

Another creative way of using time-evolution to prepare the ground-state of a physical system is the "Quantum Imaginary Time Evolution" (QITE)

This algorithm is inspired by classical methods which uses the fact that

$$\lim_{\tau \rightarrow \infty} e^{-(H-E_0)\tau} |x\rangle = \lim_{\tau \rightarrow \infty} \sum_{\alpha} e^{-(E_\alpha - E_0)\tau} |\psi_\alpha| x \rangle |\psi_\alpha\rangle \\ = |\psi_0| x \rangle |\psi_0\rangle$$

$$\text{where } H|\psi_0\rangle = E_0|\psi_0\rangle. \text{ and } \langle x|\psi_0\rangle \neq 0$$

meaning that if one starts for some arbitrary state $|x\rangle$ with non zero overlap with true $|\psi_0\rangle$ and let it evolve in imaginary time, after some time (again defined by the gap of the sysl ham), the sysl gets purified into its ground state $|\psi_0\rangle$. (because components of $|x\rangle$ along excited states are expo suppressed).

Typically not necessary to know E_0 , but upper bound E_T ($E_T - E_0 \leq \epsilon$) is enough. ($E_0 \leq E_T \leq E_1$)

Now to do that on a QC, the issue is that

$e^{-(H-E_0)G}$ is not unitary

so similarly to LCU one has to work in an extended Hilbert space and find unitary operators that act as $e^{-(H-E_0)G}$ on the (sub) system of interest.

Define $\hat{Q}(z)$ nn unitary acting on $|k\rangle\langle k|$:

$$\begin{aligned}\hat{Q}(z) &= A(z) e^{-(H-E_0)G} \\ &= \frac{e^{-(H-E_0)G}}{\sqrt{1 + e^{-2(H-E_0)G}}} \\ &\xrightarrow[G \rightarrow \infty]{} e^{-(H-E_0)G}\end{aligned}$$

Now embed it into a unitary acting on a larger system ($|\text{lancilla}\rangle\langle x|$):

↓
1 qubit

$$\begin{aligned}\hat{U}(z) &= \begin{pmatrix} \hat{Q}(z) & \hat{A}(z) \\ \hat{A}(z) & -\hat{Q}(z) \end{pmatrix} \\ &= \hat{Z} \otimes \hat{Q}(z) + \hat{X} \otimes \hat{A}(z)\end{aligned}$$

it is easy to see that $U(B)$ is unitary:

$$\begin{aligned}
 U^+ U &= (Z \otimes Q + X \otimes A)^+ (Z \otimes Q + X \otimes A) \\
 &= (Z \otimes Q^+ + X \otimes A^+) (Z \otimes Q + X \otimes A) \\
 &= \underbrace{Z^2}_{\text{I}} \otimes Q^+ Q + \underbrace{ZX}_{-iY} \otimes Q^+ A \\
 &\quad + \underbrace{XZ}_{-iY} \otimes A^+ Q + \underbrace{X^2}_{\text{I}} \otimes A^+ A
 \end{aligned}$$

$$\begin{aligned}
 Q^+ Q &= \left[A e^{-i(H-E_0)G} \right]^+ A e^{-i(H-E_0)G} \\
 &= e^{-i(H-E_0)G} \underbrace{A^+ A}_{A^2} e^{-i(H-E_0)G} \quad (\text{A Hermitian}) \\
 &= e^{-2(H-E_0)G} A^2 \quad ([A, Q] = 0)
 \end{aligned}$$

$$\Rightarrow \text{Term } iY \otimes (Q^+ Q + A^+ A) = iY \otimes \underbrace{\left(e^{-2(H-E_0)G} + I \right)}_{A^2} A^2 = 0$$

$$\text{and term } iY \otimes [\underbrace{Q^+ A - A^+ Q}_{A^+ Q^+}] = 0 . \quad \checkmark$$

Now

$$U(3) |10\rangle \otimes |x\rangle$$

$$= |10\rangle \otimes Q(3)|x\rangle + |11\rangle \otimes A(3)|x\rangle$$

measure ancilla and keep only
states which have collapsed to $|10\rangle$
 \Rightarrow the state for the global syst has
collapsed to

$$\propto |10\rangle \otimes Q(3)|x\rangle$$

\hookrightarrow normalization.

\Rightarrow one has now generated a time
evolved state, which, for long \mathcal{T} ,
converges towards the ground state.

(The non-unitary nature of the evolution
has been implemented by the non-unitary
nature of the measurements)

But again proba of success is related
to fraction of events where ancilla
collapses to $|10\rangle$, which itself depends
on spectrum of physical system.

* Initializing syst $|x\rangle$ to something close to
 $|4_0\rangle$ will provide better approx to $|4_0\rangle$

and reduce circuit size.

* it can also be helpful to Trotterize -

At each Trotter step we measure and get a state a bit closer to the true gs.

Summary:

If one can prepare a state with large overlap with exact eigenstate \rightarrow QPE, QITE can provide energy eigenvalues and Hami' eigenstates with great accuracy -

However, even though the scaling of the circuit size is $\text{poly}(n)$,

the circuit depths are still too long to obtain meaningful results with current (noisy) quantum computers

(because the run times are too long and decoherence occurs before the end of the calculation.)

Such algorithms will be useful when new-generation quantum computers (less noisy, "fault tolerant") will be available.

In order to take advantage of current quantum computers, other kinds of algo have been developed -

Such algorithms are typically "hybrid" classical-quantum algo , in the sense that part of the computation is done on the QC , while another part is done classically .

This allows for reductions of quantum circuits and for meaningful results even with noisy quantum computers .

One of the most popular / advanced hybrid algo for finding hamiltonian ground states is called

"Variational Quantum Eigensolver".

Peruzzo et al. , Nature Comm. 5 , 4213 (2014)

This algo is based on minimization of the energy (variational principle) and has a wider scope of application (in principle can be used to minimize any cost function) .

The algorithm works in the following way :

① Start from the Hamiltonian of the system of interest, and map it to a qubit Hamiltonian:

$$H_{\text{sys}} \rightarrow H_{\text{qubit}} \text{ expressed in terms of } x, y, z, t -$$

Example : Hamiltonian responsible for the hyperfine structure of the Hydrogen

$$H_{\text{Hydrogen}} = \alpha \vec{\sigma} \cdot \vec{\sigma} \quad (\text{when the proton and } e^- \text{ only have spin degrees of freedom})$$

$$\rightarrow H_{\text{qubit}} = \alpha(xx + yy + zz) \equiv H.$$

(Note:

so far we have considered Hamiltonians for systems of spins $\frac{1}{2}$, so the mapping to qubits is trivial - Next, we will see how this can be done for more general systems.)

② Choose an ansatz for the ground-state that you know how to prepare with a quantum circuit.

The idea is to parametrize the state by a set of angles : $|4\rangle \equiv |4(\vec{\theta})\rangle$
 $\vec{\theta} = (\theta_0, \theta_1, \dots)$
 and the VQE algorithm will determine the angles that minimize the energy

$$E(\vec{\theta}) = \langle 4(\vec{\theta}) | \hat{H} | 4(\vec{\theta}) \rangle$$

In principle, circuits can be built for arbitrary n -qubit states.

For example :

- 1-qubit states $|4\rangle$ can be parametrized by 2 complex numbers (ie 4 real numbers)
 This can be further reduced to 2 angles using normalization $|a|^2 + |b|^2 = 1$ and the fact that global phases can be dropped:

$$|4\rangle = \cos(\Theta/2) |0\rangle + e^{i\phi} \sin(\Theta/2) |1\rangle$$

Such state can be prepared from the state $|0\rangle$ by applying a general unitary $\in SU(2)$

$$U(\vec{n}, \theta) = e^{-i\frac{\theta}{2} \hat{\vec{n}} \cdot \vec{\sigma}}$$

or

$$U(\alpha, \beta, \gamma) = R_z(\gamma) R_y(\beta) R_z(\alpha)$$

(Euler decomposition)
(2 ≠ parametrizations).

In Qiskit:

$$U(\theta, \phi, \lambda) = \begin{pmatrix} \cos(\theta/2) & -e^{i\lambda} \sin(\theta/2) \\ e^{i\phi} \sin(\theta/2) & e^{i(\phi+\lambda)} \cos(\theta/2) \end{pmatrix}$$

so that

$$U(\theta, \phi, \lambda) |0\rangle = \cos(\theta/2) |0\rangle + e^{i\phi} \sin(\theta/2) |1\rangle$$

- 2-qubit states

$$|14\rangle = \alpha_{00} |00\rangle + \alpha_{01} |01\rangle + \alpha_{10} |10\rangle + \alpha_{11} |11\rangle$$

can be prepared by applying SU(4) transformations -

SU(4) has $4^2 - 1 = 15$ generators, so in general $U \in \text{SU}(4)$ requires 15 angles -

It has been shown that such unitary can be decomposed as:

$$\hat{U}_{\text{SU}(4)} = \hat{K}_1' \hat{K}_2' \hat{C} \hat{K}_1 \hat{K}_2$$

where the K_j' , K_j' are SU(2) (1-qubit) unitaries (each requires 3 angles)

while

$$\hat{C} = e^{-\frac{i}{2}(\Theta_7 XX + \Theta_8 YY + \Theta_9 ZZ)}$$

(ref: Khaneja, Glaser aux: 0010100
(2000))

Remember that XX , YY and ZZ commute -

$$\Rightarrow \hat{C} = e^{-\frac{i}{2}\Theta_7 XX} e^{-\frac{i}{2}\Theta_8 YY} e^{-\frac{i}{2}\Theta_9 ZZ}$$

\uparrow
exact.

\Rightarrow we know how to implement $\hat{U}_{\text{SU}(4)}$.

using 1 qubit gates and, for ex,

staircase algo for the 2 qubit gates $e^{-\frac{i}{2}\Theta_7 XX, YY, ZZ}$.

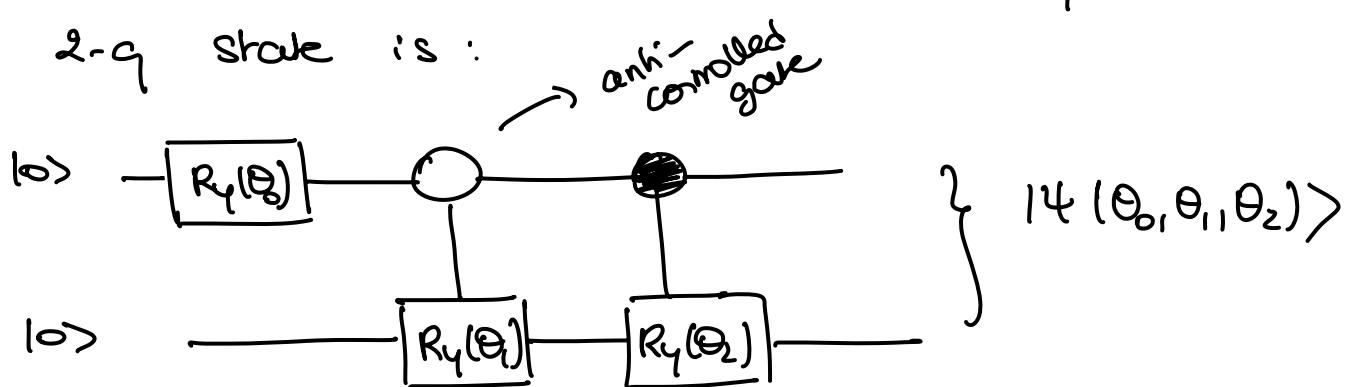
- This can be generalized to $n > 2$ qubits but the circuit size scales expo(n).

Typically the Hamiltonian will have certain symmetries, which reduces the number of angles parametrizing the state.

For ex, the Hami in quantum chem, nuclear phys ... are often invariant under CP / time-reversal which means that the eigenstates can be chosen to be real in that case

- 1-qubit states require 1 angle
- 2-qubit states require 3 angles

A circuit to initialize an arbitrary real 2-q state is:



$$\text{where } \hat{R}_y(\theta_j) = \exp\left(-i \frac{\theta_j}{2} \hat{Y}\right)$$

it is easy to check that :

$$|14\rangle = \cos\left(\frac{\theta_0}{2}\right) \cos\left(\frac{\theta_1}{2}\right) |00\rangle + \cos\left(\frac{\theta_0}{2}\right) \sin\left(\frac{\theta_1}{2}\right) |10\rangle \\ + \sin\left(\frac{\theta_0}{2}\right) \cos\left(\frac{\theta_2}{2}\right) |01\rangle + \sin\left(\frac{\theta_0}{2}\right) \sin\left(\frac{\theta_2}{2}\right) |11\rangle$$

In our example [2-qubit Hydrogen atom]
the ground state can be chosen to be
real, and we will choose such above
formulation.

(# of angles goes
is $\exp(n)$)

For systems with large #'s of qubits
it is not practical to consider exact forms
of the state, and approximations have to be made.
Physical intuition often helps in finding
a form (ansatz) for the ground state
(or other Hami. eigenstate).
We will see some examples later.

- ③ Prepare the state for an initial
set of parameters $\vec{\Theta}_{in}$

4

Measure the energy on the quantum computer : $\langle 4(\vec{\theta}_n) | H | 4(\vec{\theta}_n) \rangle$

Since \hat{H} is a sum of strings (tensor products of Pauli operators) this is easy to do by using identities relating x, y to z . (since we can only measure along the z-axis in practice).

$$\text{Example} : H = \alpha(xx + yy + zz)$$

$$\Rightarrow \langle 4(\vec{\theta}) | \hat{H} | 4(\vec{\theta}) \rangle = \langle \hat{H} \rangle_{\vec{\theta}}$$

$$\begin{aligned} &= \alpha \left(\langle 4(\vec{\theta}) | xx | 4(\vec{\theta}) \rangle \right. \\ &\quad + \langle 4(\vec{\theta}) | yy | 4(\vec{\theta}) \rangle \\ &\quad \left. + \langle 4(\vec{\theta}) | zz | 4(\vec{\theta}) \rangle \right) \end{aligned}$$

Possibility #1 :

$$\langle zz \rangle_{\vec{\theta}} = \langle z_1 z_0 \rangle_{\vec{\theta}}$$

$$= |\langle 4(\vec{\theta}) | 00 \rangle|^2 + |\langle 4(\vec{\theta}) | 11 \rangle|^2$$

$$- |\langle 4(\vec{\theta}) | 01 \rangle|^2 - |\langle 4(\vec{\theta}) | 10 \rangle|^2$$

$$= p_4(00) + p_4(11) - p_4(01) - p_4(10)$$

$$\text{where we used } \vec{zz} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix} =$$

$$= |00\rangle\langle 00| + |11\rangle\langle 11| - |01\rangle\langle 01| - |10\rangle\langle 10|$$

since $X = HzH$, $\Psi = SH \vec{z} (SH)^+$

we can obtain

$$\begin{aligned}\langle XX \rangle_{\vec{\theta}} &\equiv \langle X_1 X_0 \rangle_{\vec{\theta}} \\ &= \langle (HzH)_1 (HzH)_0 \rangle_{\vec{\theta}} \\ &= \langle H_1 H_0 z_1 z_0 H_1 H_0 \rangle\end{aligned}$$

which be obtained by transforming

$$|\Psi(\vec{\theta})\rangle \mapsto H_1 H_0 |\Psi(\vec{\theta})\rangle \equiv |\Psi'(\vec{\theta})\rangle$$

and measuring $z_1 z_0$.

$$\Rightarrow \langle XX \rangle_{\vec{\theta}} = p_{\Psi'}(00) + p_{\Psi'}(11) - p_{\Psi'}(01) - p_{\Psi'}(10)$$

$\xrightarrow{\text{prob of outcome } |00\rangle}$
when measuring in state $|\Psi'(\vec{\theta})\rangle$

and the same can be done for

$$\langle YY \rangle_{\vec{\theta}} \text{ by transforming } |\Psi(\vec{\theta})\rangle \mapsto (SH)_1^+ (SH)_0^+ |\Psi(\vec{\theta})\rangle$$

While the procedure above works, it requires to build \neq circuits to measure $\langle XX \rangle$, $\langle YY \rangle$ and $\langle ZZ \rangle$.

Since XX , YY and ZZ commute, it is in fact possible to measure them simultaneously. This is what you showed in tutorial #8.

Indeed there is a $\xrightarrow{\text{common}} \text{transfo}$ U which brings XX , YY and ZZ to a diagonal form



$$\left\{ \begin{array}{l} U^\dagger XX U = I \otimes Z \\ U^\dagger YY U = -Z \otimes Z \\ U^\dagger ZZ U = Z \otimes I \end{array} \right.$$

$$\Rightarrow \langle 4(\vec{\theta}) | XX | 4(\vec{\theta}') \rangle$$

$$\begin{aligned} &= \langle 4(\vec{\theta}) | U (I \otimes Z) U^\dagger | 4(\vec{\theta}') \rangle \\ &= \langle \widetilde{4(\vec{\theta}')} | I \otimes Z | \widetilde{4(\vec{\theta}')} \rangle \end{aligned}$$

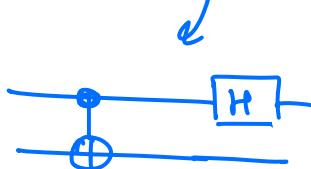
$$= \tilde{p_4}(00) - \tilde{p_4}(01) + \tilde{p_4}(10) - \tilde{p_4}(11)$$

since

$$\tau \otimes z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$= |00\rangle\langle 00| - |01\rangle\langle 01| + |10\rangle\langle 10| - |11\rangle\langle 11|$$

→ need to prepare $|4(\vec{\theta})\rangle = u + |4(\vec{\theta})\rangle$



Similarly for $\langle 44 \rangle_{\vec{\theta}}$ and $\langle 22 \rangle_{\vec{\theta}}$

(5) Optimize the parameters $\vec{\theta}$ on the classical comp.

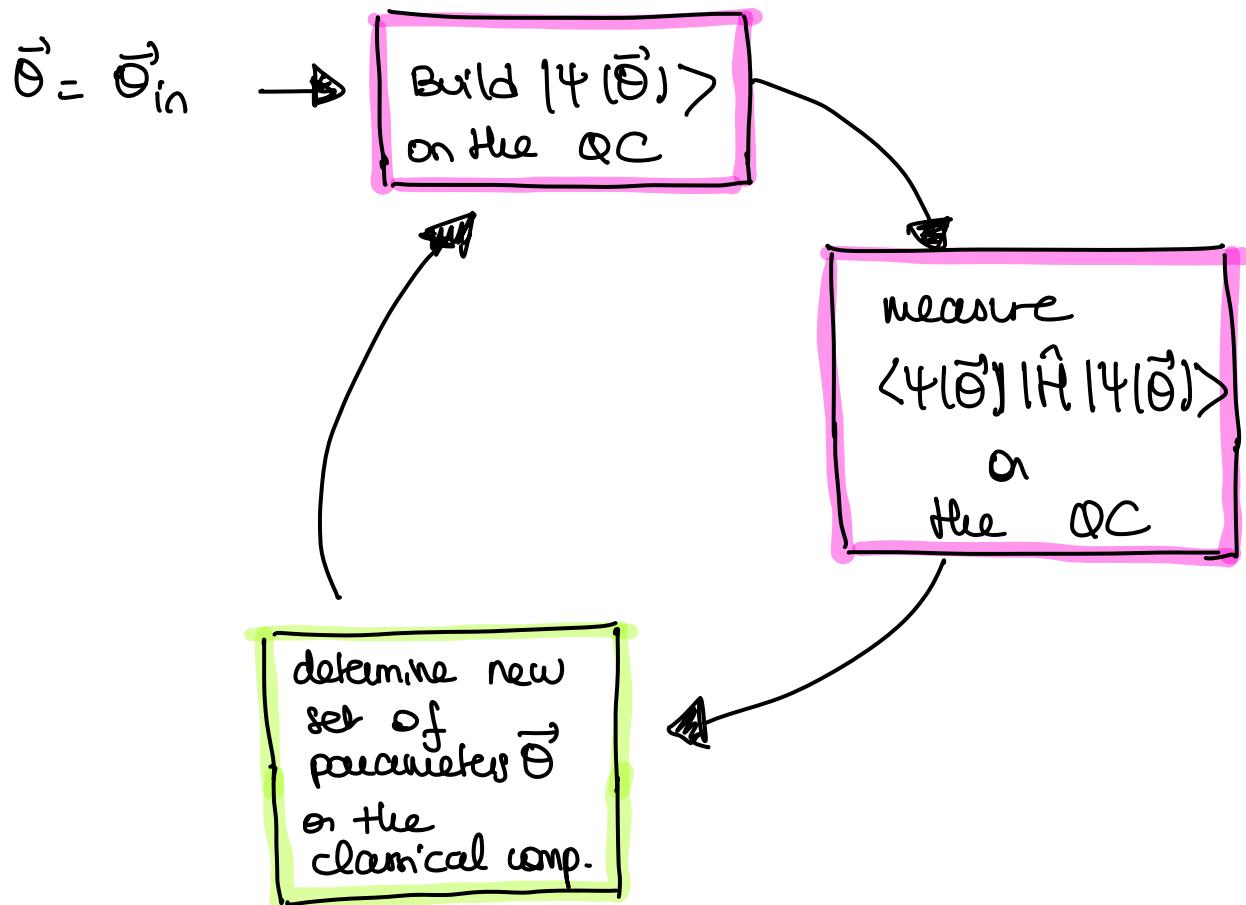
For instance use gradient descent

$$\Theta_k^{\text{new}} = \Theta_k^{\text{initial}} - \eta \frac{\partial E}{\partial \Theta_k} |_{\Theta_k^{\text{initial}}}$$

learning rate η

(6) Go back to step ③ with the new set of parameters and repeat until convergence.

In summary :



Note that there are several optimizers that one can use with Qiskit (for example can import package "minimize" from `scipy.optimize`)

in the hydrogen atom example
with the ansatz ($\vec{\theta} = (\theta_0, \theta_1, \theta_2)$)

$$|4(\vec{\theta})\rangle = \cos\left(\frac{\theta_0}{2}\right) \cos\left(\frac{\theta_1}{2}\right) |00\rangle + \cos\left(\frac{\theta_0}{2}\right) \sin\left(\frac{\theta_1}{2}\right) |10\rangle \\ + \sin\left(\frac{\theta_0}{2}\right) \cos\left(\frac{\theta_2}{2}\right) |01\rangle + \sin\left(\frac{\theta_0}{2}\right) \sin\left(\frac{\theta_2}{2}\right) |11\rangle$$

one converges to a ground-state energy

$$E(\vec{\theta}_{\text{opt}}) = -3\alpha$$

and ground-state which the "singlet"
spin state (Bell state) -