Seminar on Selected Topics from Quantum Technology (Theory) – Advanced Quantum Algorithms

VARIATIONAL QUANTUM ALGORITHMS

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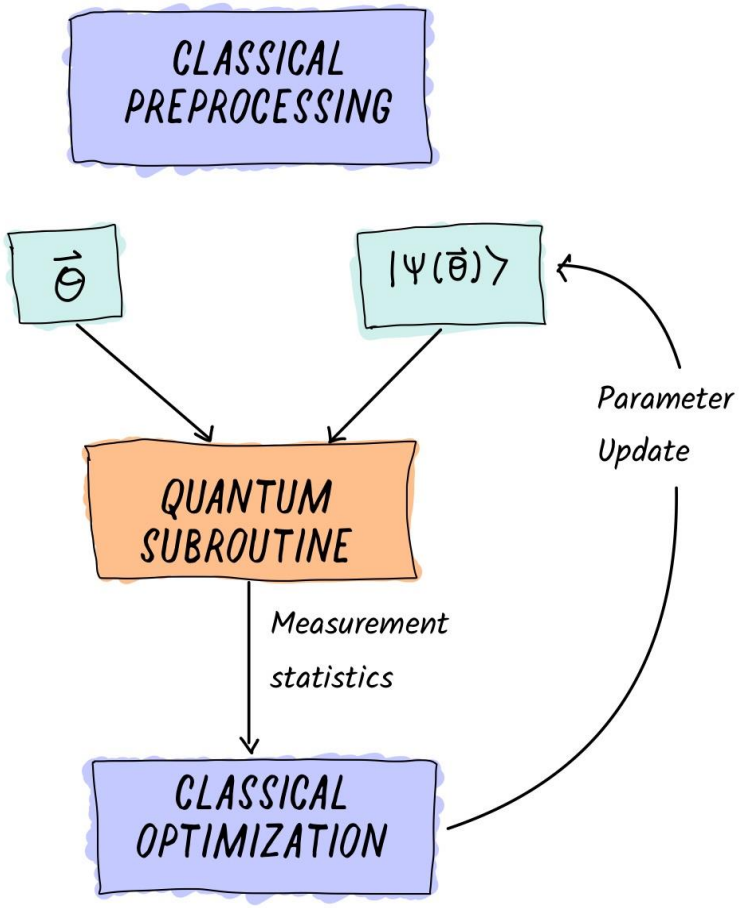
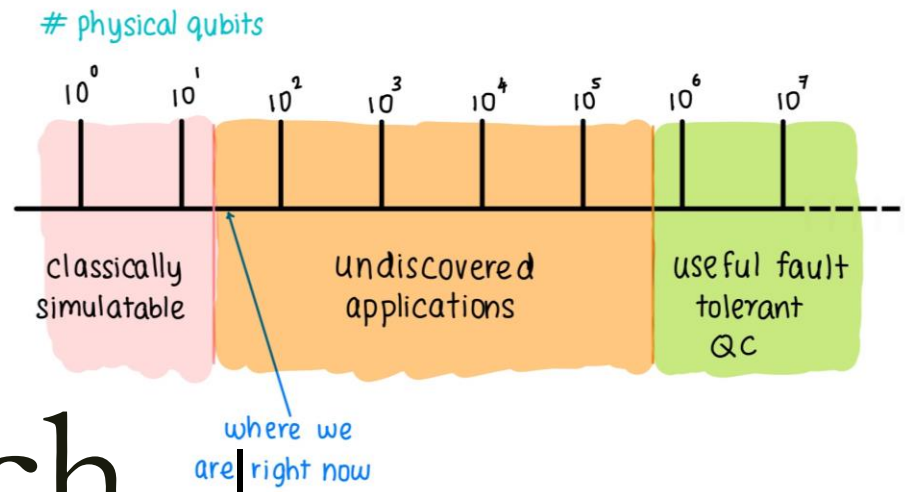
Bavithra Govintharajah

Supervisor : Prof Fabian Hassler

OUTLINE



1. Hybrid Approach and NISQs
2. Anatomy of a Variational Algorithm
3. Mapping → Classical pre-processing
4. Variational Quantum Circuit → QPU
5. Optimization → Classical post-processing
6. An example with VQE

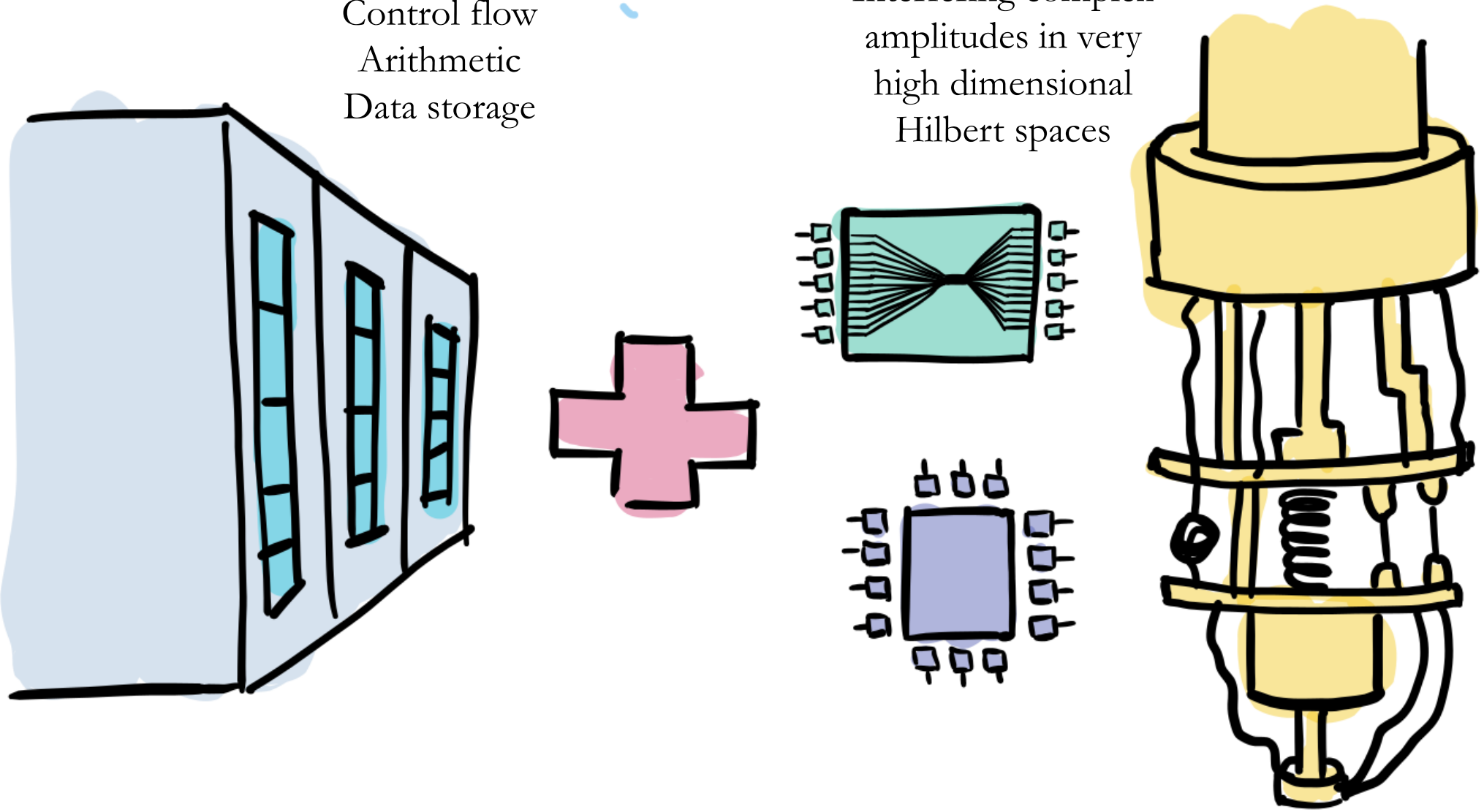


Hybrid approach & NISQs

Division of Labour

Control flow
Arithmetic
Data storage

Interfering complex amplitudes in very high dimensional Hilbert spaces



Why bother ?

Electronic Structure problem → QMA complete

Motivation

Can we do anything interesting before the advent of fault tolerant quantum computation with what we have right now?

- Use of Phase Estimation Algorithm (PEA)[1]
  - Asymptotically better scaling in terms of precision[2]
  - Stringent requirements on long and coherent gate sequences
  - Costly nature of Trotterization errors
- Variational Quantum Eigensolver (VQE) as an alternative
  - Requires only short state preparation and measurement sequences
  - Possible without the overhead of error correction

QUANTUM CHEMISTRY – test bed + 'killer' applications !

- Chemical accuracy (1 kcal/mol) classically intractable for systems with strong correlations
- Start small and go towards a quantum system that cannot be efficiently simulated classically

  # qubits → grows linearly with the number of basis functions

  # gates → grows polynomially with qubits [3]

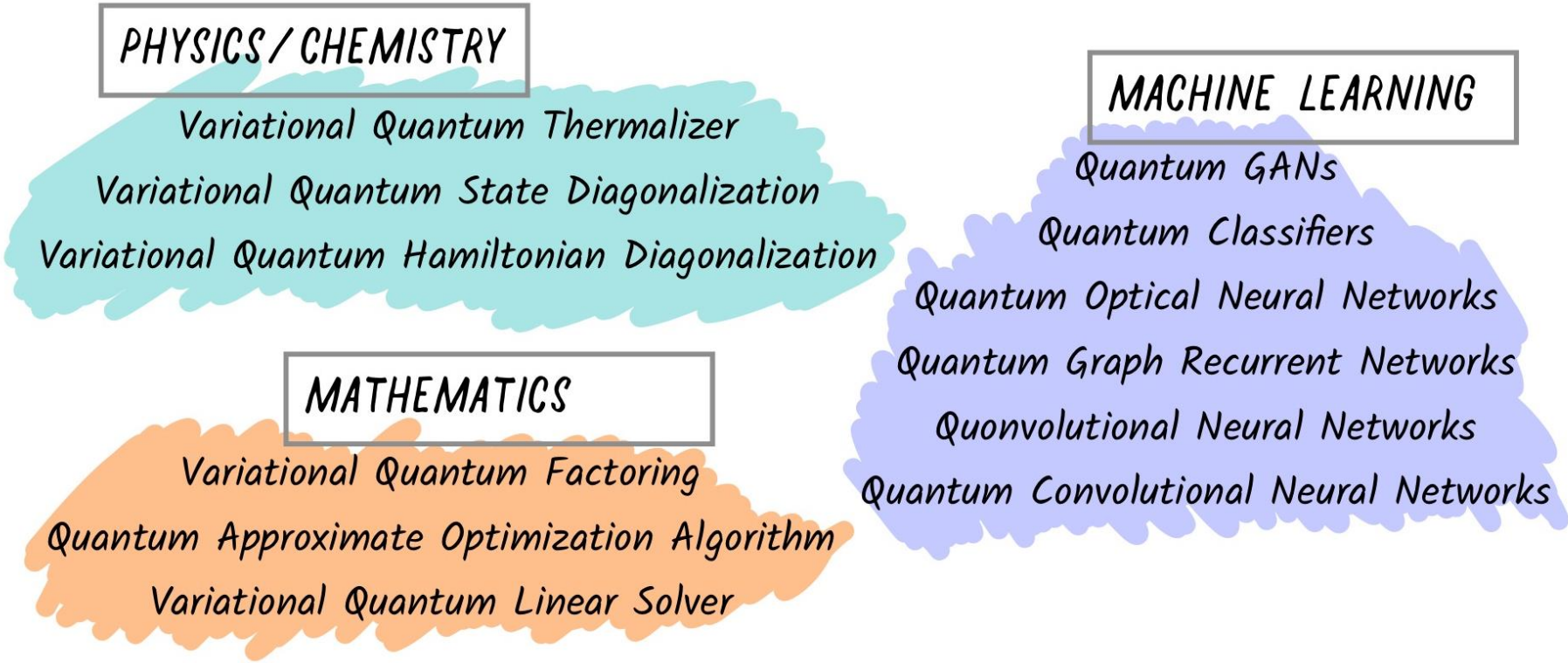
  ~ 20 spatial orbitals → quantum simulation competes with classical simulation

[1] Phys. Rev. Lett. 79, 2586
[2] Phys. Rev. X **6**, 031007
[3] Science.1113479

Why these adaptive variational methods are perfect for near term devices?

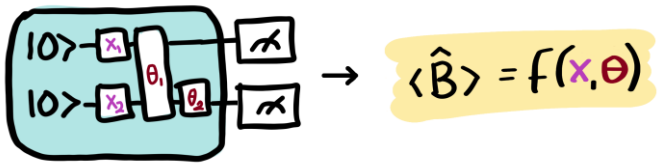
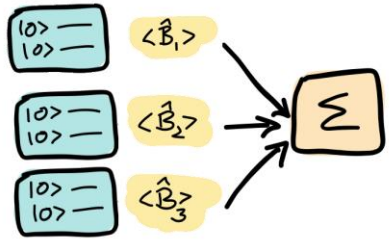
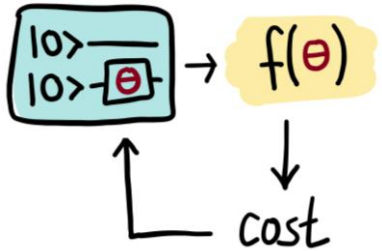
Resilience for pre-error corrected quantum computing than traditional gate model algorithms (e.g., PEA)

- ✓ Found to absorb errors in rotation angles [1]
- ✓ Classical outer loop → avoid systematic errors [2]

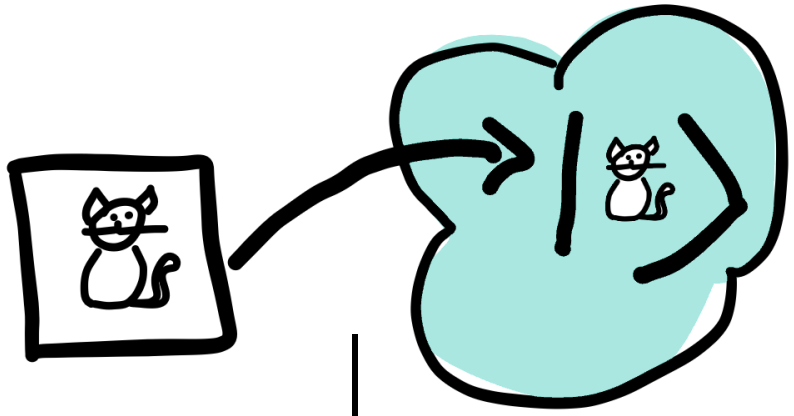


[1] Phys. Rev. X **6**, 031007
[2] Phys. Rev. Lett. 112, 240504

Anatomy of a Variational Algorithm

	Variational Quantum Eigensolver (VQE)[1]	Quantum Approximate Optimization Algorithm (QAOA)[2]
 Variational Ansatz	Unitary Coupled Cluster Singles and Doubles (UCCSD)	Repeated time evolutions of "cost" and "mixer" unitaries
 Cost function	Expectation value of a molecular Hamiltonian	Expectation value of a "cost" Hamiltonian that encodes a discrete optimization problem
 Training procedure	Gradient descent using the parameter shift rule	Gradient descent using a shots frugal optimizer

[1] Nature Comms. volume 5: 4213
[2] arXiv:1411.4028
Images from GitHub/PennyLaneAI



Mapping

Classical

Translator

Electronic structure problem needs to be translated to qubits → transfer both wavefunction and operators

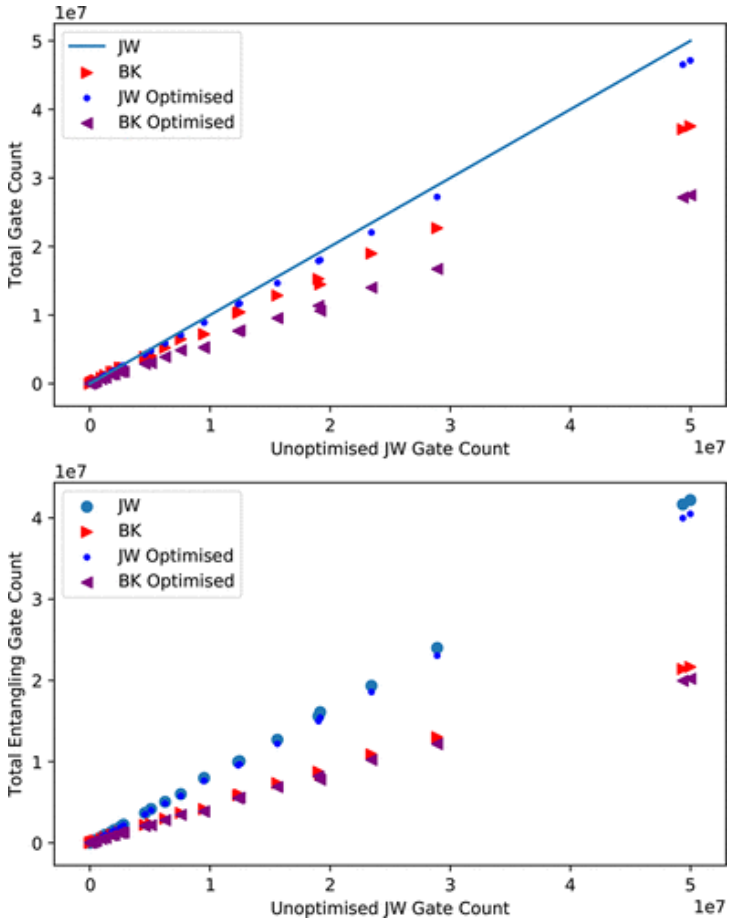
> Given a k-local Hamiltonian $\hat{H}$, composed of terms that on at most k-qubits, the solution to the local Hamiltonian problem amounts to finding its ground state eigenvalue E_G and ground state $|\Psi_G\rangle$, which satisfy $\hat{H}|\Psi_G\rangle = E_G|\Psi_G\rangle$.[1]

Use Second Quantization : Easiest form of the electronic structure theory for transformation to a qubit form

What influences the choice of mapping?

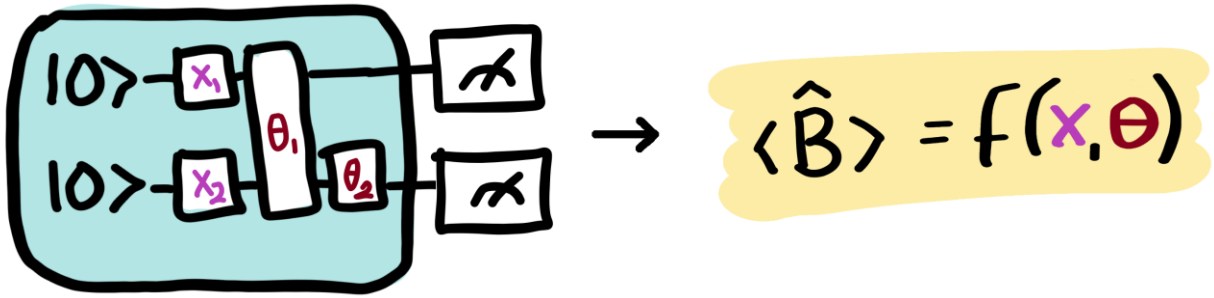
- Determines the # gates we need to apply
- Basis depends on the symmetries of our problem
  - Chemistry oriented → atomic / molecular orbitals
  - Solid State → plane wave

Jordan – Wigner [2]	**Bravyi – Kitaev** [3]
Length – $O(n)$ Pauli strings	Length – $O(\log n)$ Pauli strings
Linear en-/decoding, No qubits saved	



J. Chem. Theory Comput. 2018, 14, 11, 5617–5630

[1] Nature 549, 242–246
[2] Zeitschrift für Physik 47,631-651
[3] Annals of Physics 298, 210-226



Variational Quantum Circuit

The Stencil

Quantum

Variational Quantum Circuit

Definition. A variational ansatz on N_p parameters corresponds to a pair $(U, |\vec{0}\rangle)$, where U is a smooth map from the *parameter space* $\vec{\theta} \in \mathbb{R}^{N_p}$ to the unitary operator $U(\vec{\theta})$ on $\mathbb{C}^{2^{N_q}}$, and $|\vec{0}\rangle \in \mathbb{C}^{2^{N_q}}$ is the *starting state*, which is acted on to generate the *variational state* $|\psi(\vec{\theta})\rangle = U(\vec{\theta})|\vec{0}\rangle$, with variational energy $E = \langle\psi(\vec{\theta})|\hat{H}|\psi(\vec{\theta})\rangle$.[1]

Starting points :

- Physics, chemistry or quantum information theory
- Structure of the problem
- Insights from classical machine learning
- Underlying hardware platform

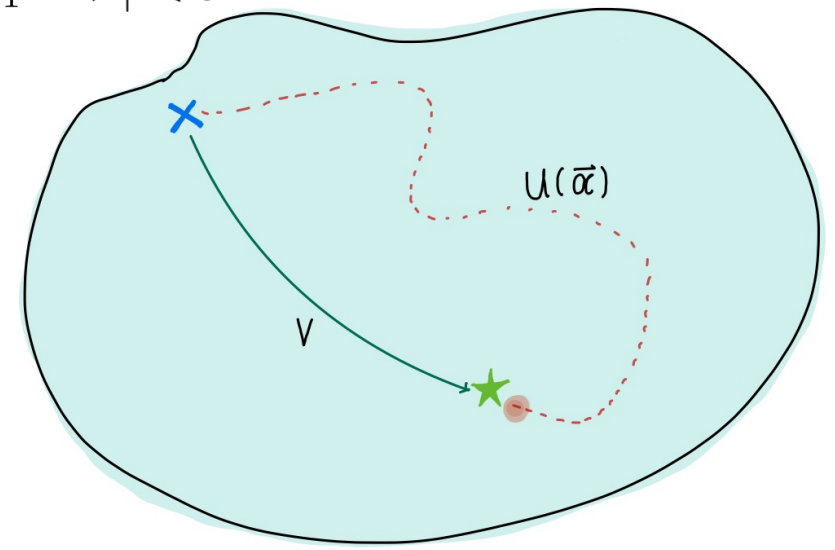
Choice affects the quality of learning ability of our model !
Many layers / circuit depth → more expressive and better learning

Hardware Efficient Ansatz

- Using native gates specific to the device running it
- Alternating gate layers in some way to span enough of the Hilbert space
- Might end up searching too much of the Hilbert space instead of narrowing down
- Worries about the optimization not being able to find good directions to go, with these circuits

The error of the approximated energy can be related to the number of layers (depth) of the circuit, by the Solovay-Kitaev theorem.

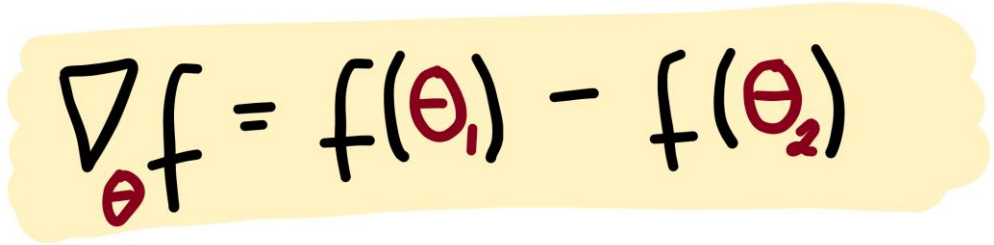
Circuit approximation to V
$|U_k \dots U_2 U_1 - V| < \delta$

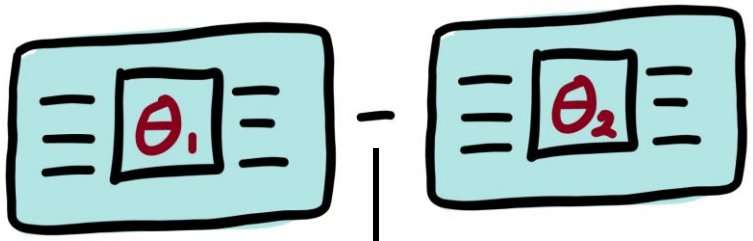


Scaling to best approximation
$k \approx O\left(\log^c \frac{1}{\delta}\right)$ operations with $1 \leq c < 4$.[1]

✓ Good Ansatz :
Shallow circuits without sacrificing exactness

× Bad ansatz leads to :
Scanning the wrong parameter space



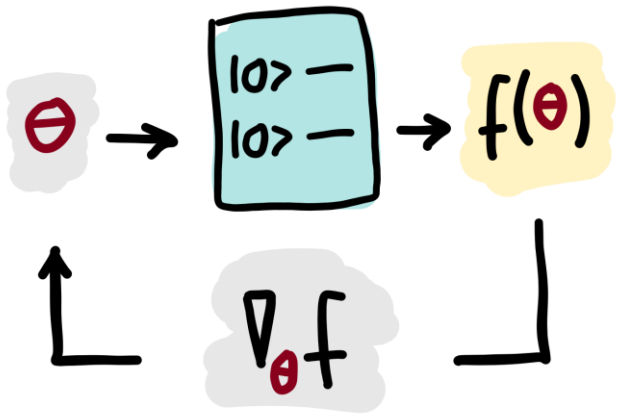


Optimization

Controller

Classical

Optimization



Popular strategy → Gradient Descent
take repetitive steps in the opposite direction of the gradient of the objective function at the current point

Commonly used:

- Constrained Optimization by Linear Approximation (COBYLA)
- Sequential Least Squares Programming (SLSQP)
- Simultaneous Perturbation Stochastic Approximation (SPSA)

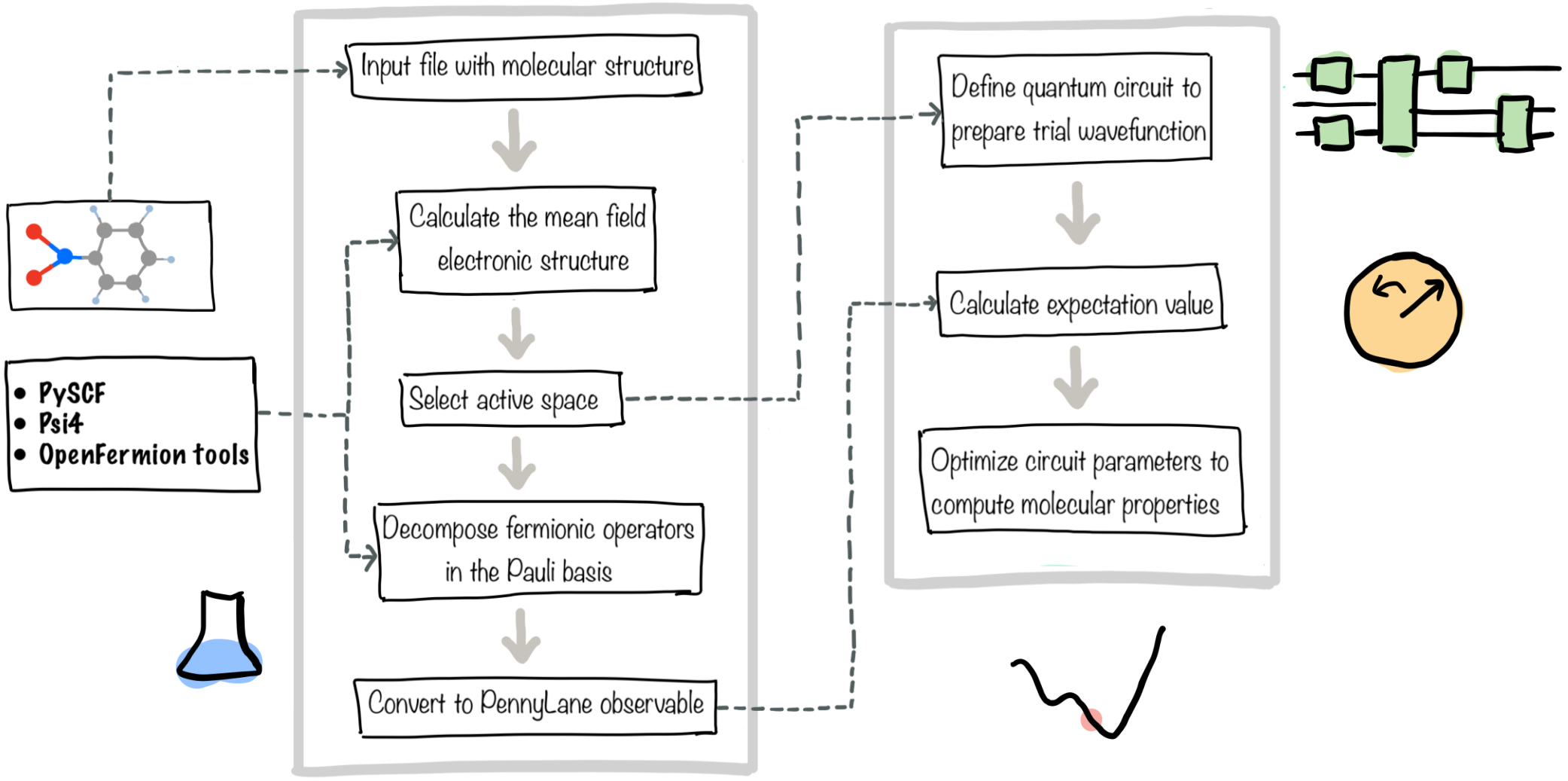
Quantum-aware optimizers:

- **Quantum Natural Gradient**→ accounts for the inherent geometry of quantum Hilbert space
- **Rotosolve/Rotoselect** → Doesn't use gradients. Directly solves for the optima w.r.t one coordinate at a time
- **iCANS/Rosalin** →shots frugal estimation of many quantities using limited samples

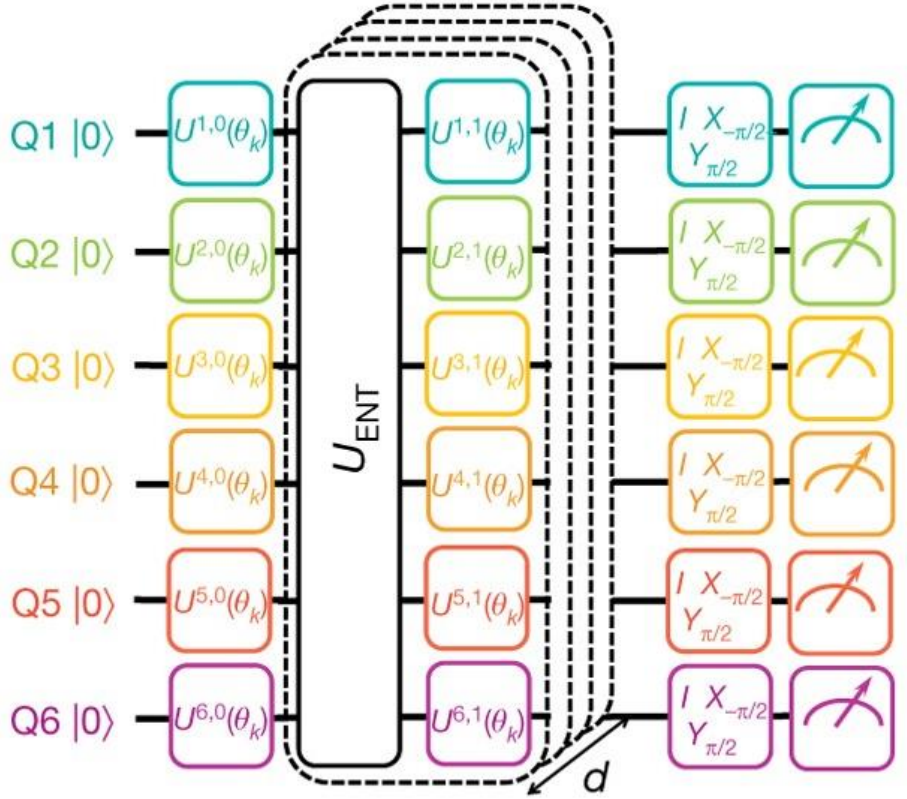
Challenges :

- Due to the noisy hardware, the objective function evaluation might not reflect the true objective function
- Some depend on the cardinality of the parameter set
- Getting stuck at a poor local optima in complicated energy landscapes
- expensive in terms of the number of circuit evaluations performed
- Barren plateaus

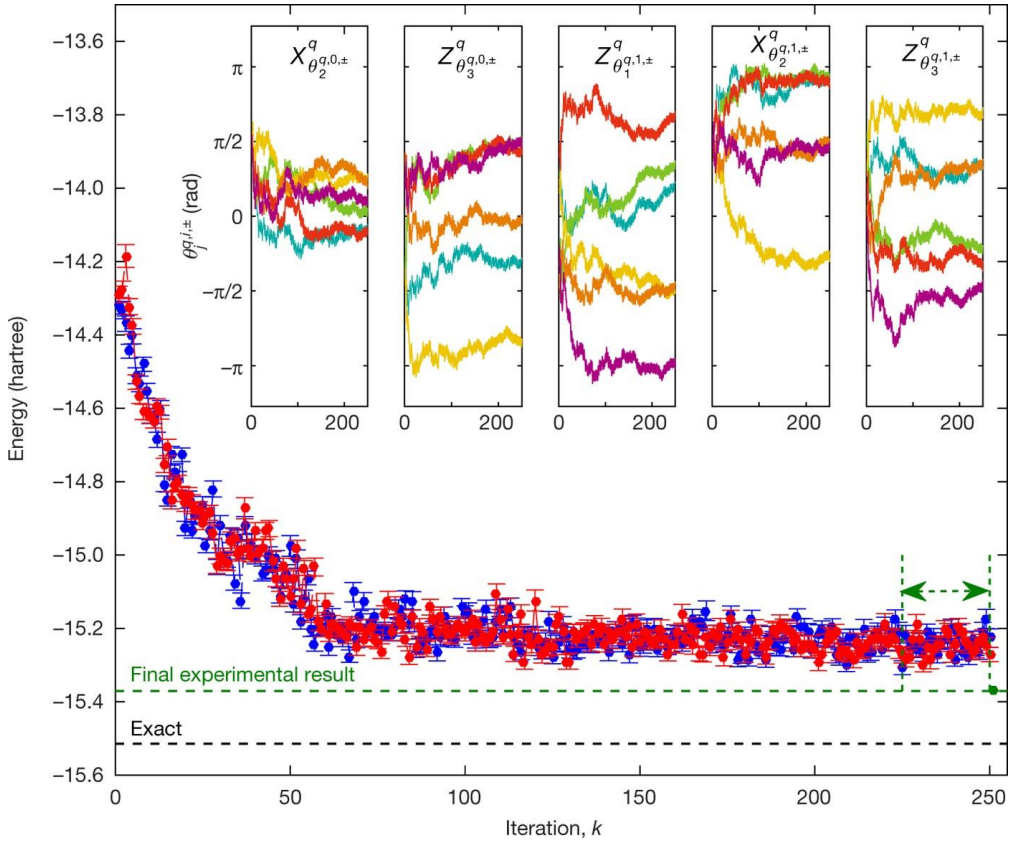
How to simulate a molecule with VQE ?



entangling unitary operations → a sequence of interleaved single-qubit rotations → final set of post-rotations → are read out is used to measure the expectation values of the individual Pauli terms in the Hamiltonian



Nature volume 549, pages242–246



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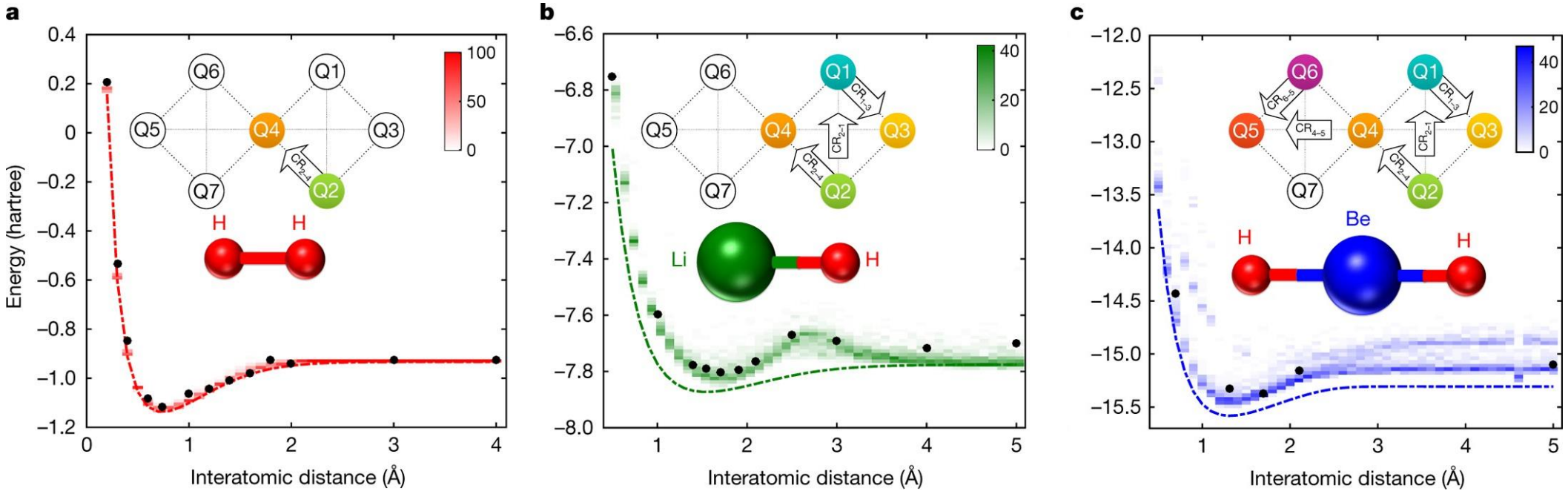

Nature volume 549, pages242–246

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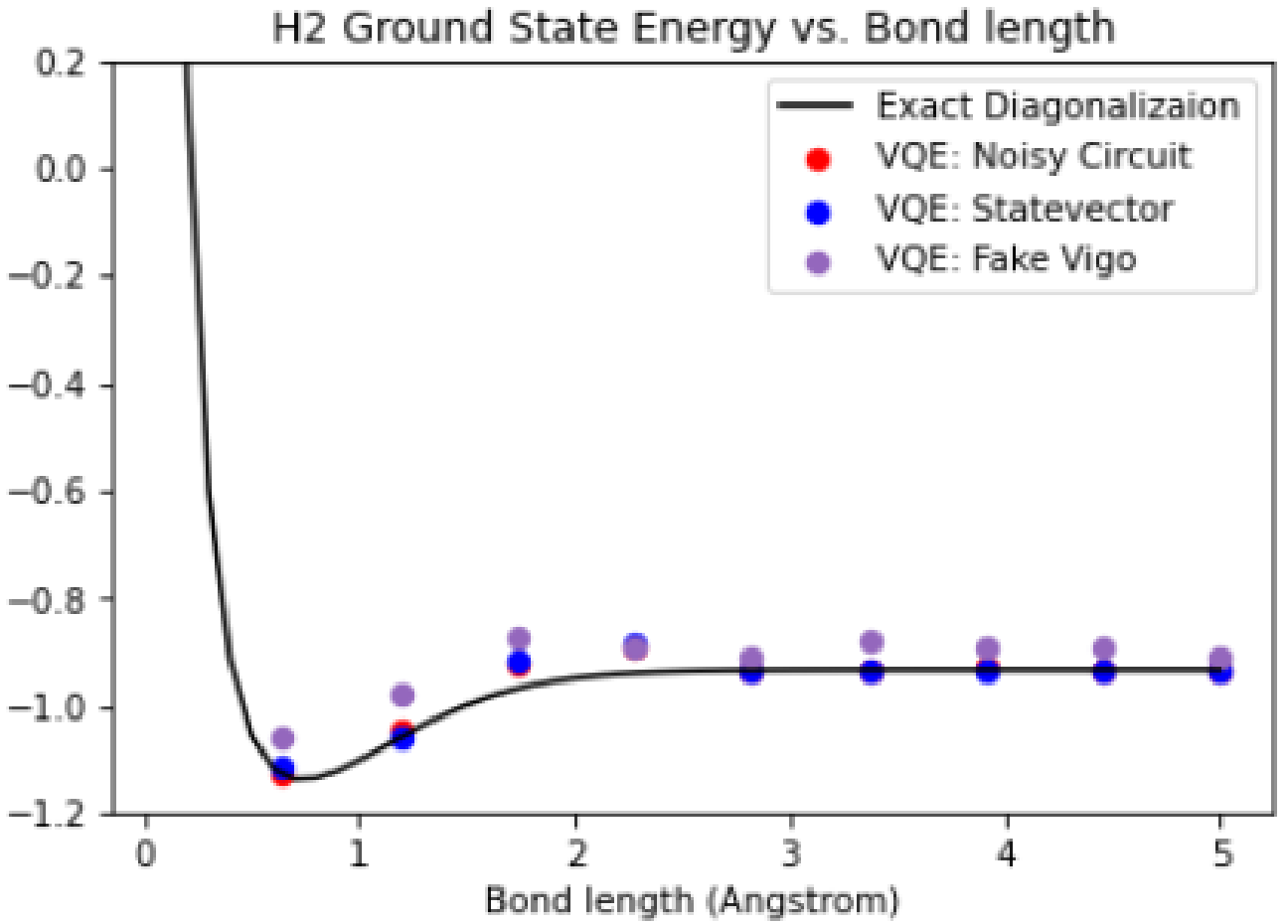
===H2 MOLECULAR INFORMATION===
Number of Electrons:     2
Number of spin orbitals  4
1st H : 1s spin up, 1s spin down; 2nd H 1s spin up, 1s spin down = 4
Number of Qubits         4
Repulsion Energy         0.7559674441714287 Hartree
```

```
===GROUND STATE INFORMATION===
We can solve small systems classically using
Exact Diagonalization methods
Ground State Wavefunction =
 [ 0.00000000e+00+0.j  0.00000000e+00+0.j  0.00000000e+00+0.j
  0.00000000e+00+0.j  0.00000000e+00+0.j -9.94506463e-01+0.j
  1.38777878e-17+0.j  0.00000000e+00+0.j  3.85185989e-34+0.j
 -3.11368744e-18+0.j  1.04675186e-01+0.j  0.00000000e+00+0.j
  0.00000000e+00+0.j  0.00000000e+00+0.j  0.00000000e+00+0.j
  0.00000000e+00+0.j]
Ground State Energy =
 -1.8921568982373507 (computed) + 0.7559674441714287 (shift)
    = -1.136189454065922 Hartree
```



So what did / do we learn?

Weigh in on Variational Methods

They were not originally presented as a faster algorithm, but rather one that has the potential to scale well and gives a chance to make use of NISQs

What do we need to get near there?

- ❑ Better coherence times and gate fidelities
- ❑ Robust algorithms

Why do even perform these experiments?

- Find out how far we are from something classically intractable
- Gives a general device level benchmark
- Study the effects of noise on algorithms and to test error mitigation ideas

Open questions:

- ❑ How to input or embed classical data as part of the ansatz effectively?
- ❑ What if we make the classical processing itself trainable?
- ❑ Scaling to larger systems

THANK YOU

Questions?