Variational Quantum Eigensolver

累了嗎？ 再讓我推薦個影片吧

- 線性代數的本質

Noisy Intermediate-Scale Quantum (NISQ)

- Quantum Computing is powerful ?
  - Quantum Algorithm Zoo
  - Quantum Complexity

- Quantum Computing is scalable
  - Need Error Correction

https://arxiv.org/abs/1801.00862

Noisy Intermediate-Scale Quantum (NISQ)

- When will quantum computer really be realized?
  - Very, very, very likely….

- Quantum Supremacy
  - 50 qubits is a significant milestone

NISQ Disadvantages

- Lots of Noise
  - Gate Errors, Readout error, etc
- Lifetime for qubits is limited
  - Lost of information was stored → number of operations you can perform in this time is limited
- Number of qubits is limited
  - Algorithm Requirements:
    - Shallow circuit depth
    - Robustness
    - Limited number of qubits and operations

VQE in nutshell

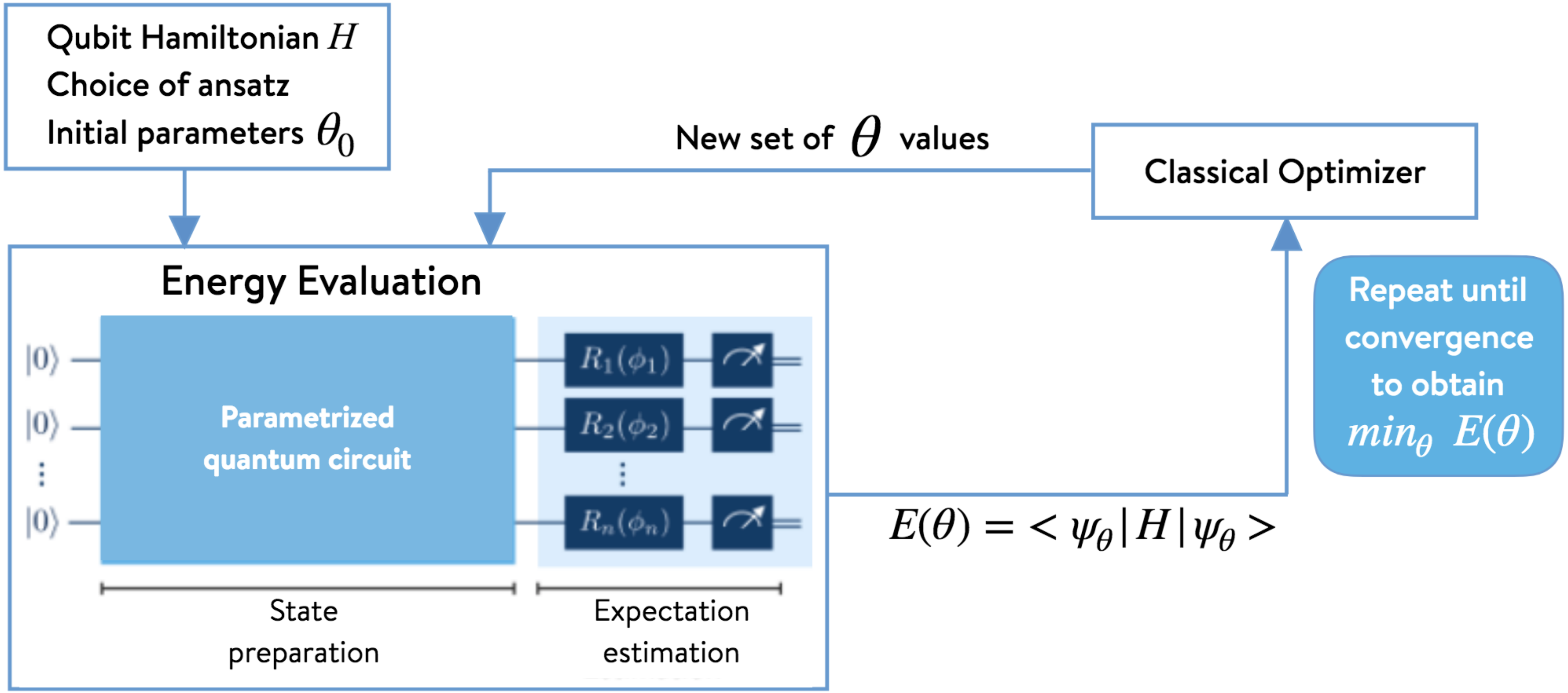
- VQE = Variational Quantum Eigensolver
  - Goal : find an upper bound of the lowest eigenvalue of a given Hamiltonian.

- Hybrid Quantum-Classical (HQC) Algorithm
  - Use both QPU and CPU, leverage strengths of quantum and classical computation.

VQE in Detail

- VQE One Two Three Four
  - One core concept : Variational Principle
  - Two parts: Quantum and Classical
  - Three Steps: Ansatz preparation, measure expectation and optimization
  - For Success!

VQE in Detail



VQE - Example

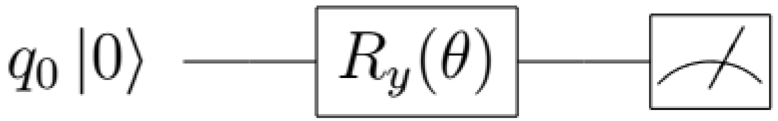
- Consider want to find the lowest eigenvalue of given Hamiltonian

$$H = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} .$$

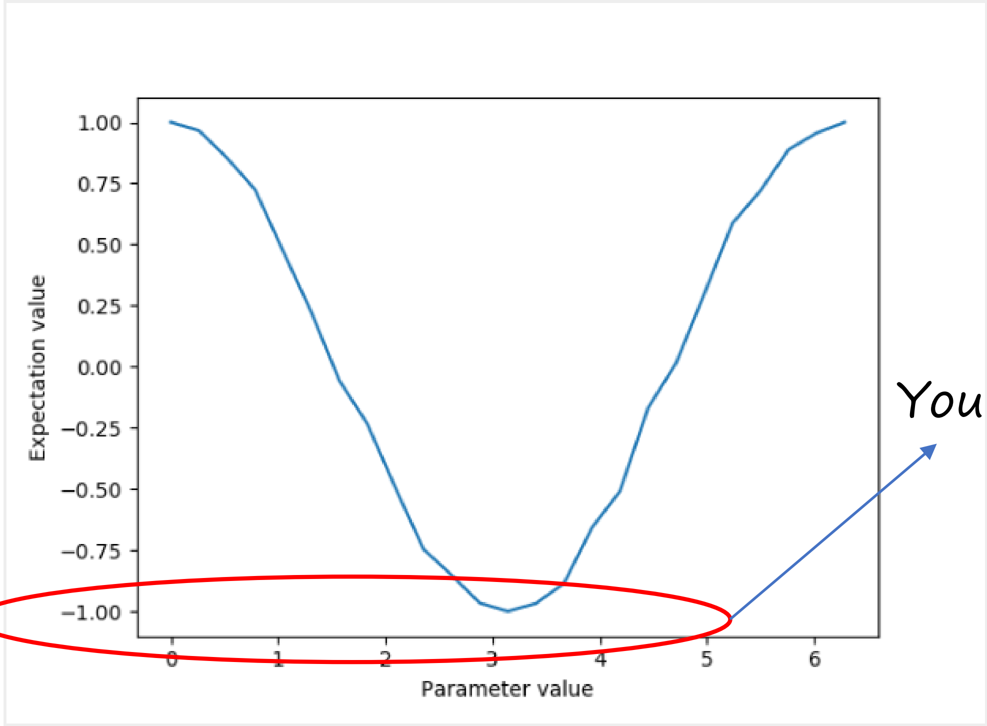
- Variational Principle:

$$\langle H \rangle_{|\psi(\vec{\theta})\rangle} = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle \ .$$

$$\langle H \rangle_{|\psi(\vec{\theta})\rangle} \geq \lambda_1 \, .$$



$$|\psi(\vec{\theta})\rangle = \mathrm{RY}\,|0\rangle$$
$$= \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
$$= \begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{bmatrix} .$$



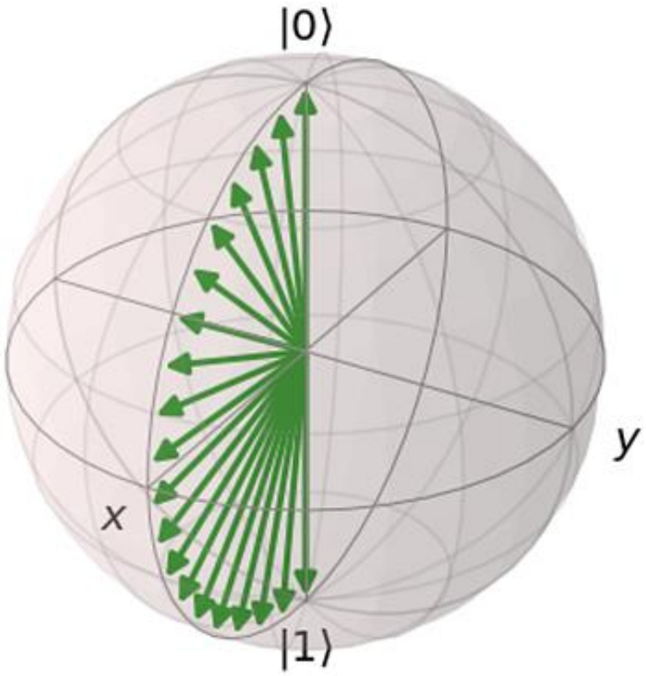
Expectation value depending on parameter in ansatz

You find minimum 1!
You get the eigenvalue and corresponding eigenvector!

LIVE DEMO-1

- VQE Algorithm Review

Variational Quantum eigensolver



EX:

1. write down the Hamiltonian

$$M = \begin{bmatrix} -0.2524859 & 0.18121 \\ 0.18121 & -1.8318639 \end{bmatrix}$$

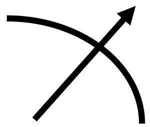
2.Tranfrom the Hamiltonian into Pauli form

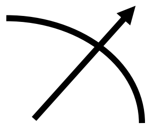
$$= -1.0421749I + 0.789689Z + 0.181210X$$

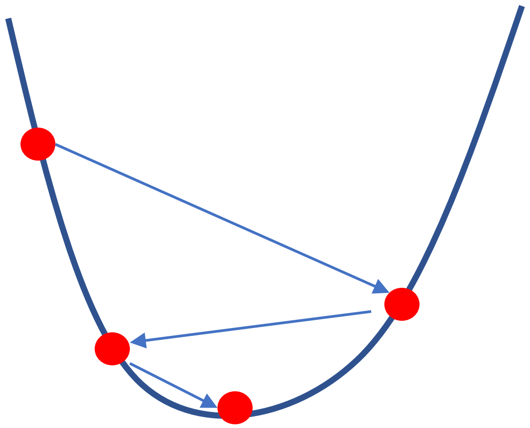
3. Determine the ansatz

$$|\psi(\theta)\rangle = \boxed{R_y(\theta)}|0\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)|1\rangle = \begin{bmatrix} \cos(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) \end{bmatrix}$$

4. Measure the expectation value term by term





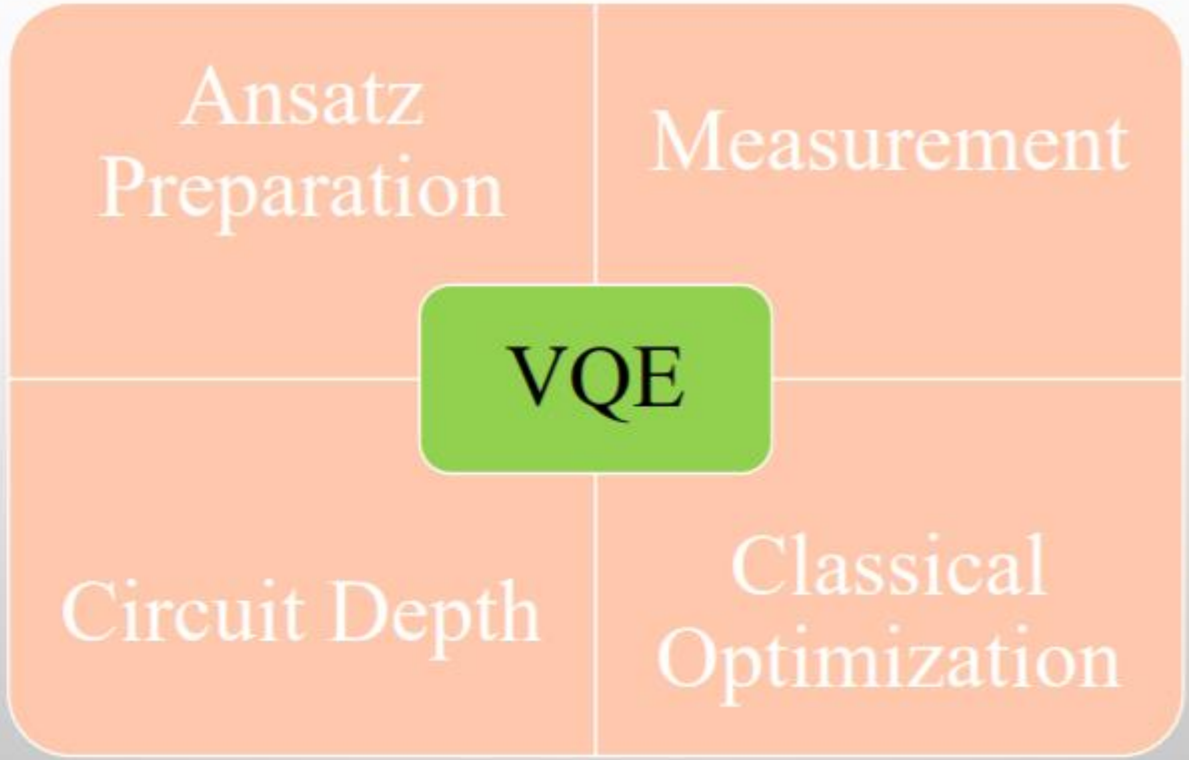


5. Sum up and minimize the expectation value

$$M_0 = \min_{\theta} \langle 0| R_y(\theta)^\dagger M R_y(\theta) |0\rangle = \min_{\theta} M(\theta)$$

VQE Challenges

- Ansatz performance sensitive to ansatz structure
- Quantum coherence is very limited



- Practical constraints, noise, etc…
- Classical optimization is not infinitely powerful