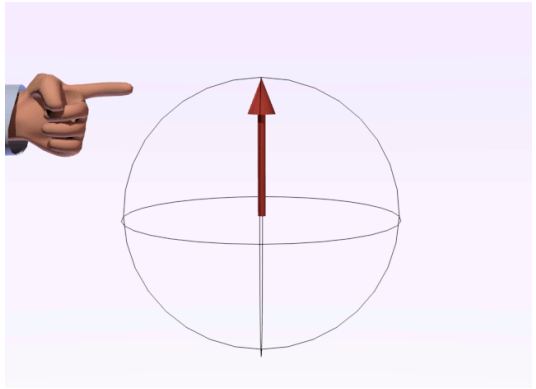
Variational Quantum Eigensolver

What is VQE?

Find the lowest eigenvalue of the cost function(M) which can be expressed in Pauli matrices.

$$M = aX + bY + cZ + const.$$



measure

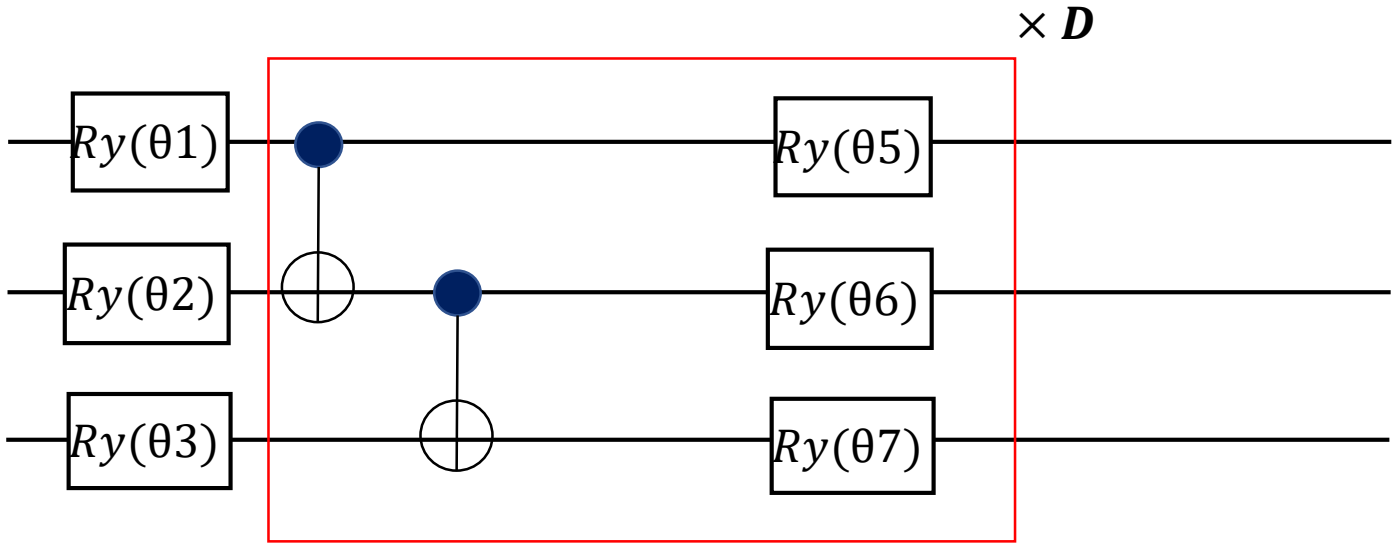
$|\psi\rangle$ is the initial state.

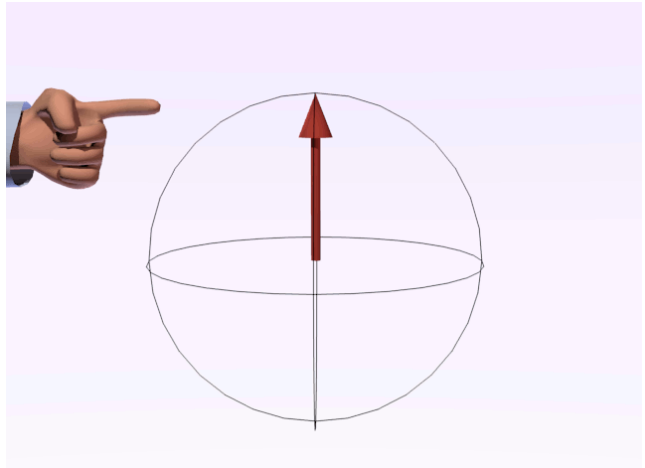
$$\langle\psi|A(\theta)MA(\theta)|\psi\rangle$$

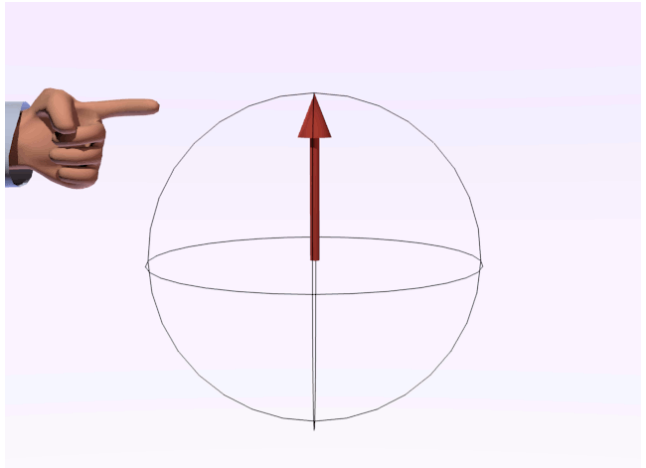
$$M_0 = \min_{\theta}\langle\psi|A(\theta)MA(\theta)|\psi\rangle$$

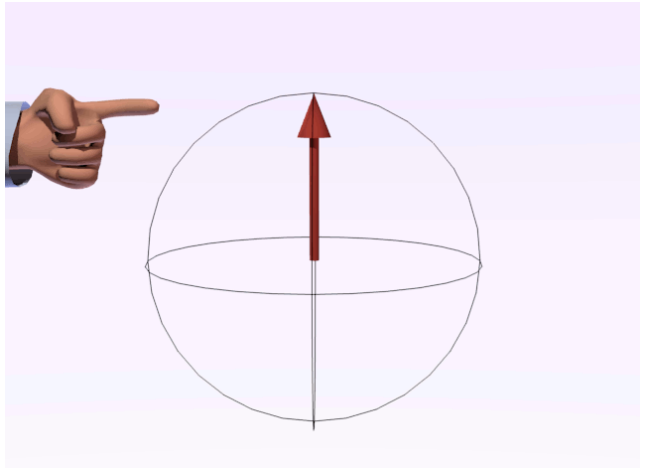
Ansatz(Ry)

Generate a trial wavefunction.









Measurement

$$|\psi\rangle = a|000\rangle + b|001\rangle + c|010\rangle + d|011\rangle + f|100\rangle + g|101\rangle + h|110\rangle + h|111\rangle$$

$$\langle\psi|ZZZ|\psi\rangle$$

$$= \underbrace{|a|^2 + |d|^2 + |g|^2 + |h|^2}_{\mathbb{P}_0} - \underbrace{|b|^2 - |c|^2 - |f|^2 - |h|^2}_{\mathbb{P}_1}$$

sum of the bit string is even

Eigenvalue=1

$a|000\rangle$

$d|011\rangle$

$g|101\rangle$

$h|110\rangle$

sum of the bit string is odd

Eigenvalue=-1

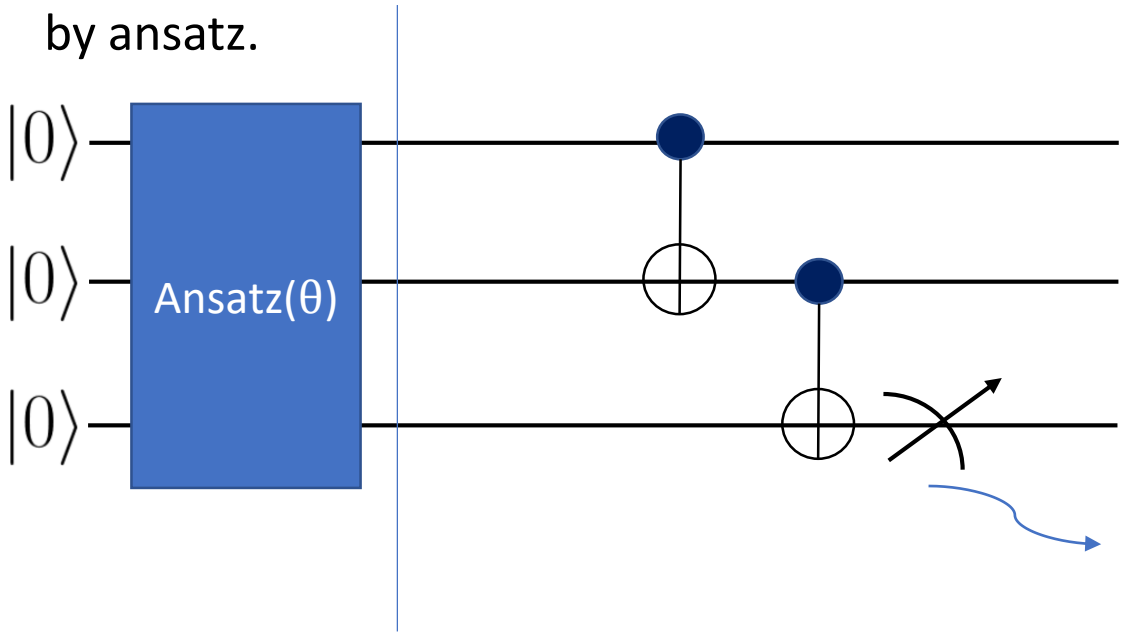
$b|001\rangle$

$c|010\rangle$

$f|100\rangle$

$h|111\rangle$

Generate a state by ansatz.



$\mathbb{P}_0$: sum of probability of the bit string being even

$\mathbb{P}_1$: sum of the bit string of the bit string being odd

Expectation Value of X

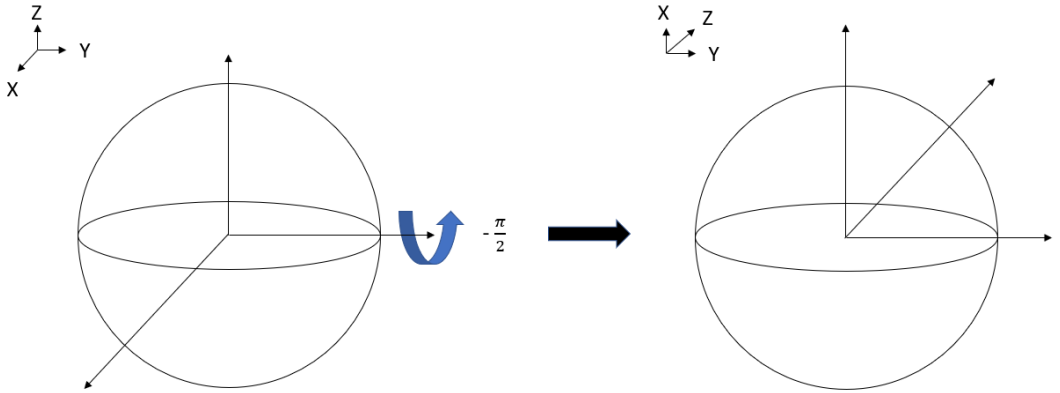
$$\begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\langle \psi | X | \psi \rangle = \langle \psi' | Z | \psi' \rangle$$

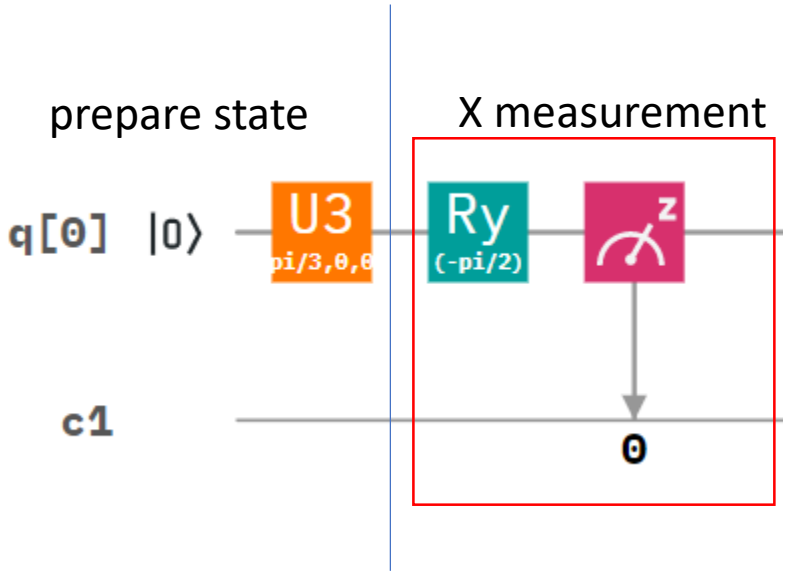
$$|\psi'\rangle = R_y(-\pi/2)|\psi\rangle$$

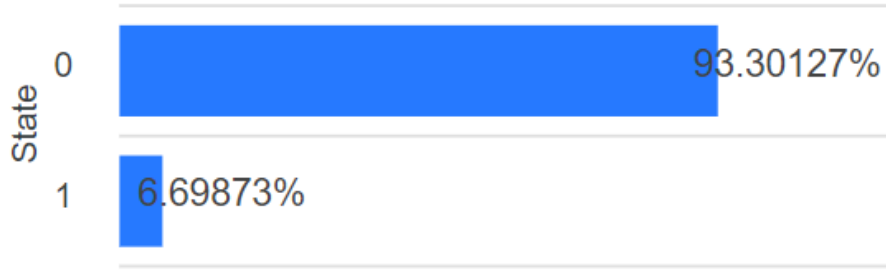
The rotation on the Bloch sphere:

$$R_y(-\pi/2) = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$



Expectation Value of X





$$\langle\psi|X|\psi\rangle = 0.933... - 0.067... = 0.866...$$

Expectation Value of Y

$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

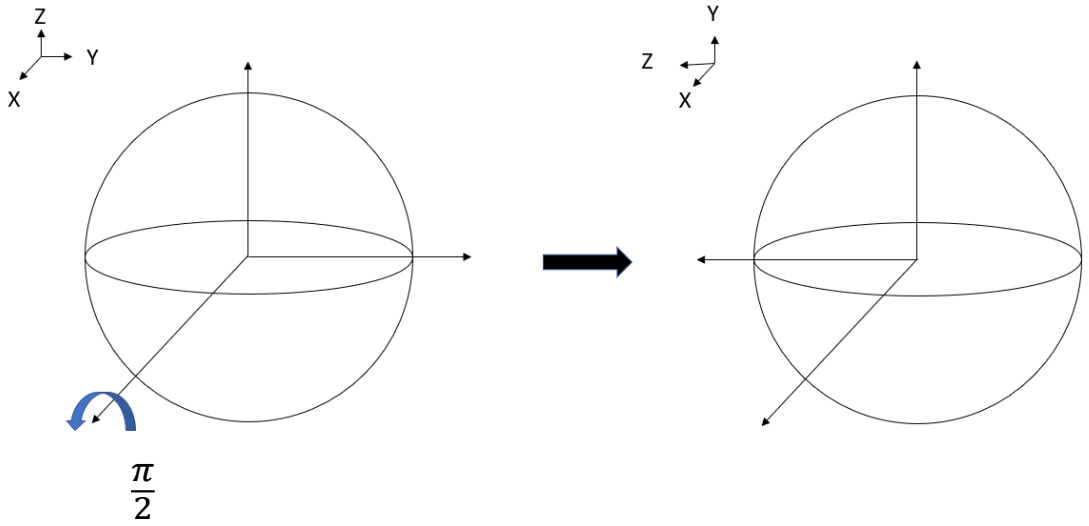
SORRY

$$\langle \psi | Y | \psi \rangle = \langle \psi' | Z | \psi' \rangle$$

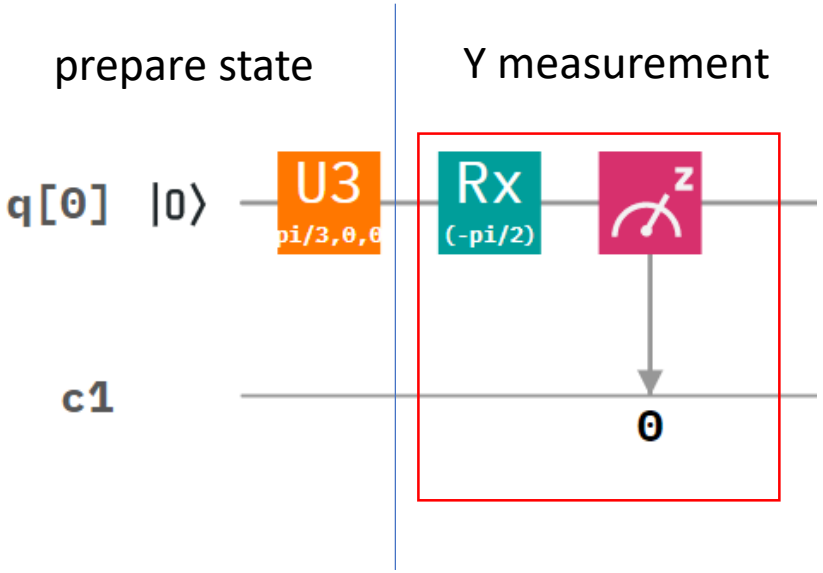
$$R_x(\pi/2)|\psi\rangle = |\psi'\rangle$$

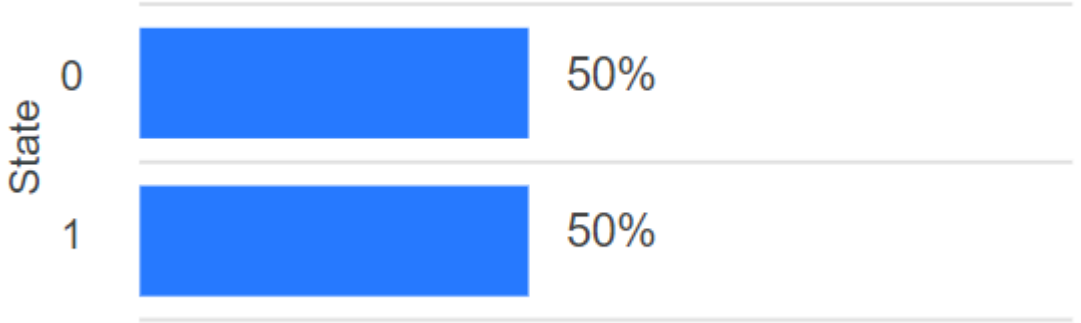
The rotation on the Bloch sphere:

$$R_x(\pi/2) = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$



Expectation Value of Y





$$\langle \psi | Y | \psi \rangle = 0.5 - 0.5 = 0$$