
0.000246549665815894
ZIXZ
-0.011962198277325331
ZIXI
-0.011962198277325331
ZZXI
0.000246549665815894

YYXX
-0.02892604472017965
YYIX
-0.0074989926703520624

XXXX
0.02892604472017965
XXII
-0.029639606309848882
IXII
0.0027917513494058743
IIXX
-0.029639606309848868
IIIX
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XIXX
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XIIX
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XXXI
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XXIX
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IXXI
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IXXX
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IXIX
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ZZXX
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ZIXX
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ZZIX
-0.0097693536789154 93
IZXX
-0.024279988585959 71
IZIX
-0.0080251584900907554

XXYY
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IXYY
-0.0074989926703520624

ZXZX
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ZXII
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IIZX
-0.0027917513494058726
ZIZX
-0.016781393784256322
ZIIX
0.016781393784256322
ZXZI
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IXZI
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ZXIX
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IXZX
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XZZZ
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XIZI
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ZXXZ
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XXXZ
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IXXZ
-0.0012708408559466 88

ZZYY
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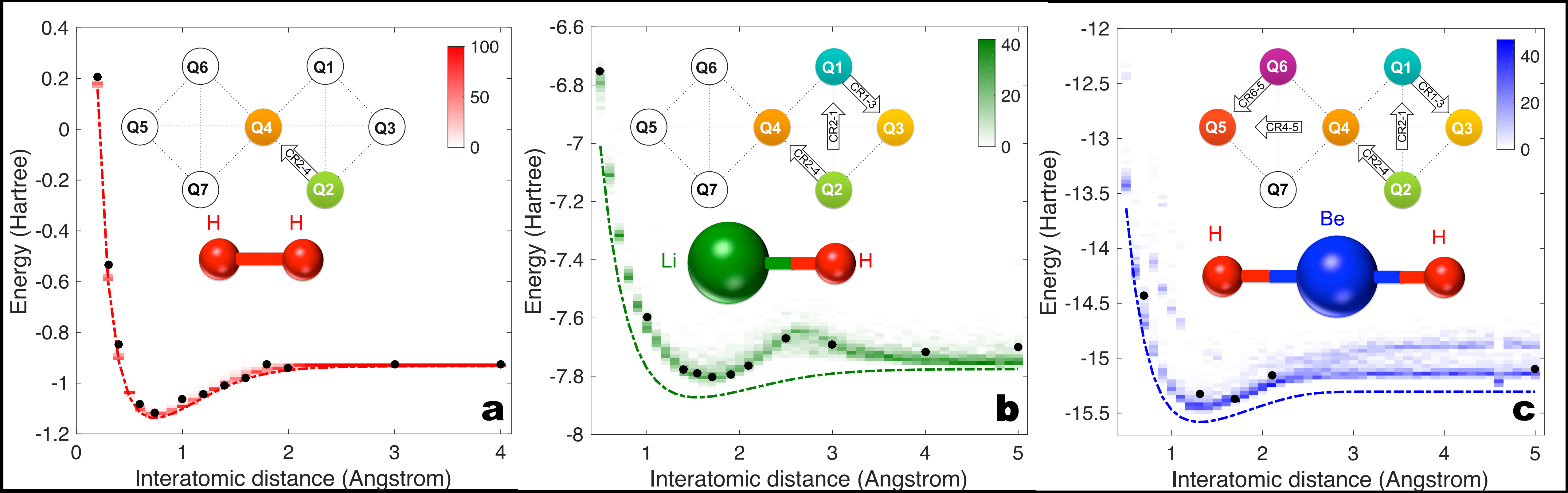
ZIYY
-0.039154818592760203
IZYY
0.024279988585959 71

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

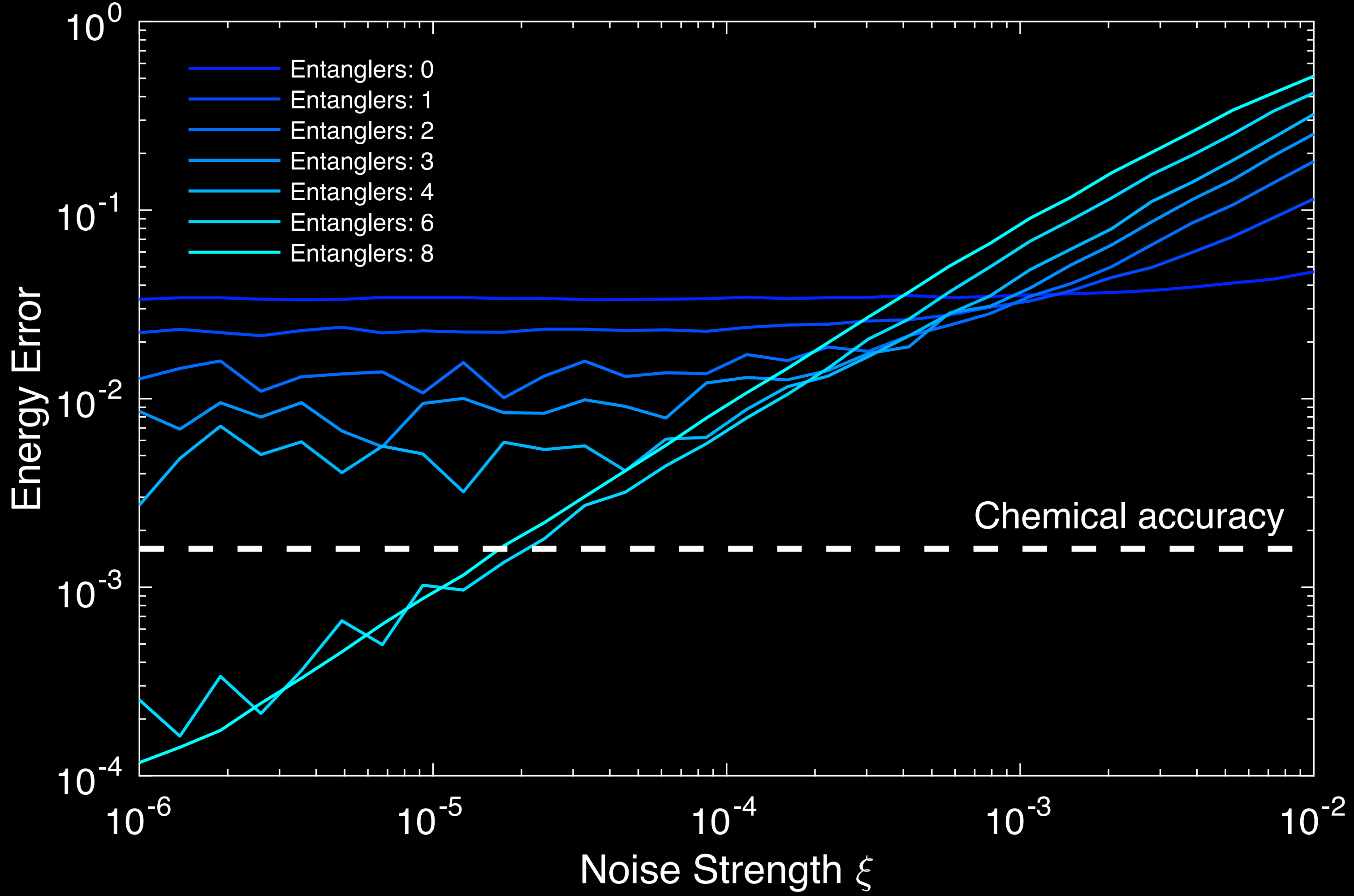
BeH_2: 6 qubits
165 pauli terms, 44 sets

- Decoherence
- Sampling error
- Limited iterations

- Accuracy of the classical optimizer
- Insufficient depth

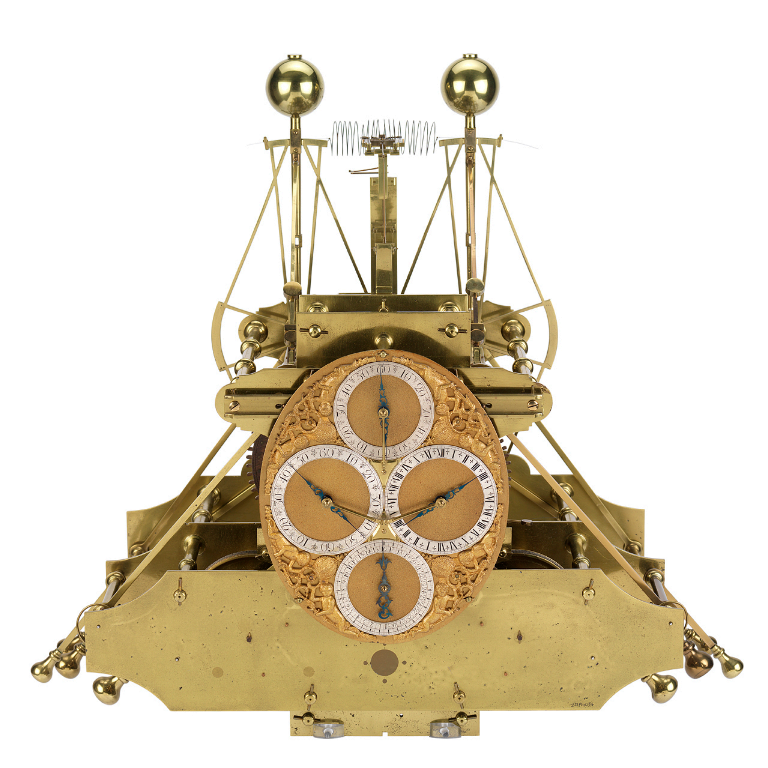
A. Kandala, A. Mezzacapo, et al, Nature **549**, 242-246 (2017)

Performance trade-off: Decoherence v/s Circuit depth

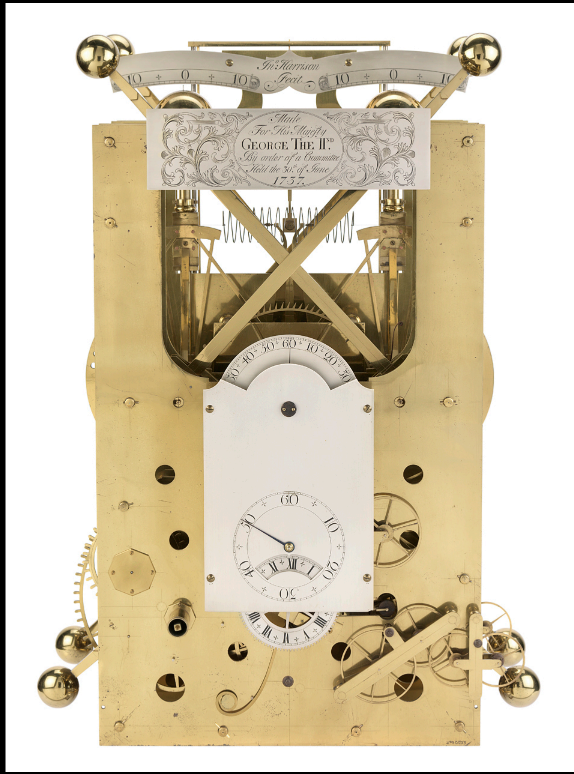


A. Kandala, A. Mezzacapo, et al,
Nature **549**, 242-246 (2017)

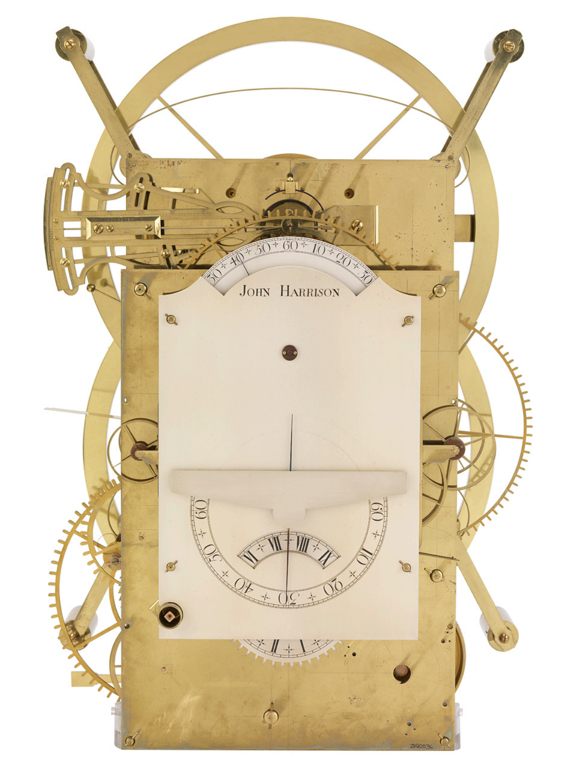
The longitude problem



H1
1730-1735



H2
1737-1739



H3
1740-1759
Invention of
Bimetallic strip

H4
1755-1759

http://collections.rmg.co.uk

Error mitigation

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)

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

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

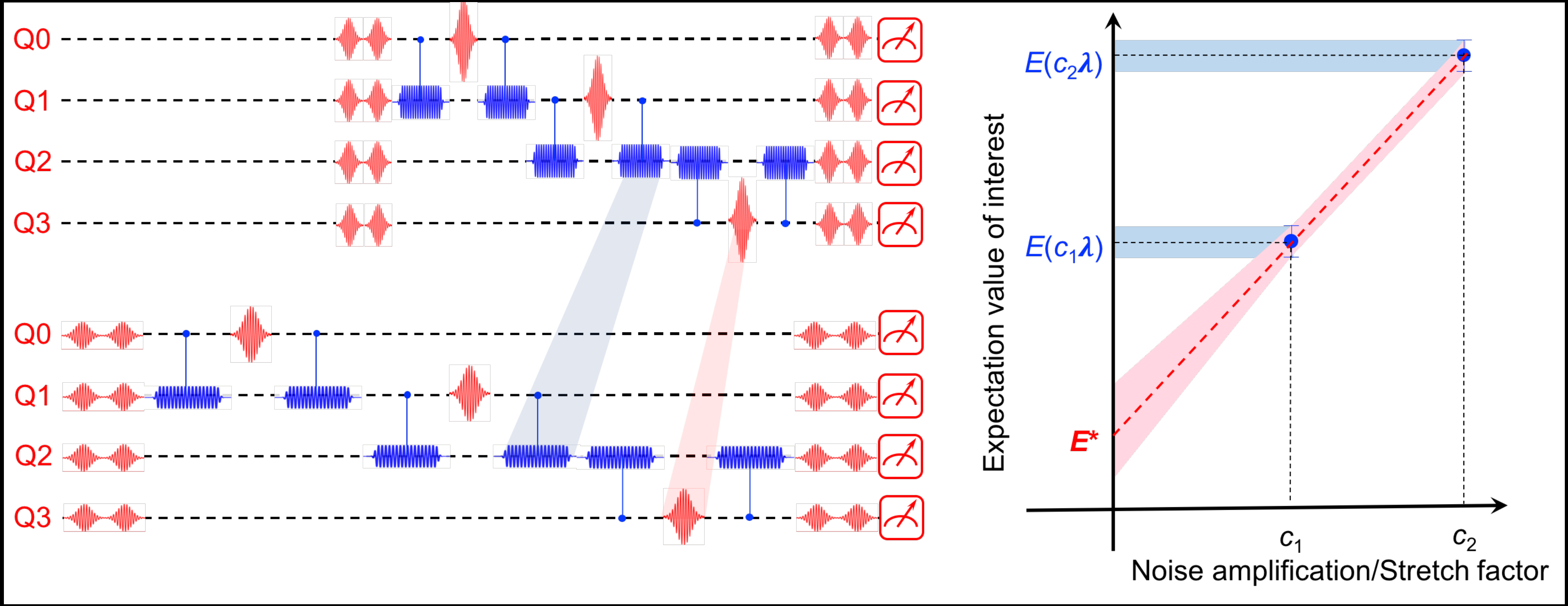
$$\hat{E}_K^2(\lambda) = \frac{cE_K(\lambda) - E_K(c\lambda)}{c-1} = E^* + \mathcal{O}(\lambda^2)$$

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

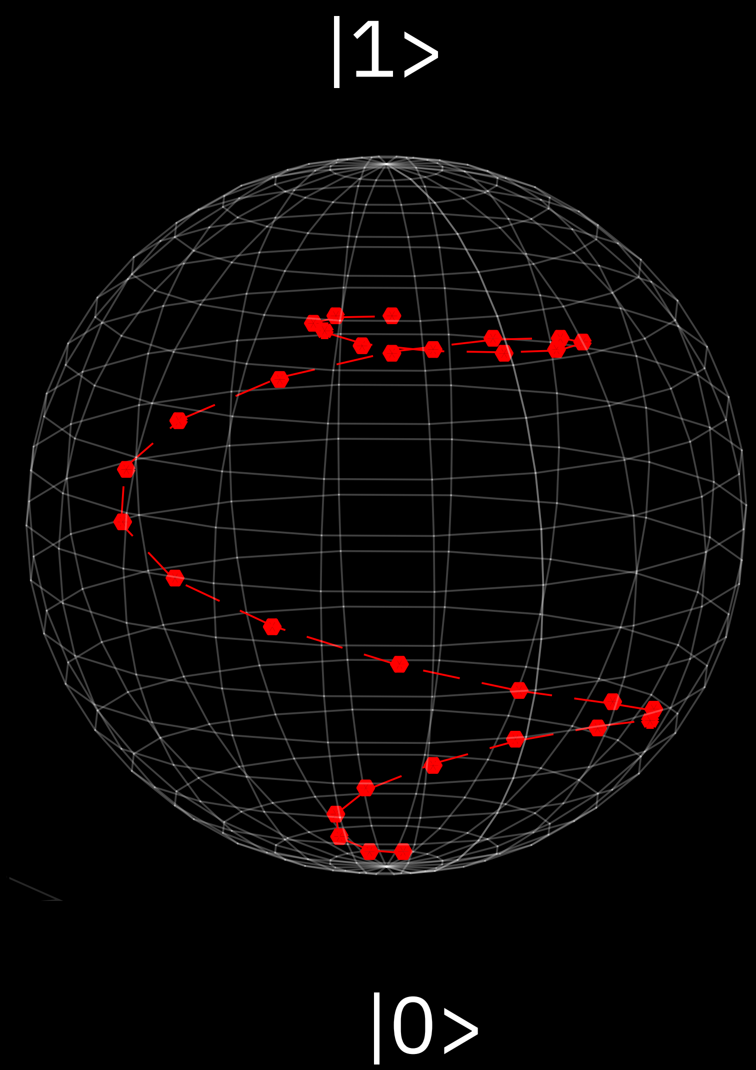
How does one measure $E(c_i\lambda)$??

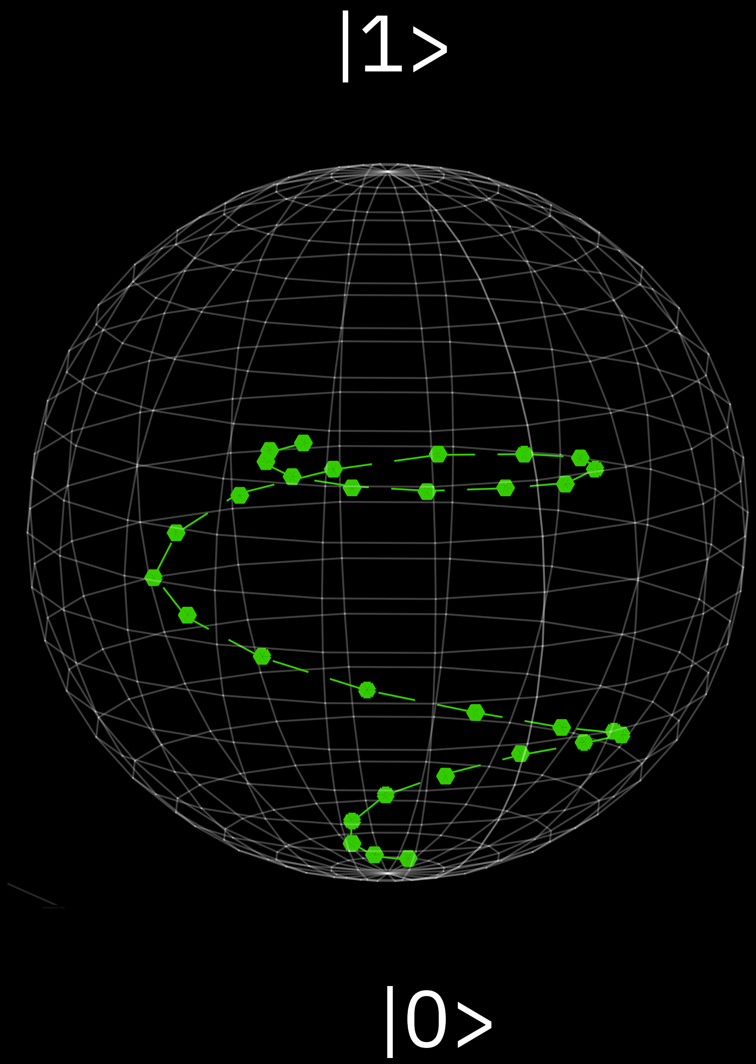
When two wrong's make a right

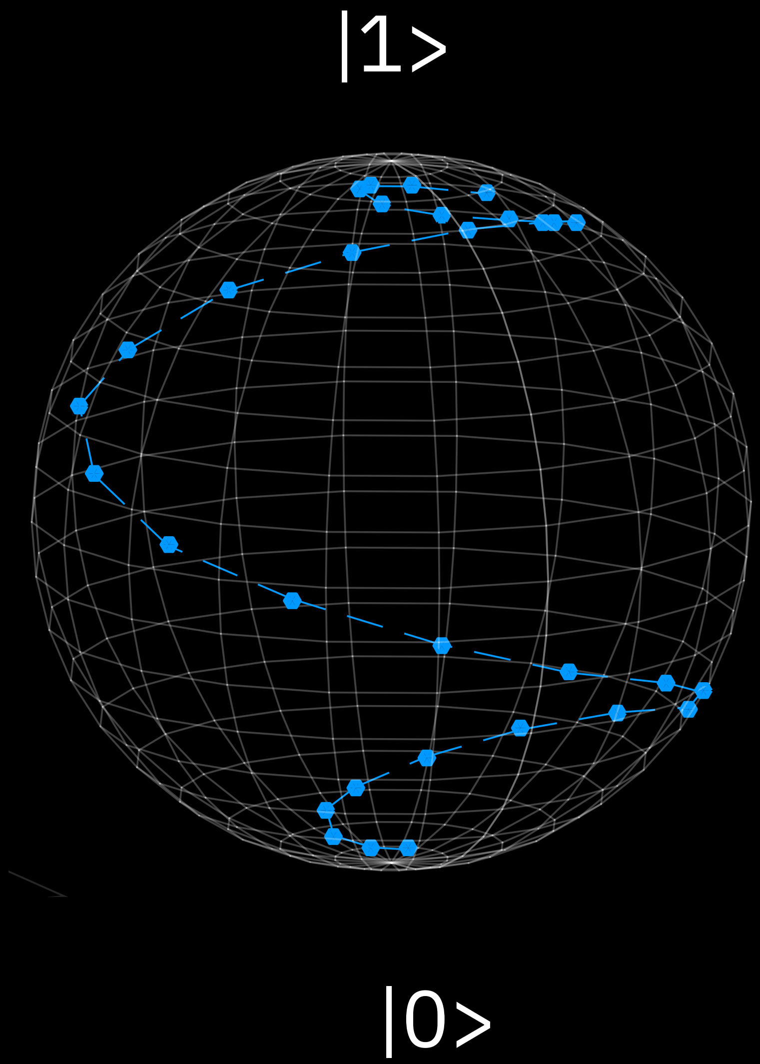
Amplifying noise strength equivalent to to rescaling dynamics under the assumption of time invariant noise.



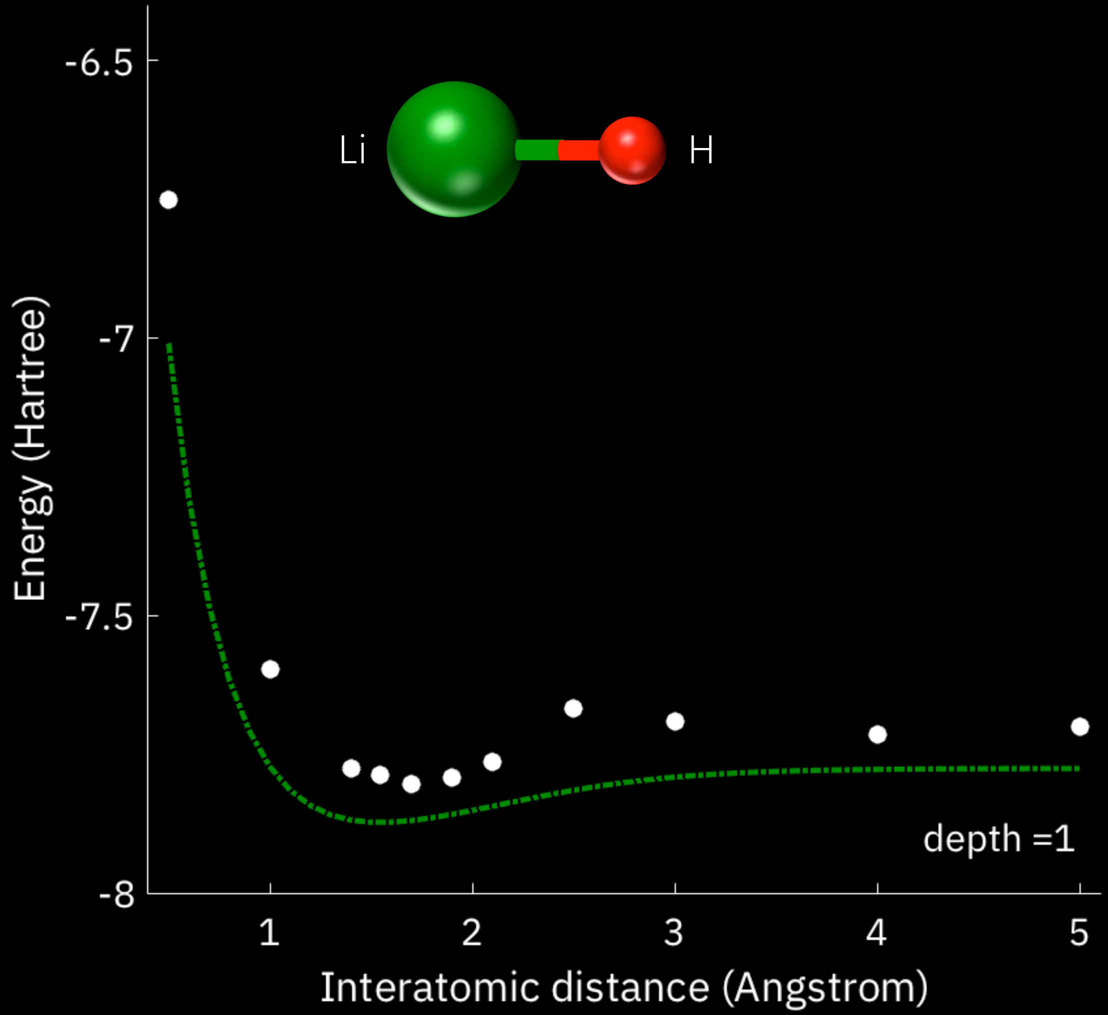
Error Mitigation: 1Q trajectory







Error Mitigation in molecular simulation: 4Q LiH



Kandala et al
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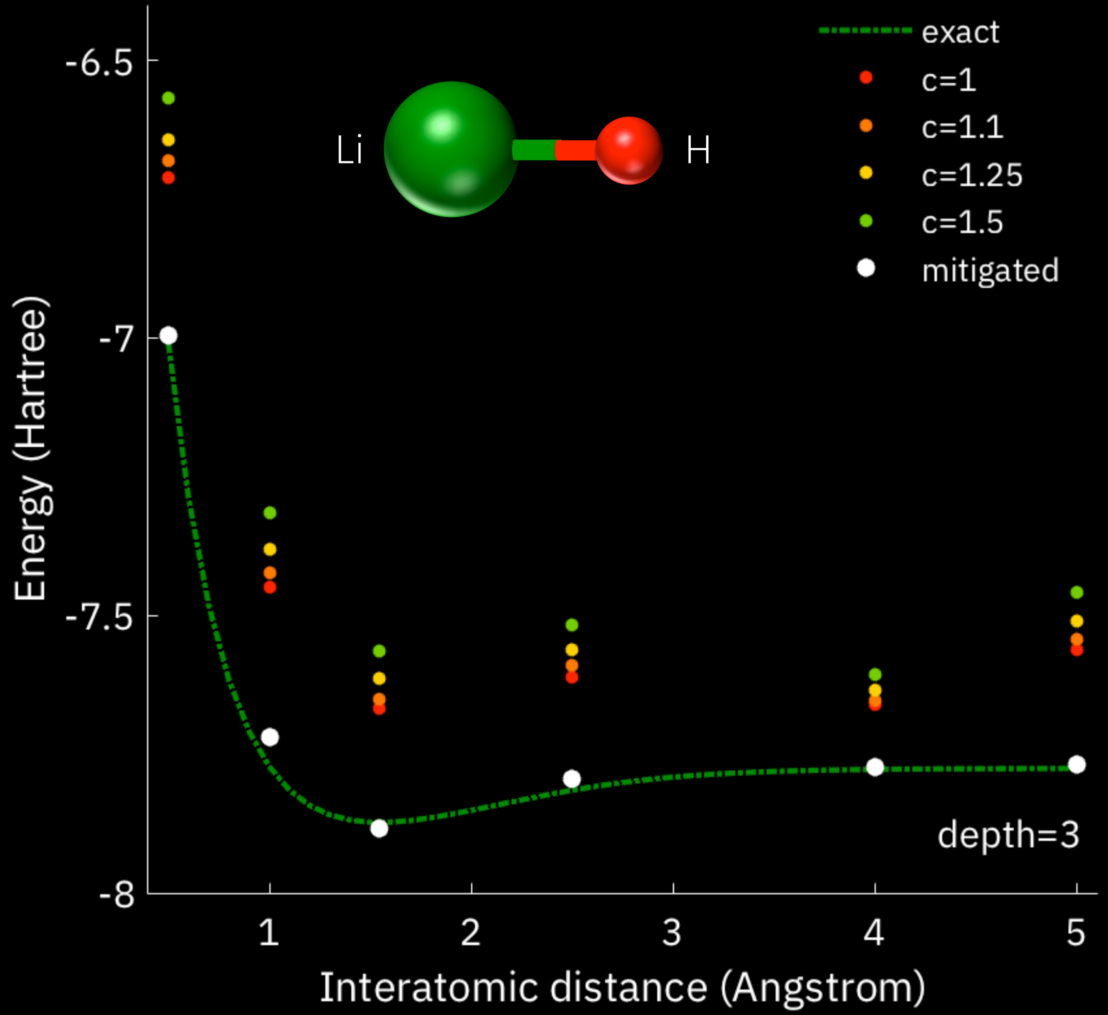
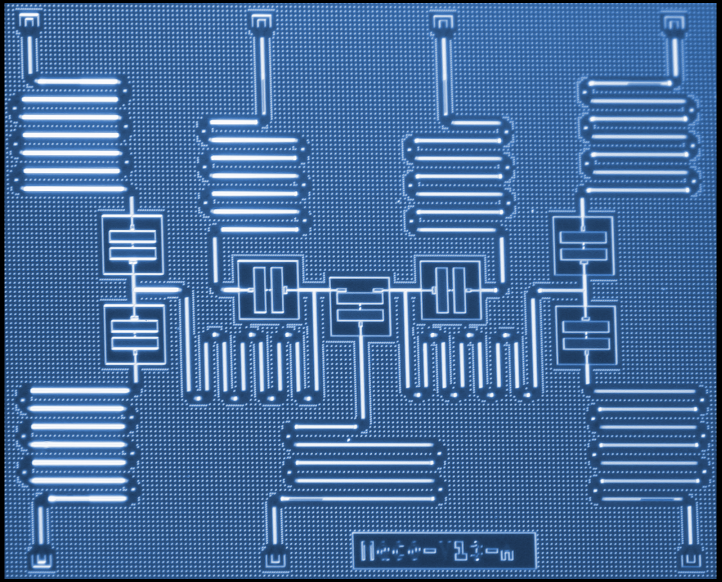
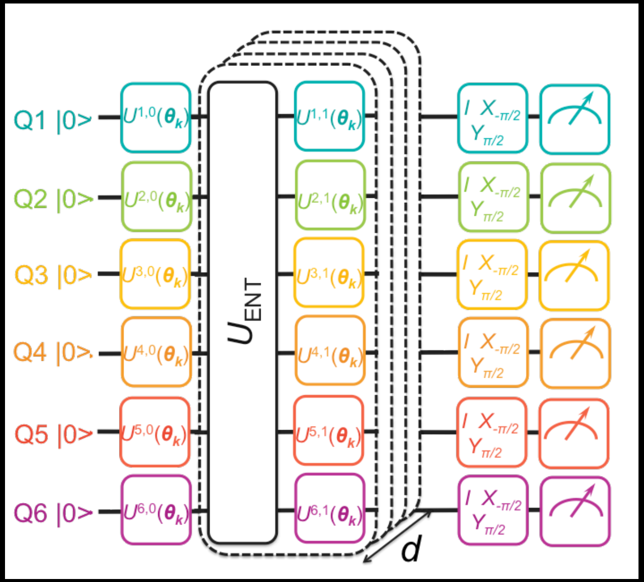
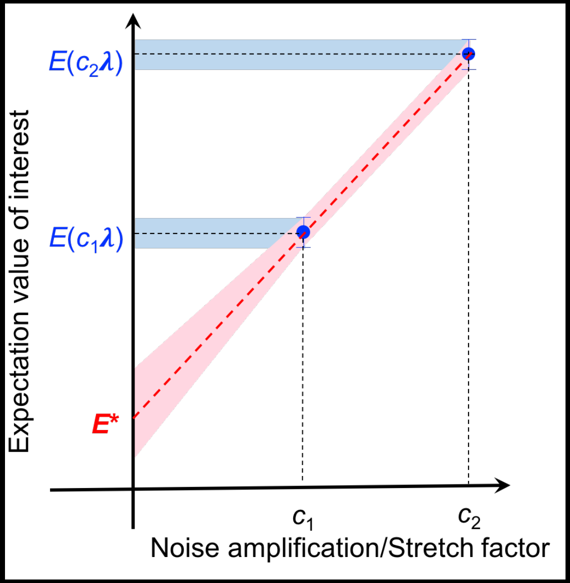


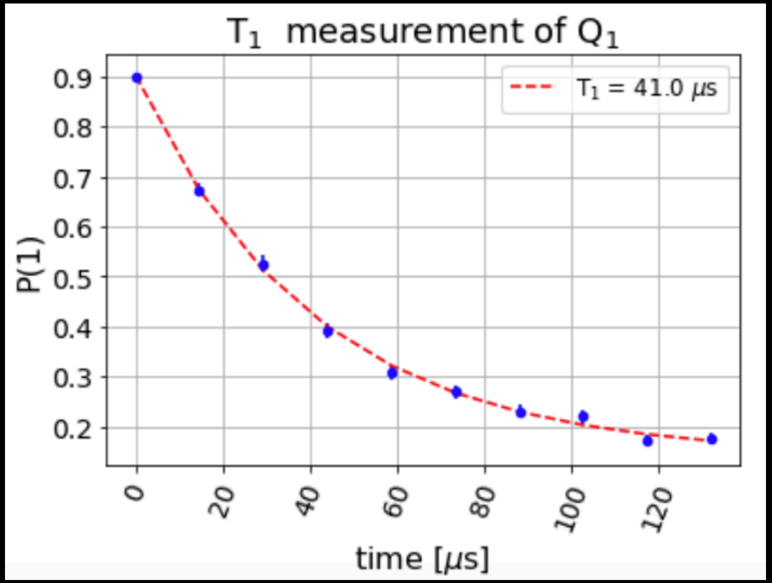
Kandala et al
Nature **567**, 491–495 (2019)

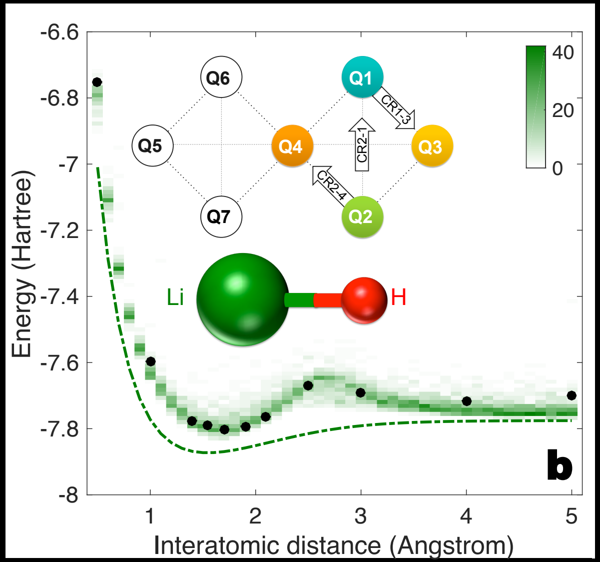
What we've covered today











Techniques go beyond just chemistry …


THANK YOU