

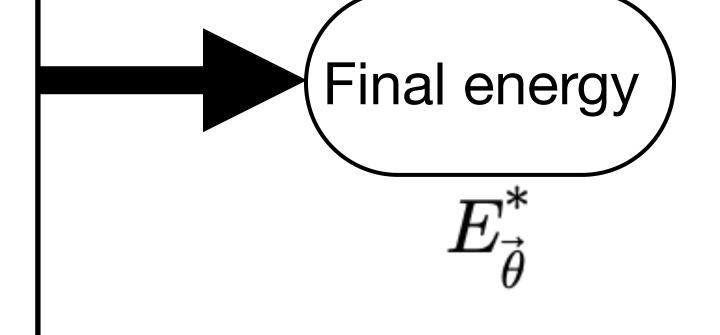
Quantum Processor Unit (QPU)

State preparation

$$|\psi_{\vec{\theta}}\rangle = U_{\vec{\theta}}|\psi_{\mathrm{HF}}\rangle$$

Energy evaluation

$$E_{\vec{\theta}} = \langle \psi_{\vec{\theta}} | H | \psi_{\vec{\theta}} \rangle$$



Classical parameters

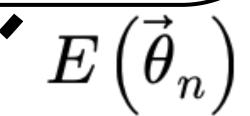
$$\vec{\theta}_{n+1}$$

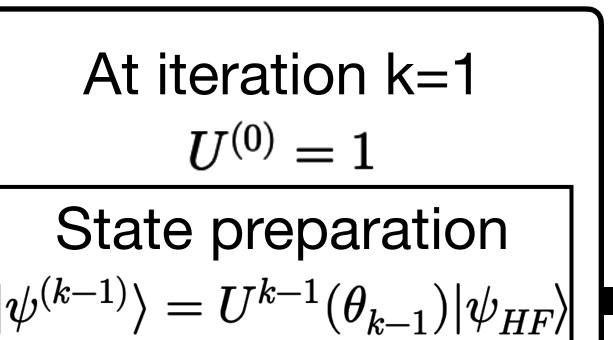
Classical Processor Unit

optimize.minimize

COBYLA, CG, BFGS,

Variational energy





START

Gradients measurement

$$\frac{\partial E^{(k-1)}}{\partial \vec{\theta}_m} = \langle \psi(\vec{\theta}_{k-1}) | [H,A_m] | \psi(\vec{\theta}_{k-1}) \rangle$$

Excitation pool operators

$$A_m = \{A_m(p,q), A_m(p,q,r,s)\}$$

 θ_{k-1} Is from previous **VQE** iteration

k - 1 = k

$$\left\| \|\vec{g}^{(k-1)}\| = \sqrt{\left(\frac{\partial E^{(k-1)}}{\partial \theta_1}\right)^2 + \dots + \left(\frac{\partial E^{(m)}}{\partial \theta_m}\right)^2} \leq \varepsilon \right\|$$

The convergence criterion

VQE: Re-optimize all parameters

$$E^{(k)} = \min_{ec{ heta}_k} \langle \psi_{ ext{HF}} | e^{- heta_1 A_1} ... e^{- heta_k A_k} H e^{ heta_k A_k} ... e^{ heta_1 A_1} | \psi_{ ext{HF}}
angle$$

Select operator with largest gradient

$$\vec{\theta}_m \to \vec{\theta}_k$$

 $ec{ heta}_m
ightarrow ec{ heta}_k$ **L** & expand the ansatz

$$|\psi^{(k)}
angle = e^{ heta_k A_k} |\psi^{(k-1)}
angle = e^{ heta_k A_k} \cdots e^{ heta_3 A_3} e^{ heta_2 A_2} e^{ heta_1 A_1} |\psi_{
m HF}
angle$$