Variational Quantum Eigensolver

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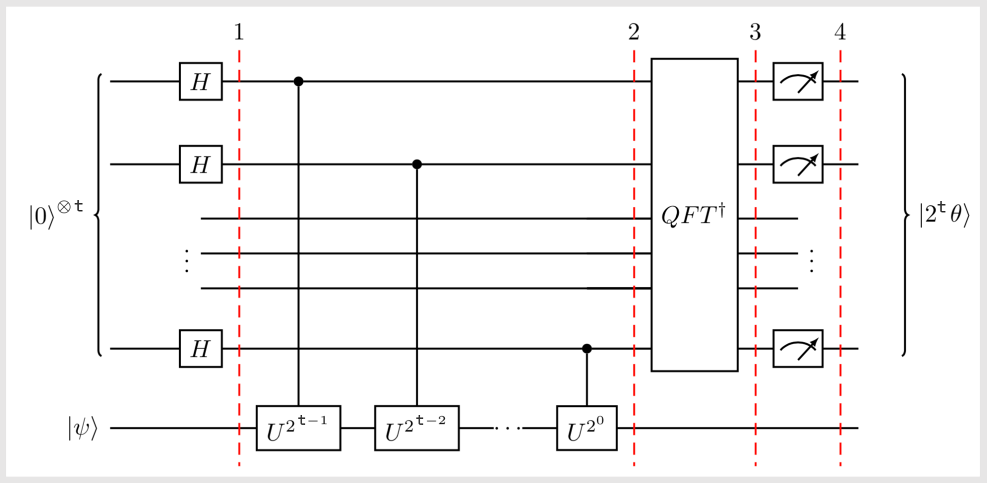
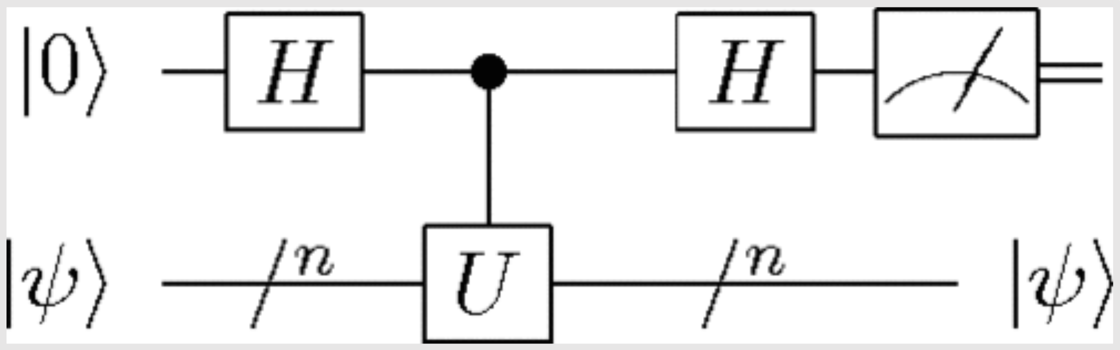
Road Map

- Build up high-level description of VQE
- Discuss theoretical underpinnings
- Sample code walk through

Quantum Phase Estimation recap



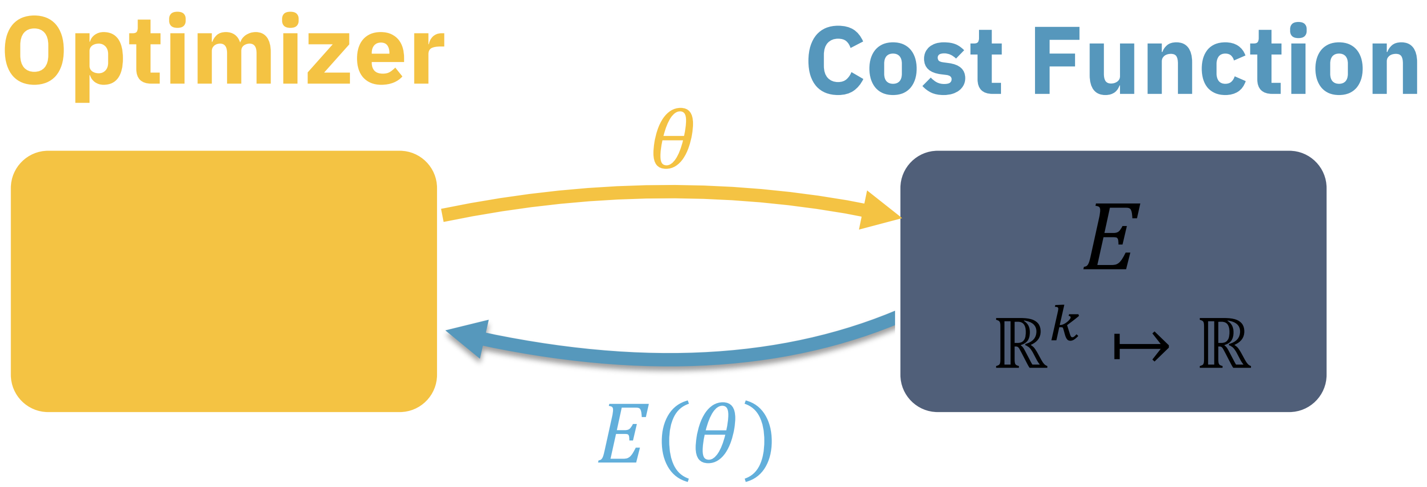
Quantum phase estimation



Iterative quantum phase estimation

VQE: Motivation

Goal: **minimize the energy of a system**



$E: \mathbb{R}^k \mapsto \mathbb{R}$

parameters

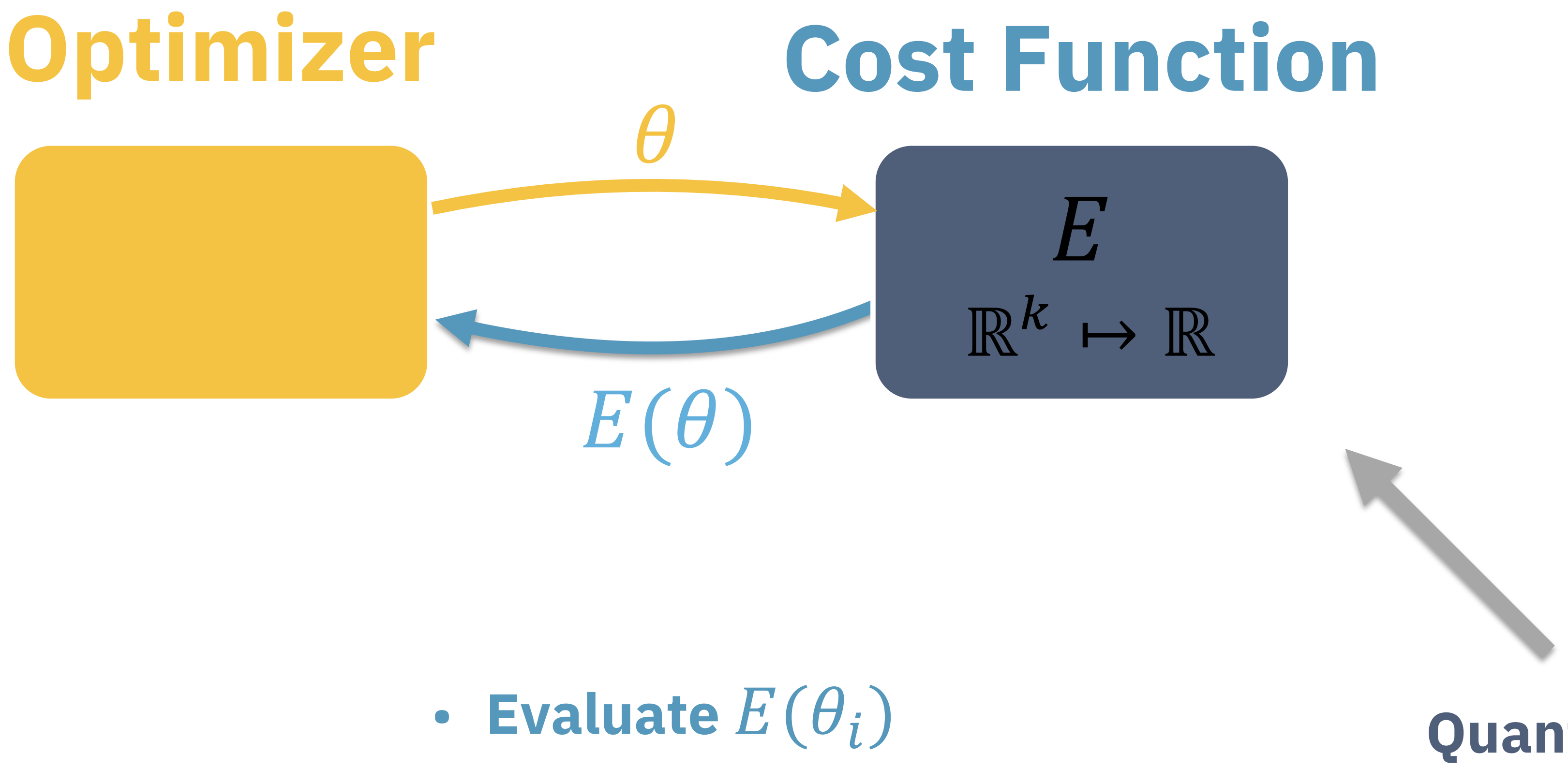
$\downarrow$

real number

- Initialize params θ_0
- Repeat:
  - **Evaluate** $E(\theta_i)$
  - **Choose** θ_{i+1}

VQE: Motivation

Goal: minimize the energy of a system



$E: \mathbb{R}^k \mapsto \mathbb{R}$

parameters

$\downarrow$

real number

- **Evaluate** $E(\theta_i)$
- **Choose** θ_{i+1}

Cost Function: What is a Hamiltonian?

If the system is in state $|\psi\rangle$,
the energy of the system is: $\langle\psi|H|\psi\rangle$

We want to know the minimum energy of H.
In other words: the lowest eigenvalue, λ_0

$$\min_{|\psi\rangle} \langle\psi|H|\psi\rangle$$
$$= \langle\psi_0|H|\psi_0\rangle$$
$$= \lambda_0$$

Trial States + The Variational Principle

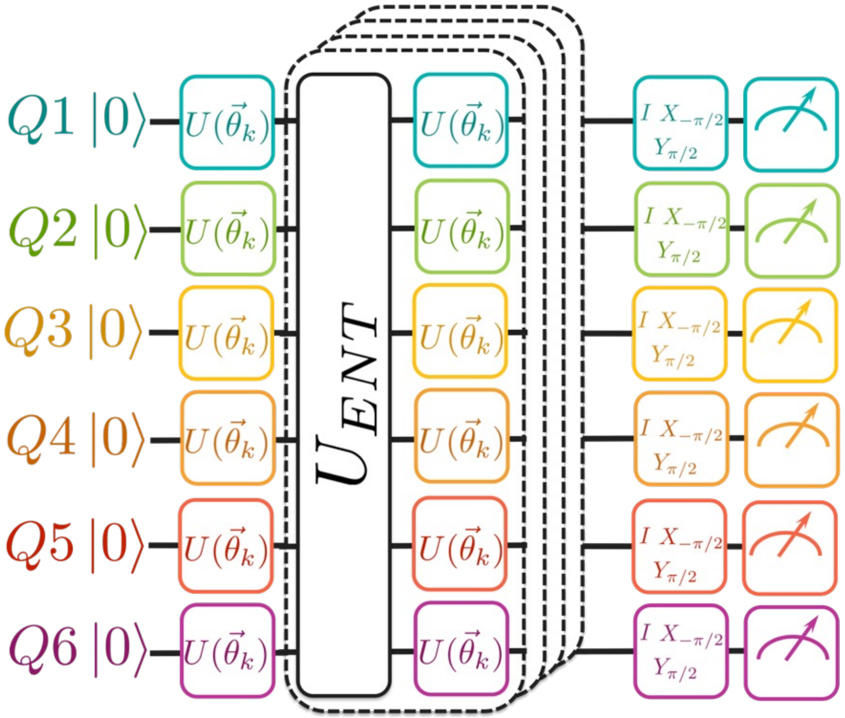
Parameterize some continuous subset M_k of quantum states

$$|\psi(\theta)\rangle \in M_k \subset \mathbb{C}^{2^n}$$

Where k = dim(θ) = $\mathcal{O}(poly)$

Note: we are not guaranteed that M_k contains the ground state!

WHP: $|\psi_0\rangle \notin M_k$



Trial States + The Variational Principle

Trial States

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The Variational Principle

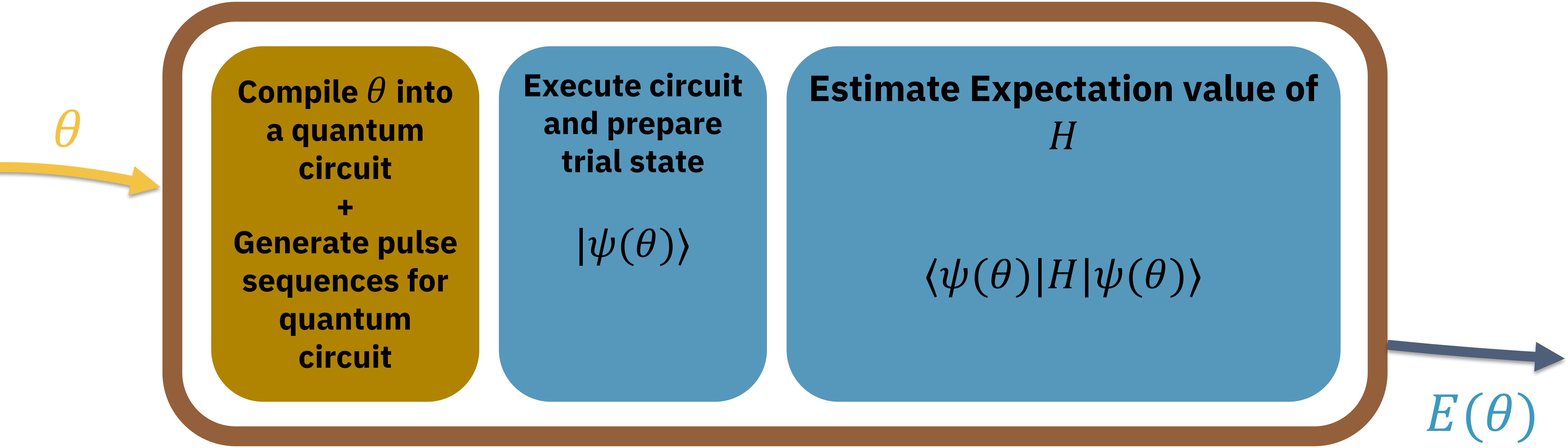
$$\langle\psi(\theta)|H|\psi(\theta)\rangle \geq \langle\psi_0|H|\psi_0\rangle$$

(Still holds if $|\psi(\theta)\rangle$ isn't pure)

$$\frac{\langle\psi(\theta)|H|\psi(\theta)\rangle}{\langle\psi(\theta)|\psi(\theta)\rangle} \geq \langle\psi_0|\psi_0\rangle$$

Proof attached after conclusion slide.

Cost Function Breakdown



Cost Function Breakdown

θ

Cost Function

Compile θ into a quantum circuit
+
Generate pulse sequences for quantum circuit

Execute circuit and prepare trial state

$|\psi(\theta)\rangle$

Measure Pauli Strings

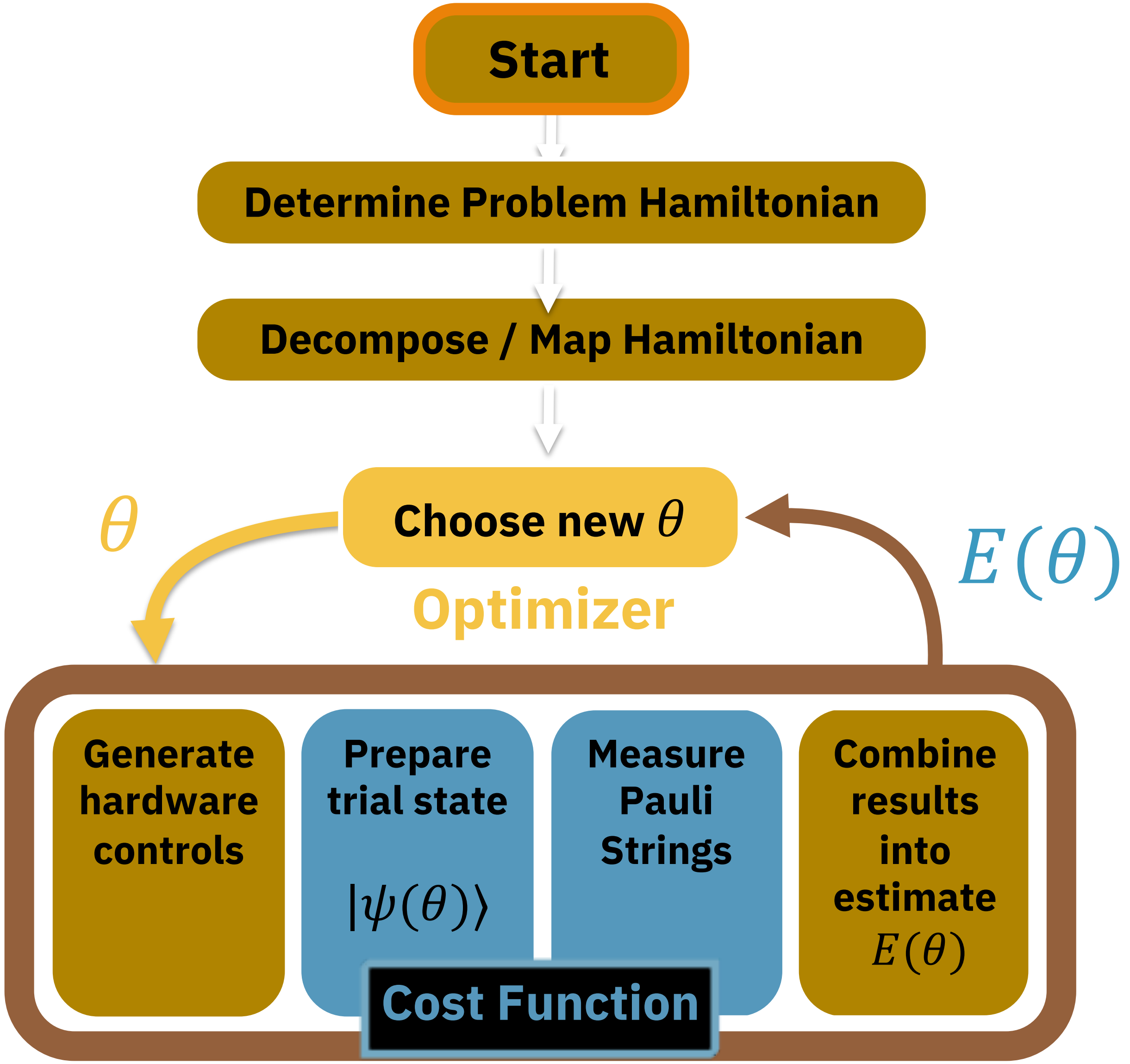
$\langle\psi(\theta)|P_i|\psi(\theta)\rangle$

Combine results to estimate

$\langle\psi(\theta)|H|\psi(\theta)\rangle = E(\theta)$

$E(\theta)$

The whole VQE-nchillada



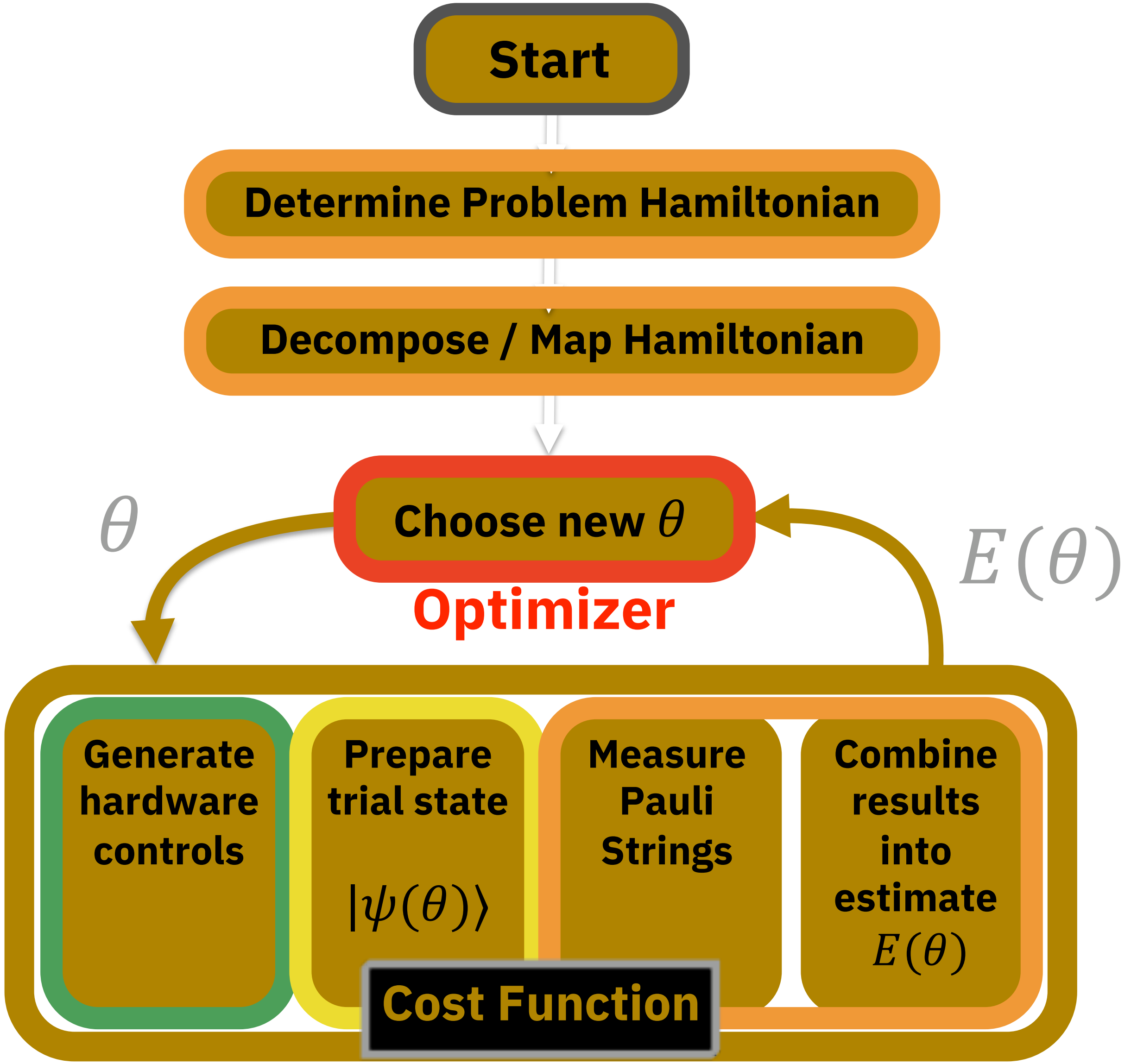
Advantages:

- Uses **shallow circuits**
- Results in an efficient representation of the ground state †

Robust to incoherent **AND** coherent noise

† Approximate representation & only when successful.

The whole VQE-nchillada

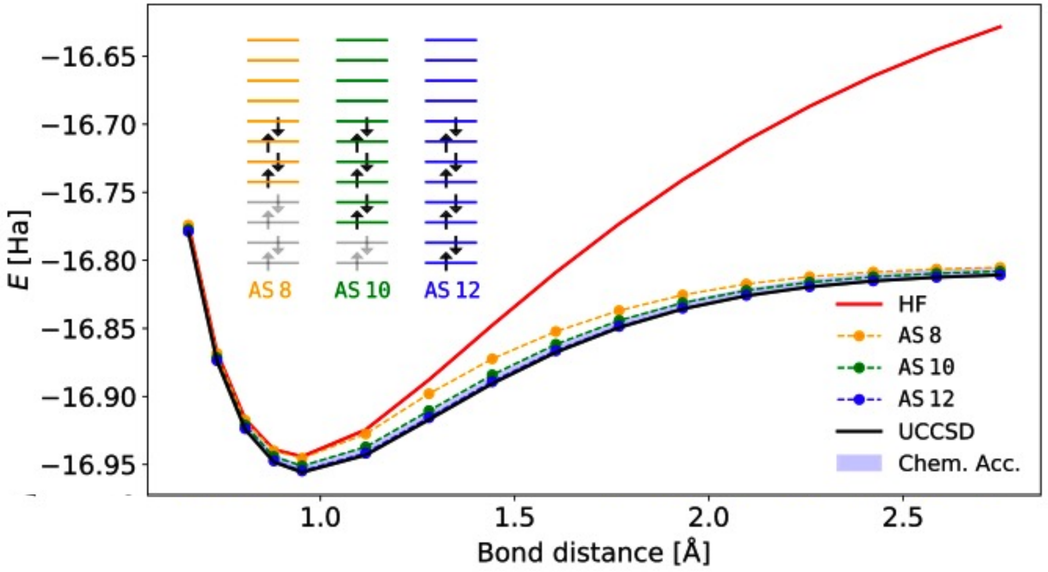


1. Optimizer
2. Hamiltonian Mapping
3. Hamiltonian Mapping & Reduction
4. Initial States + Variational Forms
5. Hardware Control
6. Error Mitigation Techniques

VQE Application Areas

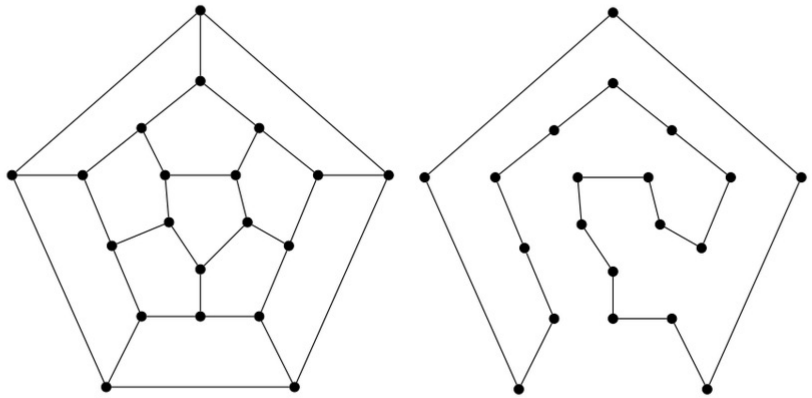
Chemistry

- Ground State Preparation
- Excited state prep



Optimization

- Constraint Satisfaction
  - Traveling Salesman
- Clustering



Computational Complexity of VQE

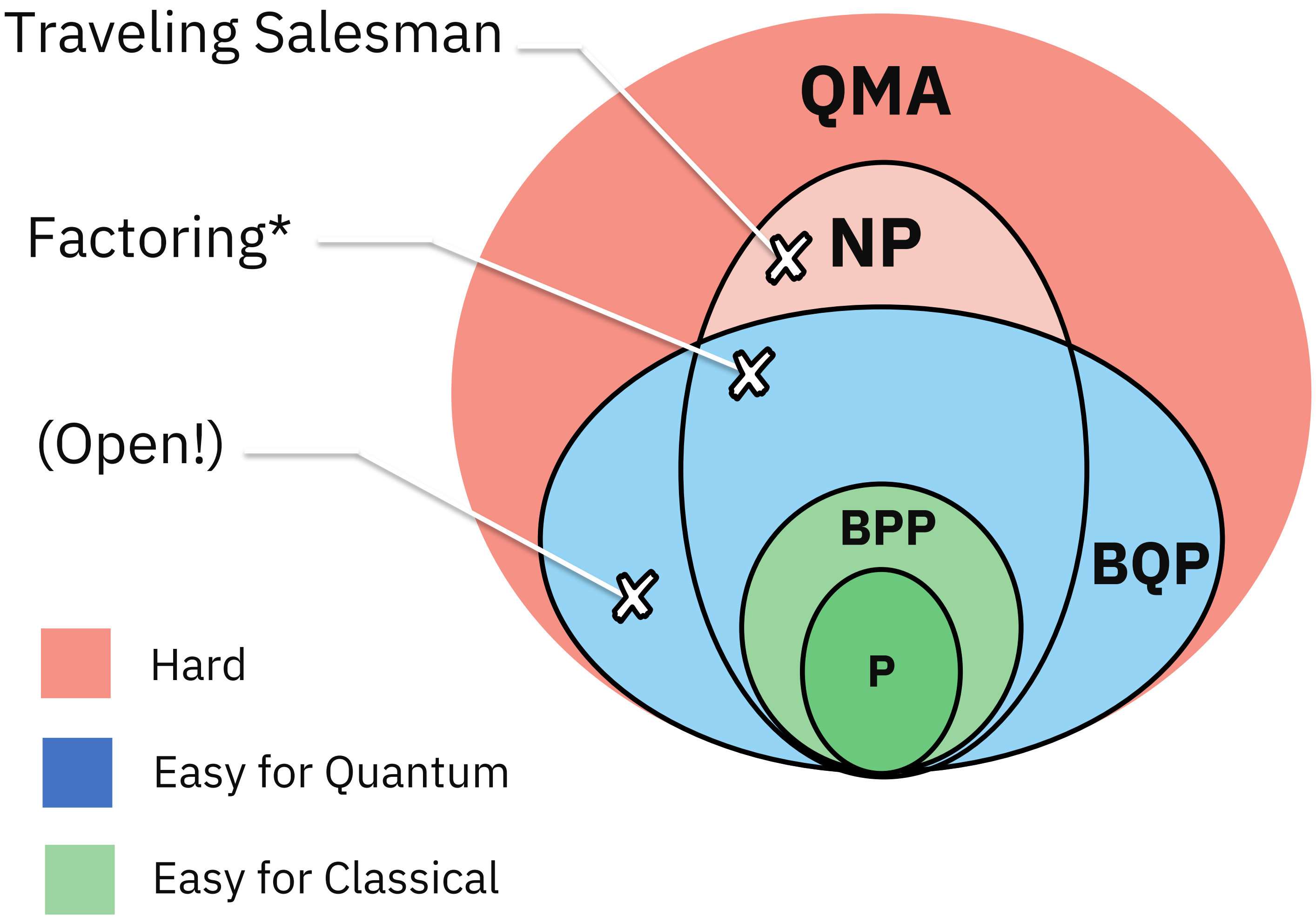
When should you try VQE?

Your problem is naturally expressed with a Hamiltonian
& the solution finding states with high ground-state overlap.

When does VQE perform well?

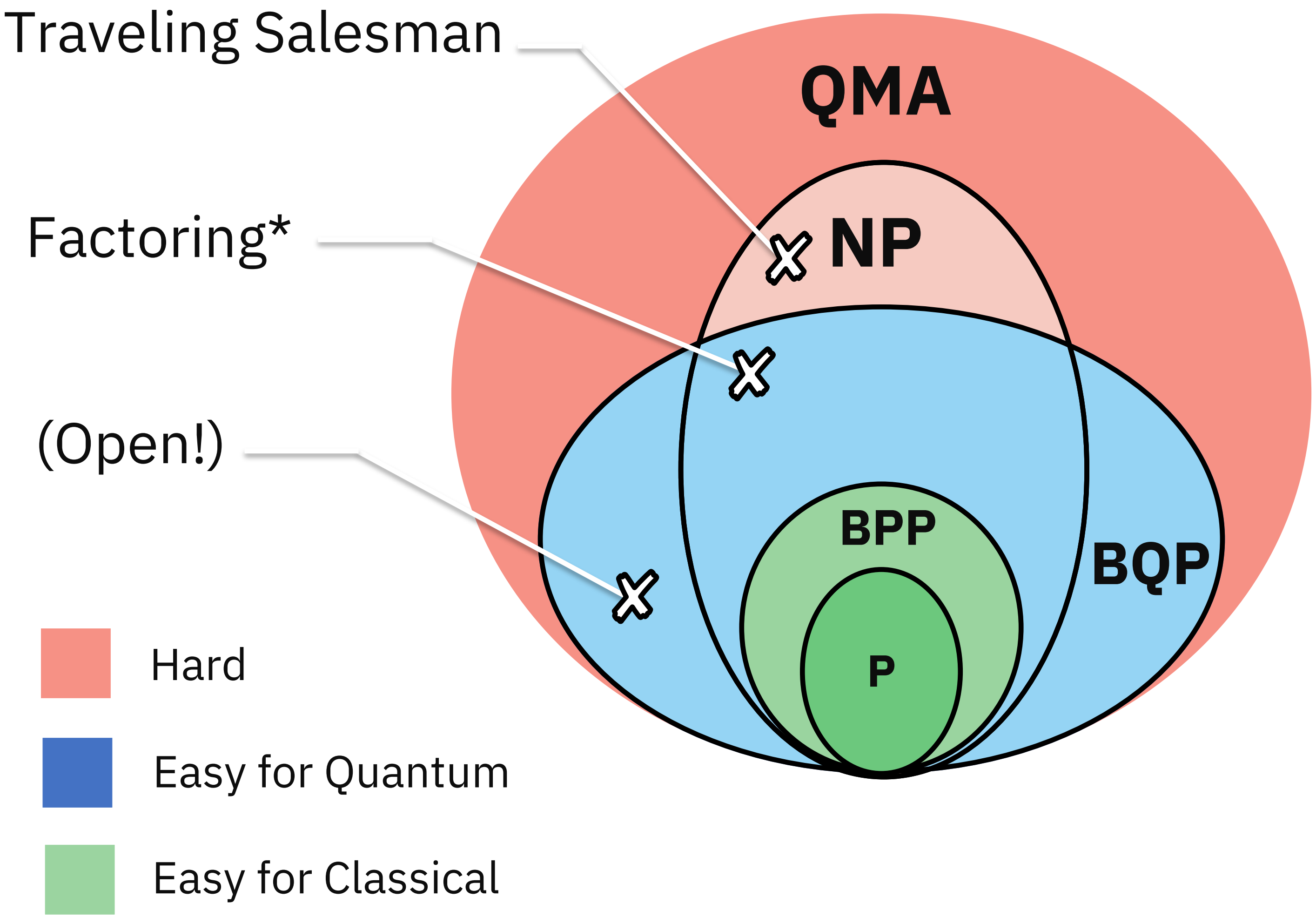
Not so easy to answer.

Computational Complexity of VQE



Computational Complexity of VQE

VQE under the following conditions:



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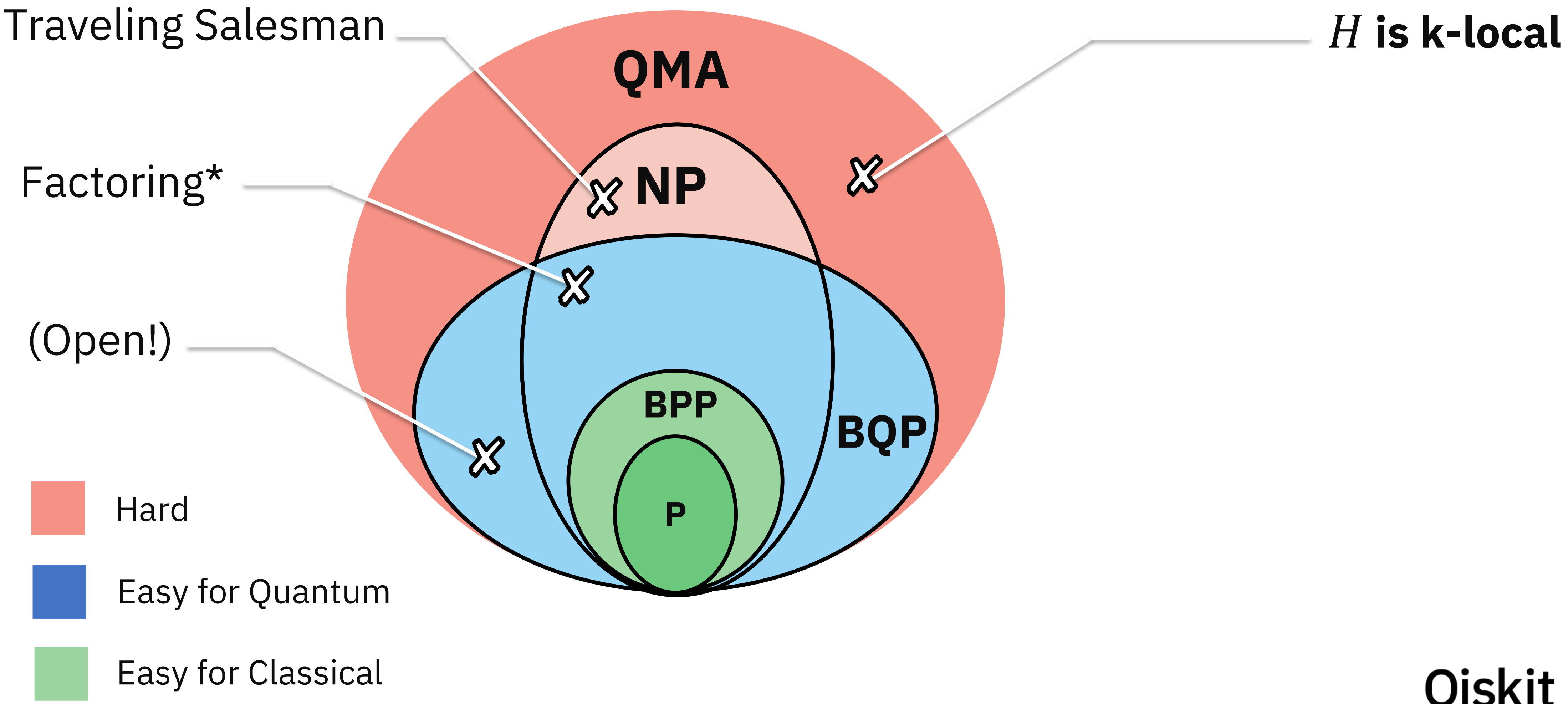


Computational Complexity of VQE

VQE under the following conditions:

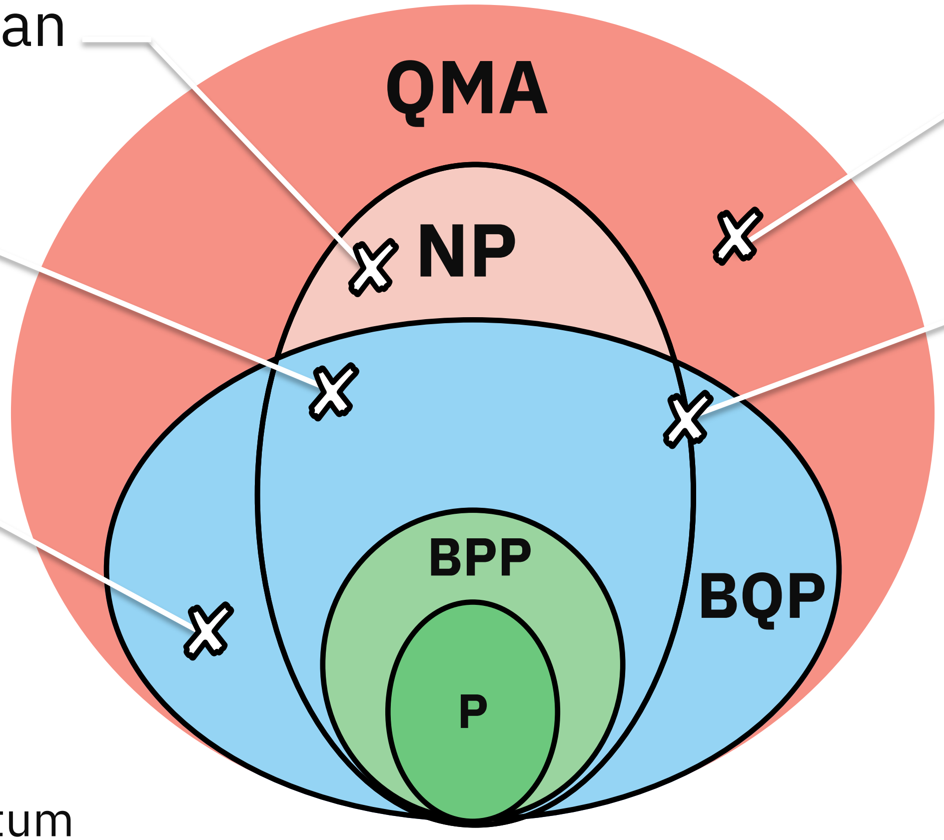
H **is k-local**

$H \geq 0^{\ddagger}$

Traveling Salesman

Factoring*

(Open!)



Hard

Easy for Quantum

Easy for Classical

‡ **Where depth and # VQE iterations is $\mathcal{O}(poly)$**

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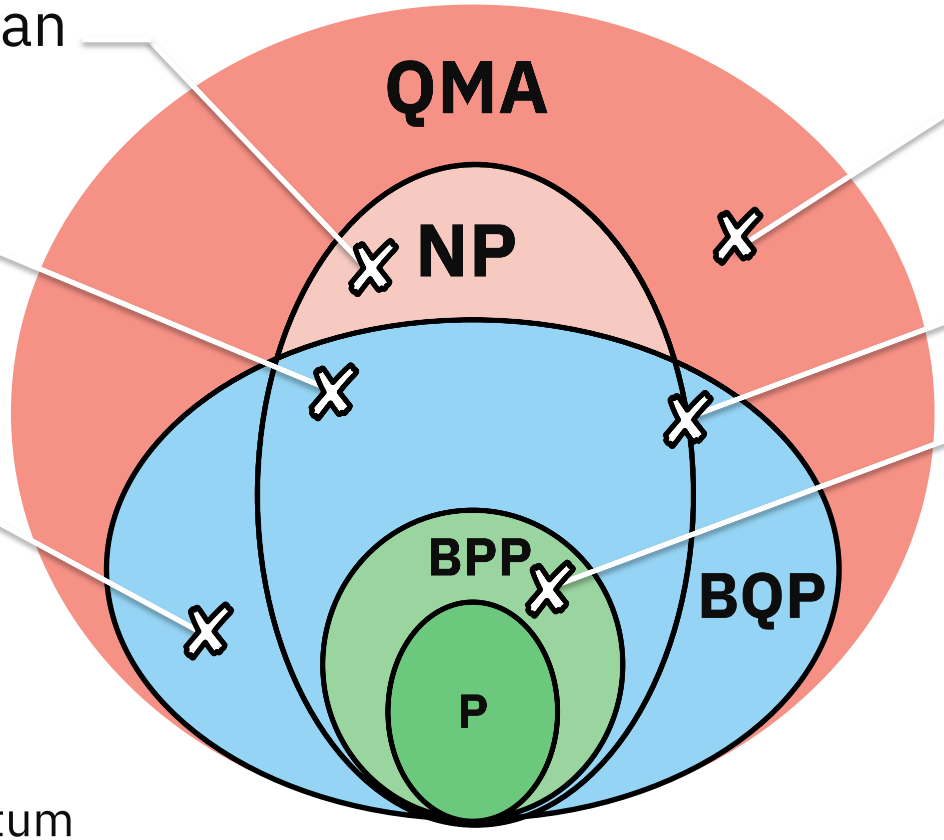

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Constant-depth

2D circuits †

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† **The VQE ansatz has 2D connectivity**

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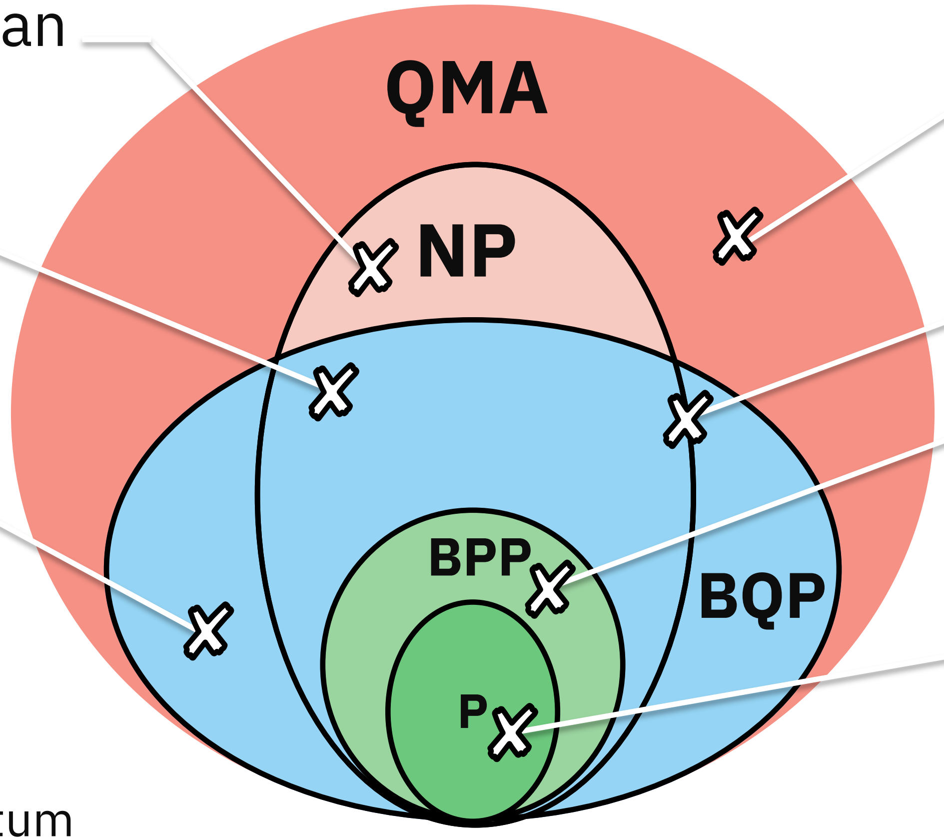

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Gapped local 1D H

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Computational Complexity of VQE

VQE under the following conditions:

Traveling Salesman

Factoring*

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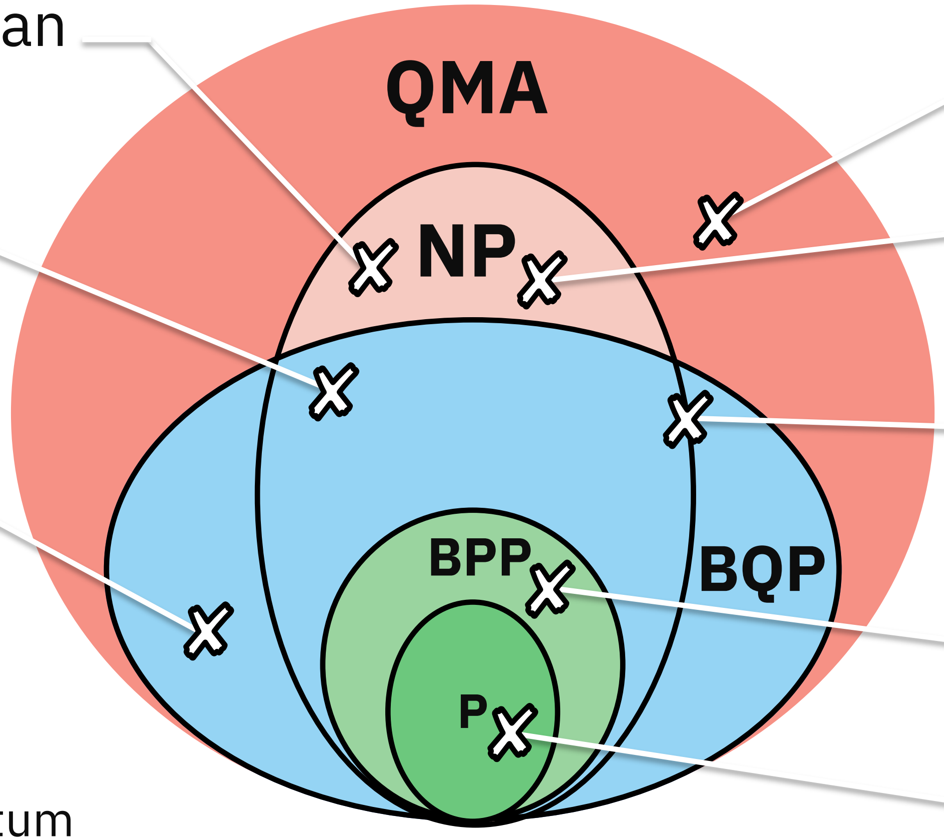

H **is k-local**

Ising model in nonuniform mag. field

$H \geq 0^{\ddagger}$

Constant-depth 2D circuits †

Gapped local 1D H

Hard

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Computational Complexity of VQE

Classical algorithms for quantum mean values

Sergey Bravyi, David Gosset, Ramis Movassagh

(Submitted on 25 Sep 2019)

The Complexity of the Local Hamiltonian Problem

Julia Kempe, Alexei Kitaev, Oded Regev

(Submitted on 24 Jun 2004 (v1), last revised 2 Oct 2005 (this version, v2))

The Power of Quantum Systems on a Line

Dorit Aharonov, Daniel Gottesman, Sandy Irani & Julia Kempe

A polynomial time algorithm for the ground state of one-dimensional gapped local Hamiltonians

Zeph Landau[1], Umesh Vazirani[1] and Thomas Vidick[2*]

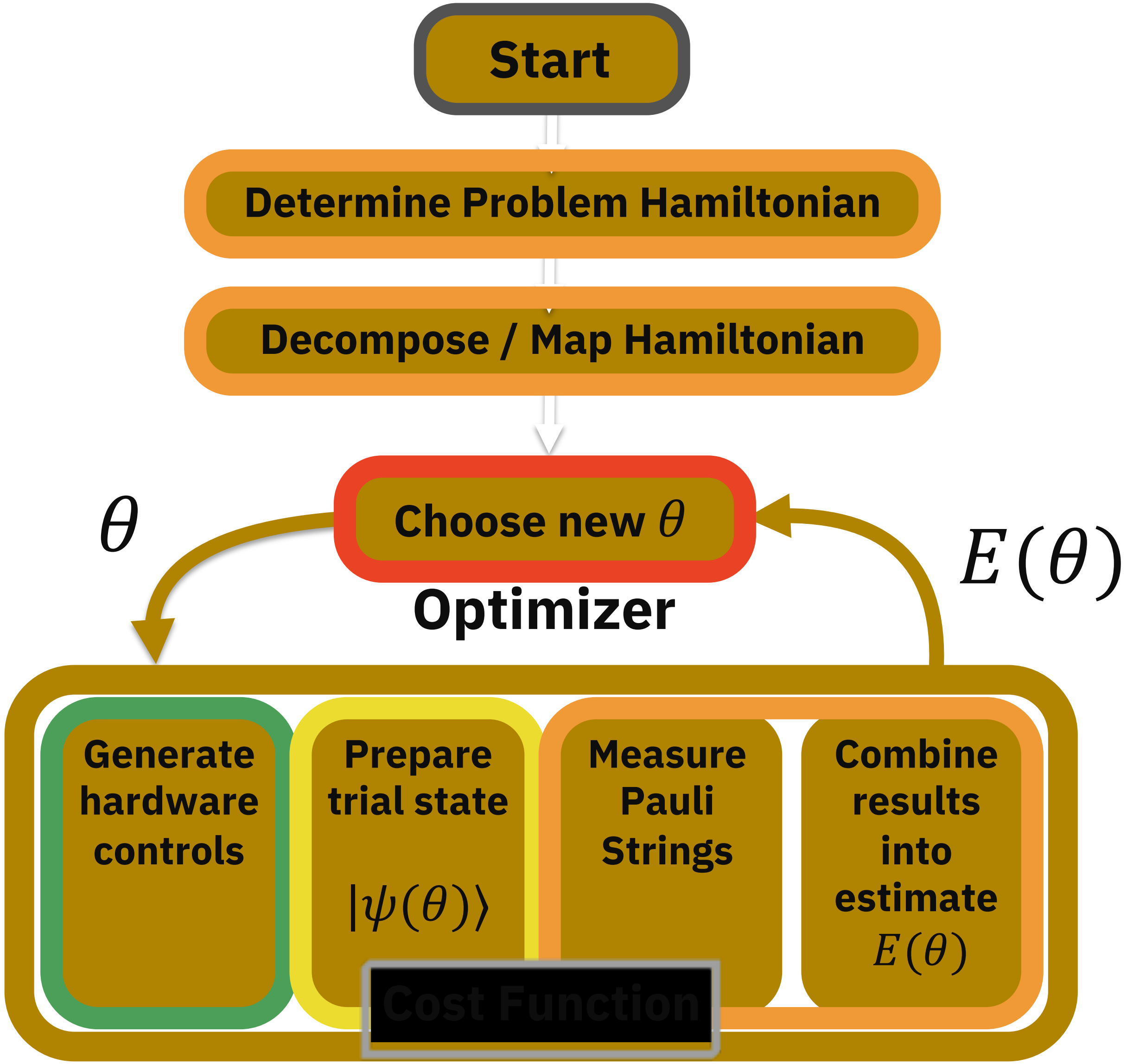
er

Key take aways

VQE is a heuristic algorithm that:

- Extends the reach of classical techniques
- Is suited to near term hardware
  - Requires only shallow circuits
  - Shows robustness to coherent and incoherent noise

The whole VQE-nchillada



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Check out Qiskit Textbook demo

https://learn.qiskit.org/course/ch-applications/simulating-molecules-using-vqe

The Variational Principle (quick proof)

Expand Hamiltonian

$$H = \sum_{i=1}^{k} \lambda_i |\psi_i\rangle\langle\psi_i| for\ eigenvalues \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_k$$

$$\langle\psi(\theta)|H|\psi(\theta)\rangle = \sum_{i=1}^{k} \lambda_i \langle\psi(\theta)|\psi_i\rangle\langle\psi_i|\psi(\theta)\rangle$$

$$\langle\psi(\theta)|H|\psi(\theta)\rangle = \sum_{i=1}^{k} \lambda_i |\langle\psi(\theta)|\psi_i\rangle|^2$$

$$min\langle\psi(\theta)|H|\psi(\theta)\rangle = \lambda_0 \rightarrow |\psi(\theta)\rangle = |\psi_0\rangle$$

Thank you