# Method 1

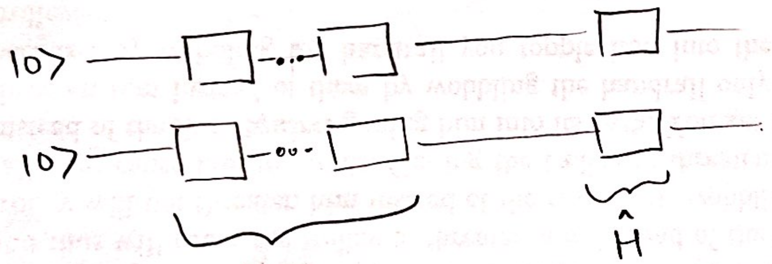
Let $H$ be the Hamiltonian, $\{E_i\}$ be the energy eigenstates and $\lambda_i$ be the corresponding eigenvalues

Suppose our VQE circuit prepares the state $|\psi\rangle$. Since $\{E_i\}$ form a complete orthonormal basis, we can write $|\psi\rangle$ as

$$|\psi\rangle = \langle E_1|\psi\rangle |E_1\rangle + \langle E_2|\psi\rangle|E_2\rangle + \ldots\ldots$$

$$|\psi\rangle = P_1|E_1\rangle + P_2|E_2\rangle + \ldots \quad P_i|E_i\rangle + \ldots \qquad ①$$

Now, let's act $H$ on our VQE circuit




$$U|00\rangle = |\psi\rangle$$

Then

$$\hat{H}|\psi\rangle = P_1 \hat{H}|E_1\rangle + P_2\hat{H}|E_2\rangle + \ldots\ldots + P_i\hat{H}|E_i\rangle + \ldots$$

$$= P_1\lambda_1|E_1\rangle + P_2\lambda_2|E_2\rangle + \ldots\ldots + P_i\lambda_i|E_i\rangle + \ldots$$

Now finding the expectation value

$$\langle\psi|\hat{H}|\psi\rangle = P_1\lambda_1\langle\psi|E_1\rangle + P_2\lambda_2\langle\psi|E_2\rangle + \ldots\ldots + P_i\lambda_i\langle\psi|E_i\rangle$$

But $\langle\psi|E_i\rangle = \langle E_i|\psi\rangle^* = P_i^*$

So,

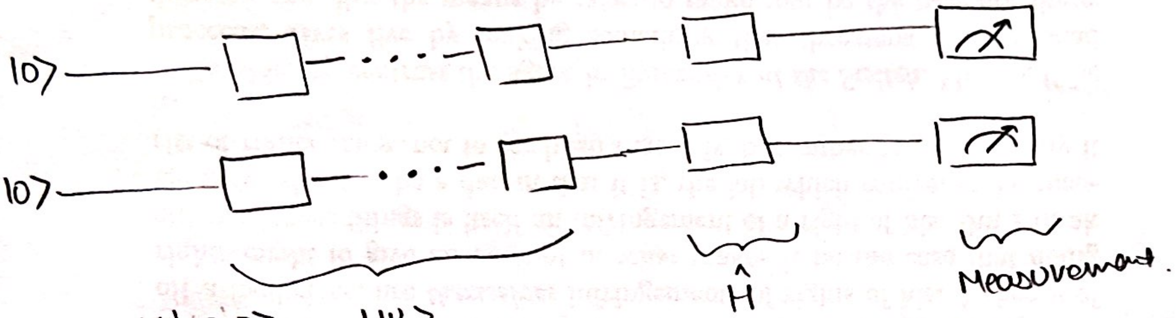
$$\langle\psi|\hat{H}|\psi\rangle = \lambda_1 P_1P_1^* + \lambda_2 P_2P_2^* + \ldots + \lambda_i P_iP_i^* + \ldots$$

$$= \lambda_1 P_1^2 + \lambda_2 P_2^2 + \ldots + \lambda_i P_i^2 + \ldots \qquad ②$$

where

$p_i^2$ = Probability with which we measure $\hat{H}|\psi\rangle$ as $|E_i\rangle$

These $p_i^2$'s are obtained by adding the measurement gates and obtaing counts correspondiy to $\{E_i\}$ states.




$U|0\,0\rangle = |\psi\rangle$

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<u>Method 2</u>

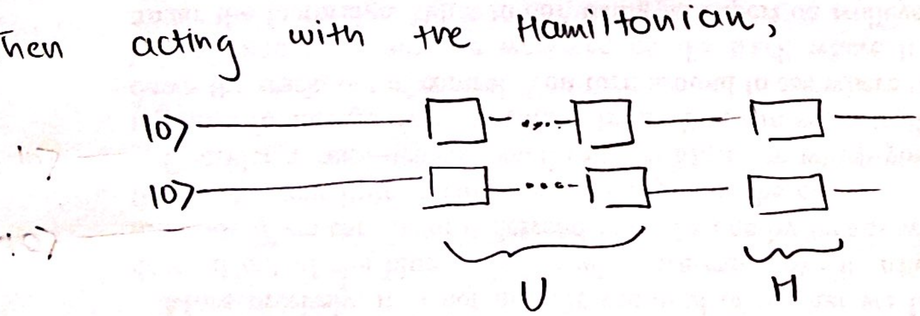
Suppose $\hat{U}|0\rangle = |\psi\rangle$

Then, expansion in energy eigen basis

$$|\psi\rangle = \hat{U}|00\rangle = \langle E_1|\hat{U}|00\rangle |E_1\rangle + \dots + \langle E_i|\hat{U}|00\rangle |E_i\rangle$$

$$= q_1|E_1\rangle + q_2|E_2\rangle + \dots + q_i|E_i\rangle$$

Then acting with the Hamiltonian,




$$\hat{H}(\hat{U}|00\rangle) = q_1\langle \hat{H}|E_1\rangle + q_2\langle \hat{H}|E_2\rangle + \dots + q_i \hat{H}|E_i\rangle$$

$$= q_1\lambda_1|E_1\rangle + q_2\lambda_2|E_2\rangle + \dots + q_i\lambda_i|E_i\rangle$$

Now we act with $U^+$ and measure probability of obtaining $|00\rangle$. That is,

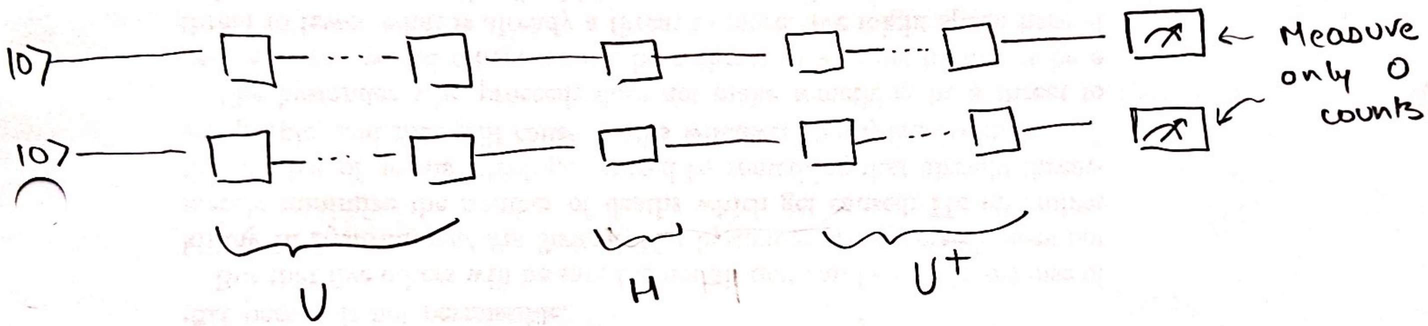
$$\langle 00| U^+ H U |00\rangle = q_1 \lambda_1 \langle 00|U^+|E_1\rangle + \dots + q_i \lambda_i \langle 00|U^+|E_i\rangle$$

Now $\langle 00|U^+|E_i\rangle = \langle E_i|U|00\rangle^* = q_i^*$

So,

$$\langle 00|U^+ HU|00\rangle = \lambda_1 q_1 q_1^* + \lambda_2 q_2 q_2^* + \dots \lambda_i q_i q_i^*$$

$$= \lambda_1 q_1^2 + \lambda_2 q_2^2 + \dots \lambda_i q_i^2 + \dots \quad (3)$$




Note that $\langle E_i|\psi\rangle = \langle E_i|U|00\rangle$

$\Rightarrow P_i = q_i$

So in (2) and (3) then,

$$\langle \psi|\hat{H}|\psi\rangle = \langle 00|U^+ HU|00\rangle$$

But there are 2 differences

1. Measurement

In method ①, we have to compute $P_i^2$ i.e. measuring counts of every eigenstate $|E_i\rangle$.

In method ②, however, we just have to only consider counts corresponding to $|00\rangle$ state.

2. Gates

Method ① involves less gate-usage than method ② because method ① doesn't have to implement $U^\dagger$