

$$\left|\psi^{(0)}
ight.
ight. = \left|\psi^{
m HF}
ight.
ight.$$

n = n + 1

Measure Gradients

$$\frac{\partial E^{(n)}}{\partial \theta_1} = \left\langle \psi^{(n)} \middle| [\hat{H}, \hat{A}_1] \middle| \psi^{(n)} \right\rangle$$

$$\frac{\partial E^{(n)}}{\partial \theta_2} = \left\langle \psi^{(n)} \middle| [\hat{H}, \hat{A}_2] \middle| \psi^{(n)} \right\rangle$$



$$rac{\partial E^{(n)}}{\partial heta_N} = \left< \psi^{(n)} \middle| [\hat{H}, \hat{A}_N] \middle| \psi^{(n)} \right>$$

Done

Yes

Converged?

No

Select operator with largest gradient

VQE: Re-Optimize all parameters

$$E^{(n+1)} = \min_{\vec{\theta}^{(n+1)}} \left\langle \psi^{\mathrm{HF}} \middle| e^{-\theta_1 \hat{A}_1} \cdots e^{\theta_{n+1} \hat{A}_{n+1}} \hat{H} e^{\theta_{n+1} \hat{A}_{n+1}} \cdots e^{\theta_1 \hat{A}_1} \middle| \psi^{\mathrm{HF}} \right\rangle$$

$$\vec{\theta}_{\mathrm{guess}}^{(n+1)} = \{\vec{\theta}^{(n)}, 0\}$$

Grow Ansatz

$$\left|\psi_{\mathrm{guess}}^{(n+1)}\right\rangle = e^{0\hat{A}_{n+1}}\left|\psi^{(n)}\right\rangle$$

