

Variational Quantum Eigensolver

Activity 3.1

QSciTech-QuantumBC virtual workshop
on gate-based quantum computing

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Topics

- 1. Variational quantum states**
- 2. Estimation of expectation values**
 - i. Measurement of 1 qubit quantum state**
 - ii. Measurement of n qubits quantum state**
- 3. Variational Quantum Eigensolver**

Our goal

Back to the future

Before even thinking of finding the **ground state** we need to be able to evaluate the energy of any **given state**.

$$E_\psi = \langle \psi | \hat{H} | \psi \rangle = \sum_i h_i \langle \psi | \hat{\mathcal{P}}_i | \psi \rangle$$

One way to **look for the ground state** is to define a **variational state** which depends on a series of **parameters**.

$$E(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | \hat{H} | \psi(\boldsymbol{\theta}) \rangle = \sum_i h_i \langle \psi(\boldsymbol{\theta}) | \hat{\mathcal{P}}_i | \psi(\boldsymbol{\theta}) \rangle$$

The variational principle states*

$$\langle \psi(\boldsymbol{\theta}) | \hat{H} | \psi(\boldsymbol{\theta}) \rangle \geq E_g$$

*Assuming normalized quantum state

Our goal

Back to the future

We will find the **ground state** if we can find the **parameters** which **minimize** the evaluated energy*.

*If the parameter space covers the ground state

$$E_0 = \min_{\theta} E(\theta) = \min_{\theta} \sum_i h_i \langle \psi(\theta) | \hat{\mathcal{P}}_i | \psi(\theta) \rangle$$

$$E_0 \sim E_g$$

Variational quantum states

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

Variational quantum states

Parametrized quantum states

A variational quantum state is a **linear combination** of the N basis states with coefficients that depend on a set of **parameters**.

Amplitude
Phase
Normalisation
Global phase

$$|\psi(\theta)\rangle = \sum_i^n \alpha_i(\theta) |\phi_i\rangle$$

There are $2N-2$ **degrees of freedom** in the choices of the coefficients. If the number of parameters is smaller, we won't be able to cover the whole state space.

A smaller space is easier to search as long as it contains what we are looking for!

Variational quantum states

As a unitary transformation

The variational state starting point can be either the **vacuum**

$$|\psi(\theta)\rangle = U(\theta) |0 \dots 0\rangle$$

or a **specific initial state**, like an approximate solution.

$$|\psi(\theta')\rangle = U'(\theta') |\psi_0\rangle$$

You'll still have to prepare this initial state.

$$|\psi_0\rangle = U_0 |0 \dots 0\rangle$$

$$U(\theta) = U'(\theta') U_0$$

Variational quantum states

A 2 qubits example

This is a 2 qubits **variational state** :

$$|\psi(\theta)\rangle = \cos \frac{\theta}{2} |00\rangle + e^{i\phi} \sin \frac{\theta}{2} |11\rangle \quad \theta = \{\theta, \phi\}$$

The **state vector** is the vector of the coefficients in a given basis.

$$\alpha_i(\theta) = \begin{pmatrix} \cos \theta/2 \\ 0 \\ 0 \\ e^{i\phi} \sin \theta/2 \end{pmatrix}$$

$$|\phi_i\rangle = \begin{cases} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{cases}$$

$$|\psi(\theta)\rangle = \sum_i^n \alpha_i(\theta) |\phi_i\rangle$$

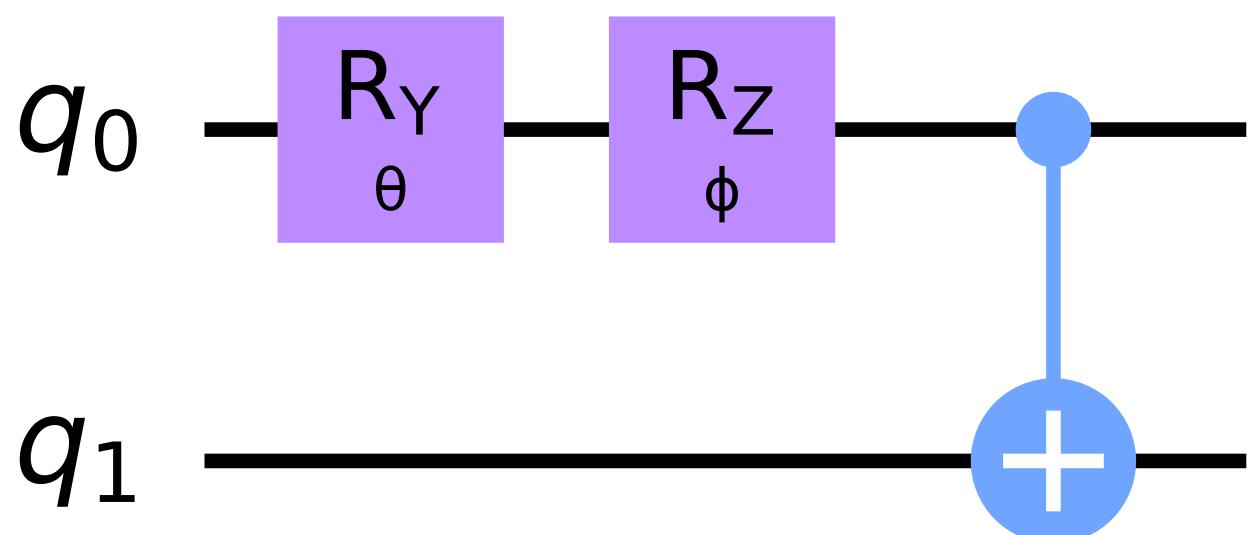
Variational quantum states

A 2 qubits example

This is a 2 qubits variational state :

$$|\psi(\theta)\rangle = \cos\frac{\theta}{2} |00\rangle + e^{i\phi} \sin\frac{\theta}{2} |11\rangle \quad \theta = \{\theta, \phi\}$$

This is a quantum circuit that prepares this variational state.

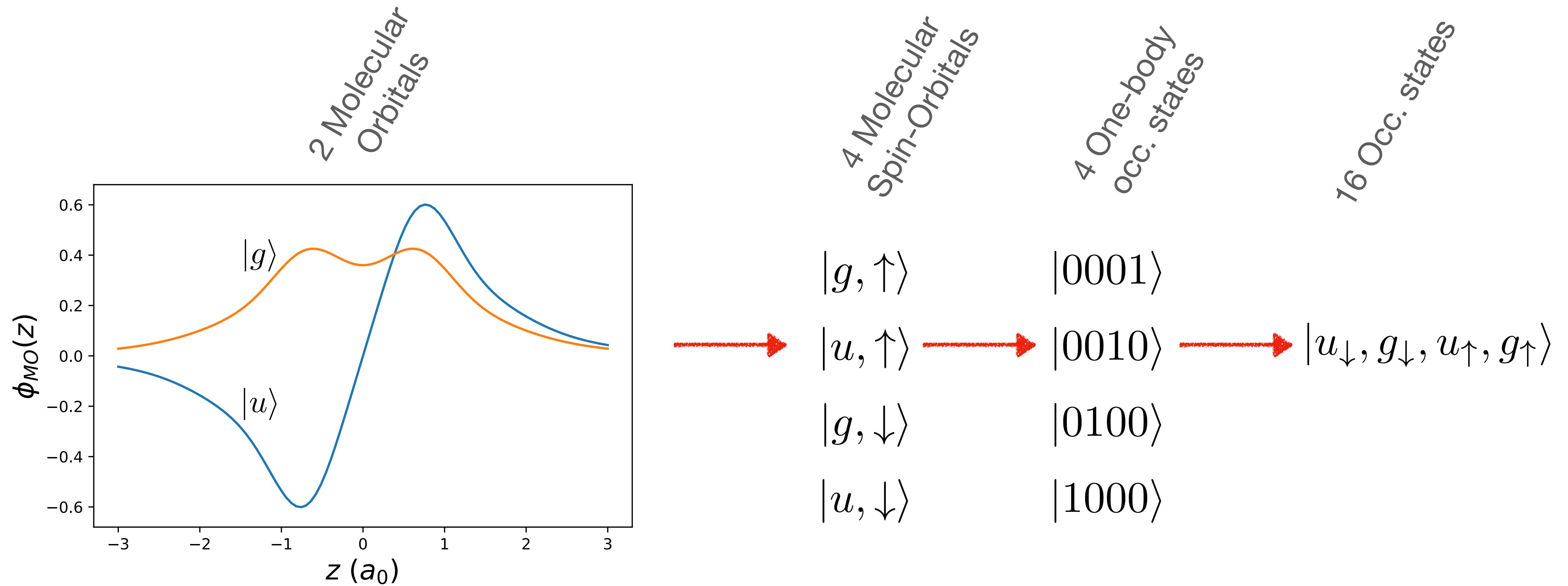


$$\begin{aligned}
 |\psi\rangle_{\text{step 0}} &= |00\rangle = |0\rangle \otimes |0\rangle \\
 |\psi\rangle_{\text{step 1}} &= |0\rangle \otimes \left(\cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle \right) \\
 &= \cos \frac{\theta}{2} |00\rangle + e^{i\phi} \sin \frac{\theta}{2} |01\rangle \\
 |\psi\rangle_{\text{step 2}} &= \cos \frac{\theta}{2} |00\rangle + e^{i\phi} \sin \frac{\theta}{2} |11\rangle
 \end{aligned}$$

Variational quantum states for H₂

Variational quantum states

Basis for the H₂ molecule



Preparation of a state

For the H₂ molecule

For a **4 qubits** system, the occupation basis counts $2^4 = 16$ base states.

$$|\phi_i\rangle = |0000\rangle, |0001\rangle, |0010\rangle, \dots, |0011\rangle, |0101\rangle, \dots, |1111\rangle$$

$\theta \rightarrow 2 \times 16 - 2 = 30$ parameters

There are only 6 states with exactly **2 electrons**.

$$|\phi_i\rangle = |0011\rangle, |0101\rangle, |1001\rangle, |0110\rangle, |1010\rangle, |1100\rangle$$

$\theta \rightarrow 2 \times 6 - 2 = 10$ parameters

And 4 states with **1 spin up and 1 spin down**.

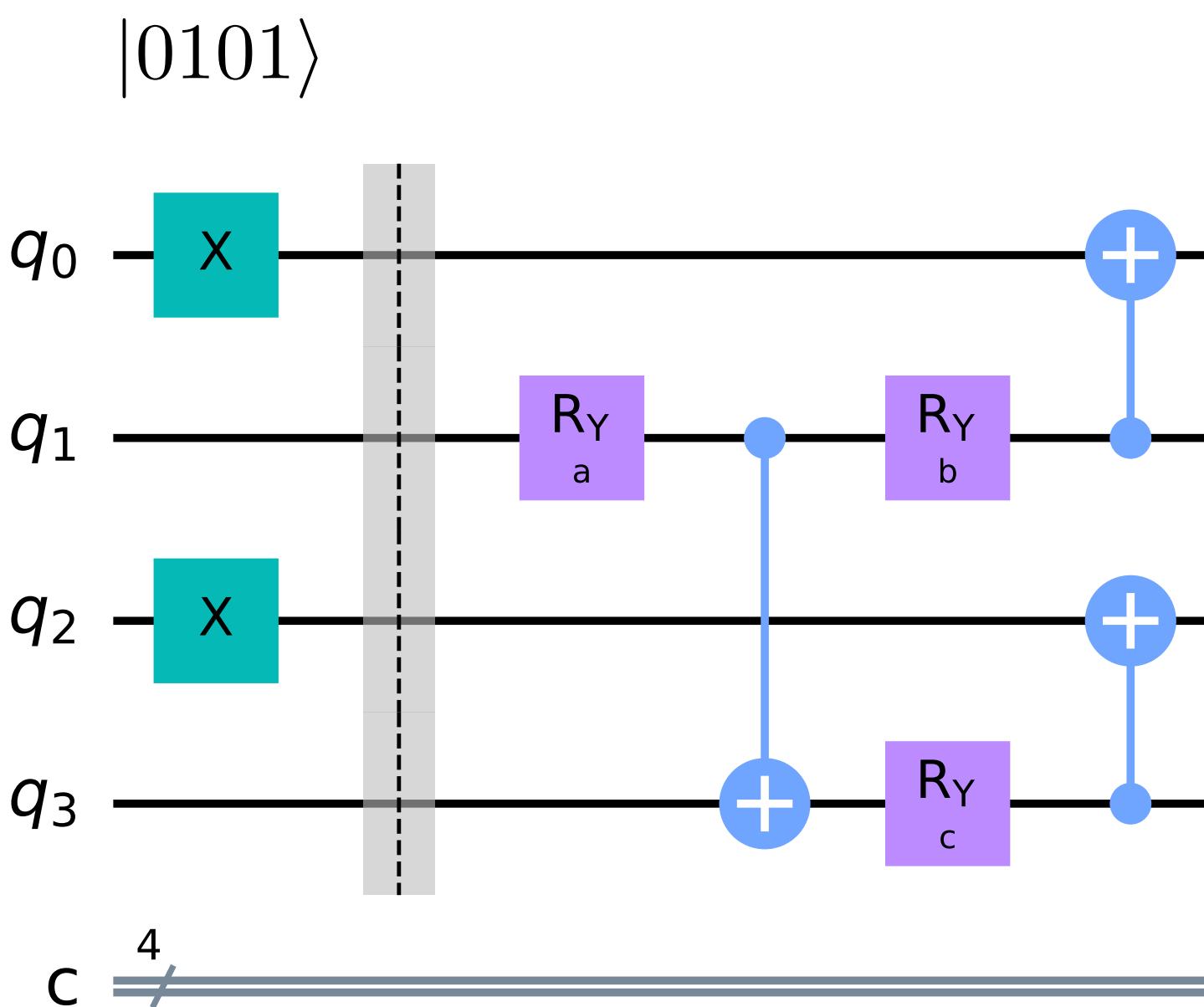
$$|\phi_i\rangle = |0101\rangle, |1001\rangle, |0110\rangle, |1010\rangle$$

$\theta \rightarrow 2 \times 4 - 2 = 6$ parameters

Preparation of a state

For the H₂ molecule

This circuit, can span the **2 electrons** (1 spin up, 1 spin down) state space with real coefficients.



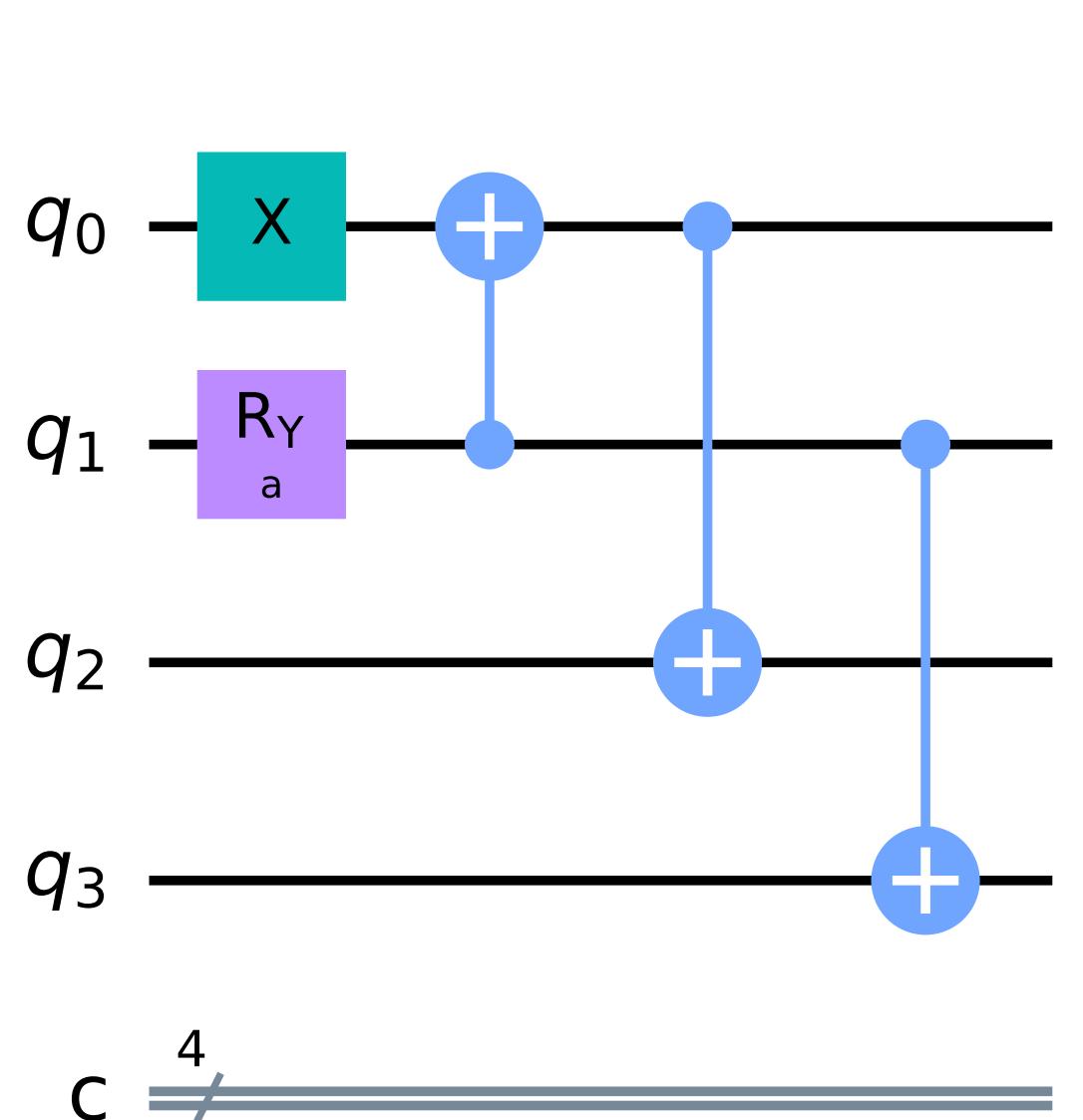
$$|\phi_i\rangle = \begin{cases} |0101\rangle \\ |1001\rangle \\ |0110\rangle \\ |1010\rangle \end{cases}$$

$$|u_\downarrow, g_\downarrow, u_\uparrow, g_\uparrow\rangle$$

Preparation of a state

For the H₂ molecule

We can span a **symmetric sub-space** with only 1 parameter!



$|u_\downarrow, g_\downarrow, u_\uparrow, g_\uparrow\rangle$

$$|\phi_i\rangle = \begin{cases} |0101\rangle \\ |1010\rangle \end{cases}$$

Evaluation of the energy or other things

Expectation value estimation

1 qubit

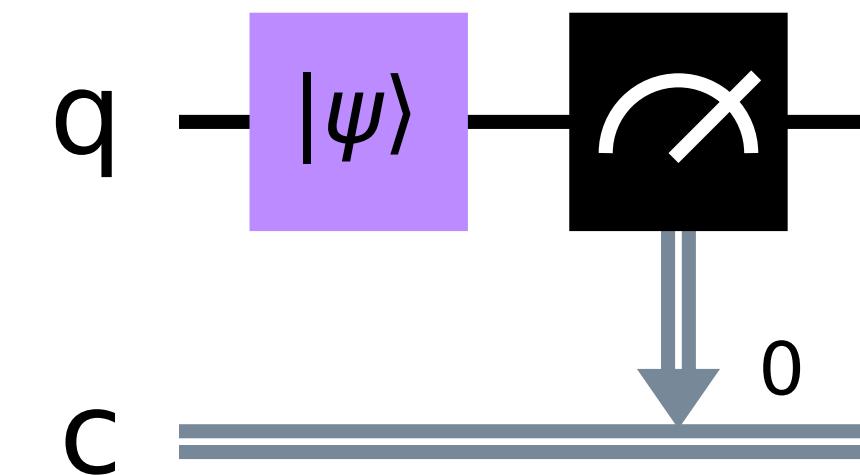
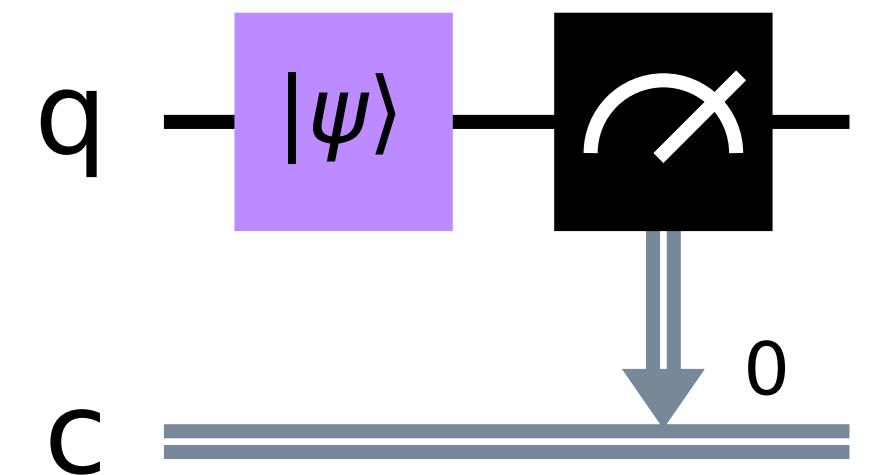
To obtain the **expectation value** of the Hamiltonian we need to compute the expectation values of several **Pauli strings**.

$$E(\theta) = \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle = \sum_i h_i \langle \psi(\theta) | \hat{\mathcal{P}}_i | \psi(\theta) \rangle$$

Expectation value estimation

1 qubit - diagonal observables

Let's start slowly with a **1 qubit** state. We can **estimate the expectation value** of a **diagonal observable** (in the computational basis) by simply **measuring the qubit many times**.



$$\langle \psi | \hat{Z} | \psi \rangle = \langle \psi | 0 \rangle \langle 0 | \psi \rangle - \langle \psi | 1 \rangle \langle 1 | \psi \rangle \approx \frac{N_0 - N_1}{N}$$

$$\langle \psi | \hat{I} | \psi \rangle = \langle \psi | 0 \rangle \langle 0 | \psi \rangle + \langle \psi | 1 \rangle \langle 1 | \psi \rangle \approx \frac{N_0 + N_1}{N} = 1$$

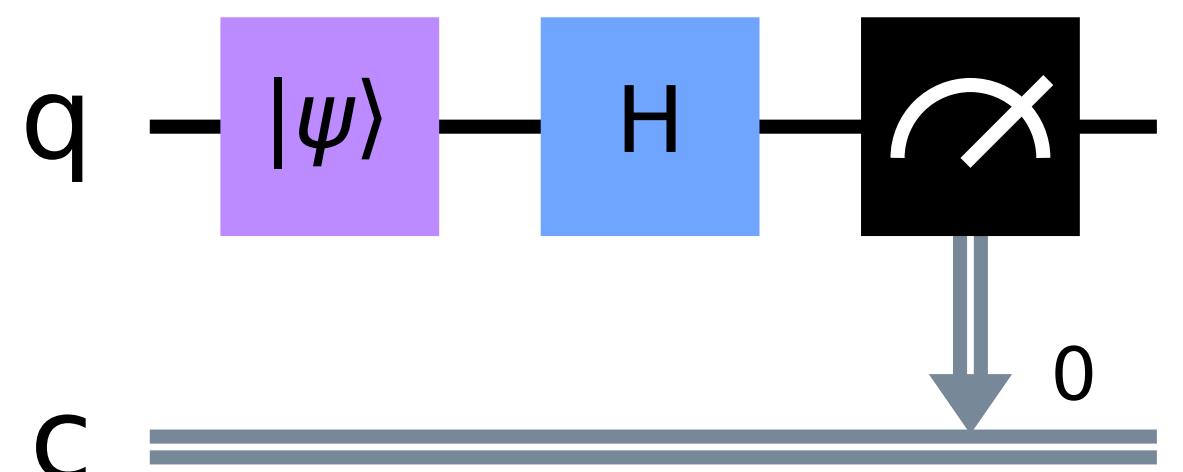
Expectation value estimation

1 qubit - non-diagonal observables

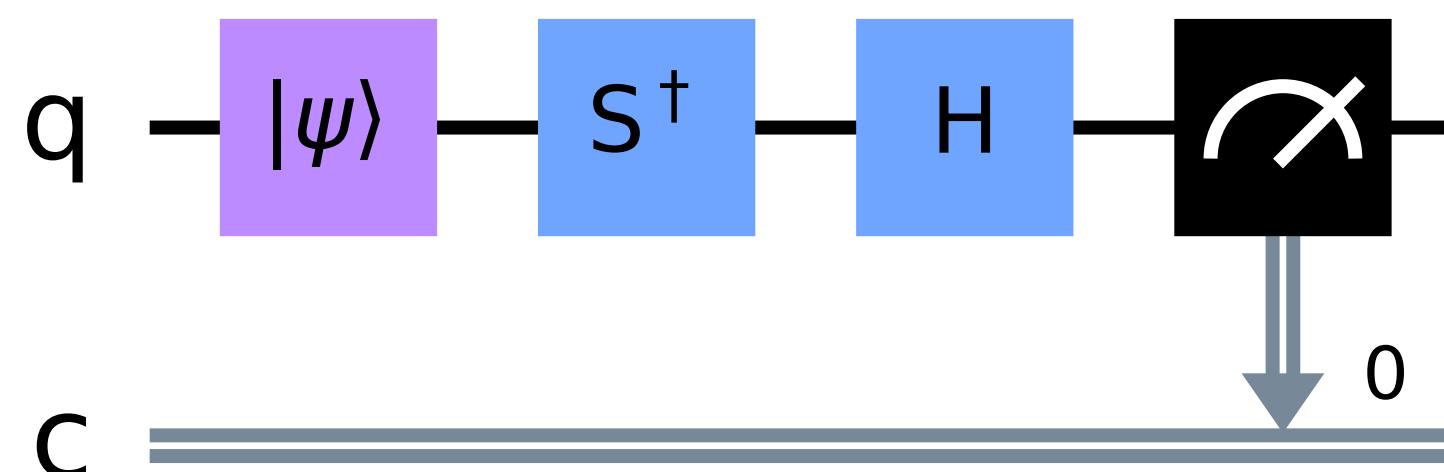
What about non-diagonal observables? We make them diagonal!

$$\begin{aligned}\langle \psi | \hat{X} | \psi \rangle &= \langle \psi | \hat{H} \hat{Z} \hat{H} | \psi \rangle \\ &= \langle \psi^{(x)} | \hat{Z} | \psi^{(x)} \rangle\end{aligned}$$

$$\begin{aligned}\langle \psi | \hat{Y} | \psi \rangle &= \langle \psi | \hat{S} \hat{H} \hat{Z} \hat{H} \hat{S}^\dagger | \psi \rangle \\ &= \langle \psi^{(y)} | \hat{Z} | \psi^{(y)} \rangle\end{aligned}$$



$$\frac{N_0 - N_1}{N_{\text{tot}}}$$



$$\frac{N_0 - N_1}{N_{\text{tot}}}$$

Expectation value estimation

many qubits - diagonal observables

The **expectation value of diagonal observable on basis state is the eigenvalue.**

Example 1 :

$$\begin{aligned} \langle 0111 | \hat{Z} \hat{I} \hat{Z} \hat{Z} | 0111 \rangle &= \langle 0 | \hat{Z} | 0 \rangle \langle 1 | \hat{I} | 1 \rangle \langle 1 | \hat{Z} | 1 \rangle \langle 1 | \hat{Z} | 1 \rangle \\ &= 1 \times 1 \times -1 \times -1 = 1 \end{aligned}$$

Example 2 :

$$\begin{aligned} \langle 1011 | \hat{Z} \hat{I} \hat{Z} \hat{Z} | 1011 \rangle &= \langle 1 | \hat{Z} | 1 \rangle \langle 0 | \hat{I} | 0 \rangle \langle 1 | \hat{Z} | 1 \rangle \langle 1 | \hat{Z} | 1 \rangle \\ &= -1 \times 1 \times -1 \times -1 = -1 \end{aligned}$$

In general :

$$\langle q | \hat{Z} | q \rangle = (-1)^{\text{number of matching 1 and } \hat{Z}}$$

Expectation value estimation many qubits - diagonal observables

The **expectation value of diagonal observable on a general state**

$$|\psi\rangle = \sum_{q=0}^{2^n} \alpha_q |q\rangle$$

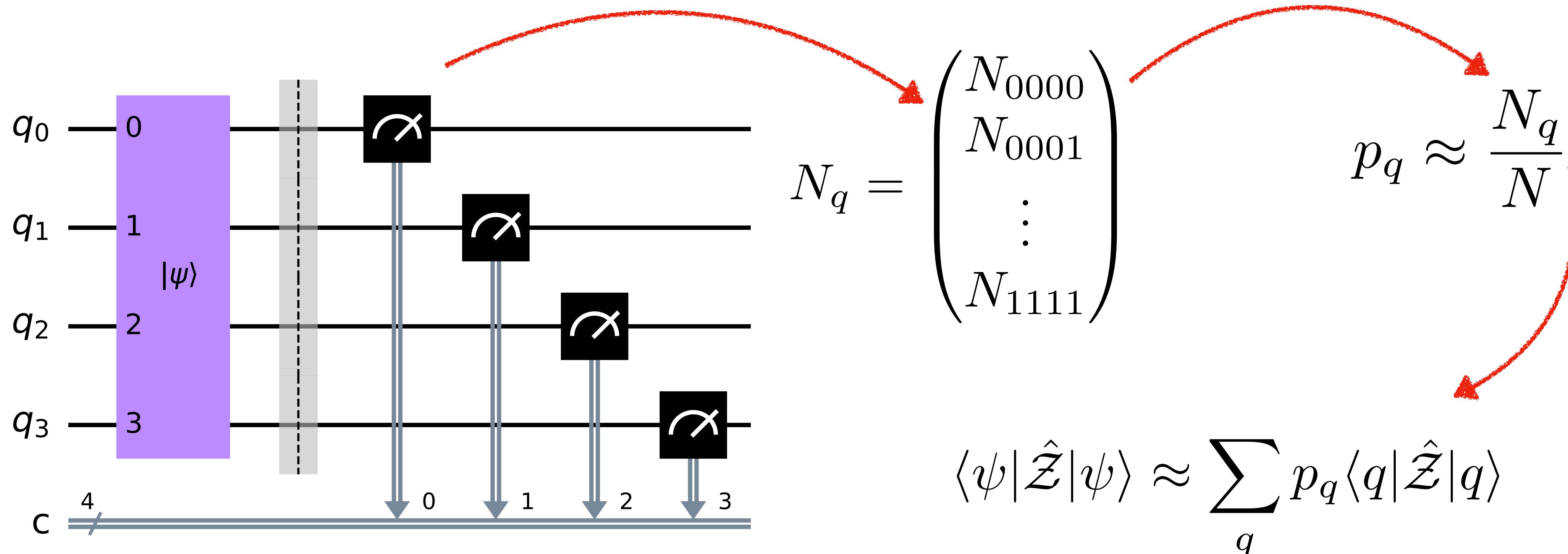
is a weighted average of the **eigenvalues** of the **basis states**.

$$\langle\psi|\hat{\mathcal{Z}}|\psi\rangle = \sum_{q=0}^{2^n-1} p_q \langle q|\hat{\mathcal{Z}}|q\rangle \quad p_q = |\alpha_q|^2$$

Expectation value estimation

many qubits - diagonal observables

We can **estimate** the **expectation value** of all the n qubits **diagonal observables** by simply measuring the qubits **many times**.



Expectation value estimation

many qubits - non-diagonal observables

For **non-diagonal** observables, simply **diagonalize** them first.

Example :

$$\begin{aligned}
 \langle \psi | \hat{Z}_3 \hat{I}_2 \hat{X}_1 \hat{Y}_0 | \psi \rangle &= \langle \psi | \hat{Z}_3 \hat{I}_2 (\hat{H}_1 \hat{Z}_1 \hat{H}_1) (\hat{S}_0 \hat{H}_0 \hat{Z}_0 \hat{H}_0 \hat{S}_0^\dagger) | \psi \rangle \\
 &= \langle \psi | (\hat{S}_0 \hat{H}_0 \hat{H}_1) \hat{Z}_3 \hat{I}_2 \hat{Z}_1 \hat{Z}_0 (\hat{H}_1 \hat{H}_0 \hat{S}_0^\dagger) | \psi \rangle \\
 &= \langle \psi' | \hat{Z}_3 \hat{I}_2 \hat{Z}_1 \hat{Z}_0 | \psi' \rangle
 \end{aligned}$$

$\hat{X} = \hat{H} \hat{Z} \hat{H}$
 $\hat{Y} = \hat{S} \hat{H} \hat{Z} \hat{H} \hat{S}^\dagger$

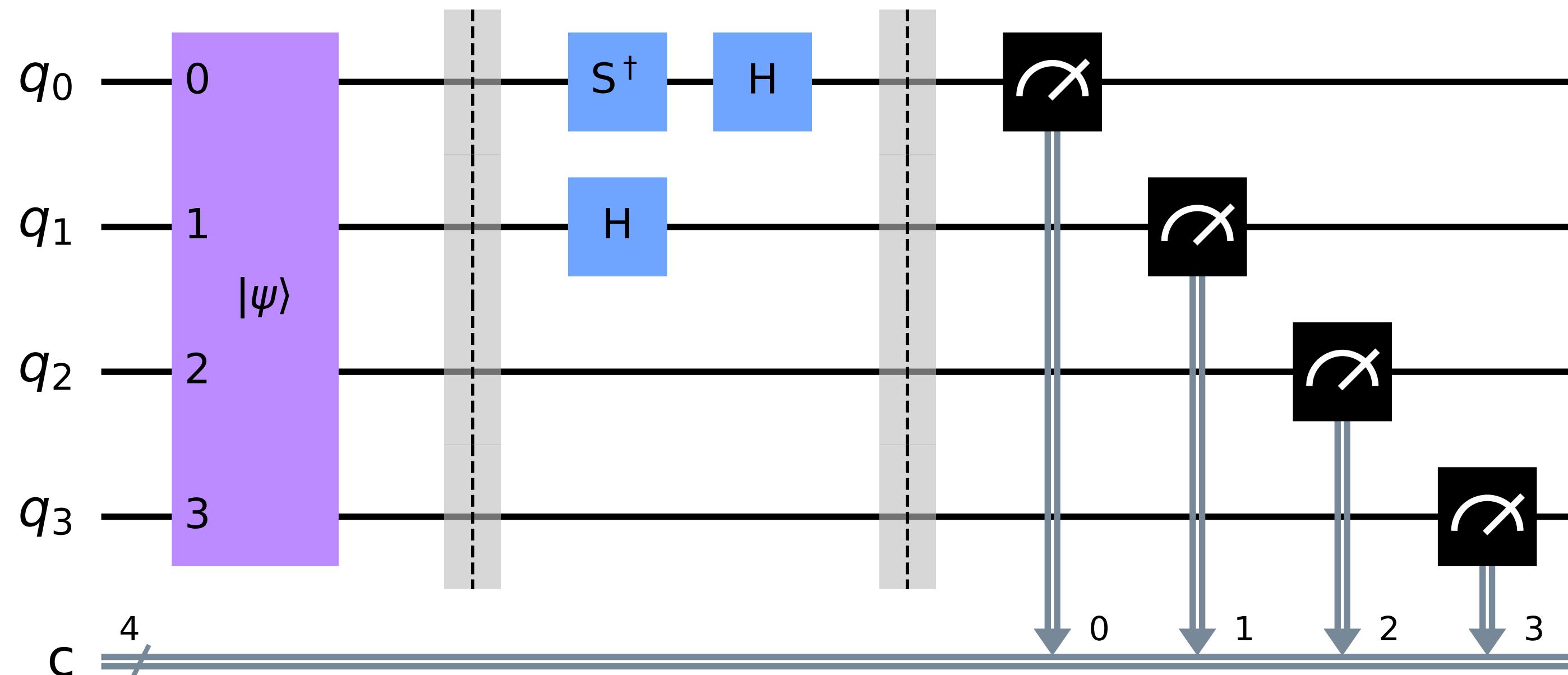
$$|\psi'\rangle = \hat{H}_1 \hat{H}_0 \hat{S}_0^\dagger |\psi\rangle$$

Expectation value estimation

many qubits - non-diagonal observables

Once it's diagonal, it is business as usual.

$$\langle \psi | \hat{Z}_3 \hat{I}_2 \hat{X}_1 \hat{Y}_0 | \psi \rangle = \langle \psi' | \hat{Z}_3 \hat{I}_2 \hat{Z}_1 \hat{Z}_0 | \psi' \rangle \quad | \psi' \rangle = \hat{H}_1 \hat{H}_0 \hat{S}_0^\dagger | \psi \rangle$$



Summary of the Estimation

Expectation value estimation

From the top

Given an **Hamiltonian** written as a linear combination of **Pauli strings**

$$\hat{H} = \sum_i h_i \hat{\mathcal{P}}_i$$

and for some **quantum state** prepared by a parametrized quantum circuit

$$|\psi\rangle = |\psi(\theta)\rangle$$

we want to **estimate the energy** as the **expectation value** of the Hamiltonian for the state

$$E(\theta) = \langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle = \sum_i h_i \langle\psi(\theta)|\hat{\mathcal{P}}_i|\psi(\theta)\rangle$$

Expectation value estimation for each Pauli string i

1. Rotate the qubits to be measured in X or Y. Transform the Pauli string into a diagonal Pauli string.

$$|\psi'_i\rangle = \hat{U}_i |\psi\rangle \quad \langle\psi|\hat{\mathcal{P}}_i|\psi\rangle = \langle\psi'_i|\hat{\mathcal{Z}}_i|\psi'_i\rangle$$

2. Measure the modified state many times to get the counts from which estimate the probabilities. Only for the basis states in the results, compute the eigenvalue.

$$N_q^{(i)} \rightarrow p_q^{(i)} \quad \langle q|\hat{\mathcal{Z}}_i|q\rangle$$

3. Get the expected value as the weighted average of the eigenvalues.

$$\langle\psi|\hat{\mathcal{P}}_i|\psi\rangle = \langle\psi^{(i)}|\hat{\mathcal{Z}}_i|\psi^{(i)}\rangle \approx \sum_q p_q^{(i)} \langle q|\hat{\mathcal{Z}}_i|q\rangle$$

Side note

Evaluation of other things

The same procedure can be used for other observables, such as the number of particles

$$\hat{n} = \sum_i \hat{a}_i^\dagger \hat{a}_i$$

First, translate the observable into a Linear Combinaison of Pauli Strings.

$$\hat{n} = \sum_j c_j \hat{\mathcal{P}}_j$$

Estimate the expected value of those Pauli strings and then sum it up.

$$\langle \psi | \hat{n} | \psi \rangle = \sum_j c_j \langle \psi | \hat{\mathcal{P}}_j | \psi \rangle$$

Variational Quantum Eigensolver

Variational Quantum Eigensolver

Summary

Using the **Linear Combinaison of Pauli Strings** representation of the Hamiltonian and the **measurements in different basis** we can estimate the expected value of the energy of a **parametrized quantum state**.

$$E(\theta) = \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle = \sum_i h_i \langle \psi(\theta) | \hat{\mathcal{P}}_i | \psi(\theta) \rangle$$

The **VQE** algorithm boils down to find the **minimum** to this **energy function**.

$$E_0 = \min_{\theta} E(\theta) \quad E_0 \sim E_g$$

Do not forget to add the Coulomb repulsion energy of the nucleus that we didn't include in the Hamiltonian.

Just code it!

Questions?