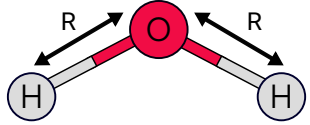

Expand Hamiltonian
in STO-6G basis set

$$\hat{H} = \sum_{ij}^{N_b} \langle i|\hat{T}_e + \hat{V}_{en}|j\rangle \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2}\sum_{ijkl}^{N_b} \langle ik|\hat{V}_{ee}|jl\rangle \hat{a}_i^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_j$$

$$\hat{a}_j \rightarrow \frac{\hat{\sigma}_x + i\hat{\sigma}_y}{2} \otimes \hat{\sigma}_z \otimes \cdots \otimes \hat{\sigma}_z$$

Qubit-mapping
Electronic Hamiltonian

$$\hat{H}_q = \sum_i c_i \prod_k^{Nb} \hat{\sigma}_k^{(i)}$$

$$|1\ 1\ 1\ 0\ 0\rangle = |\Phi_0\rangle$$

Qubit-mapping
Electronic States

$$C(\boldsymbol{\theta}) = \sum_i c_i \langle \Phi_0|\hat{U}^\dagger(\boldsymbol{\theta}) \prod_k^{N_b} \hat{\sigma}_k^{(i)} \hat{U}(\boldsymbol{\theta})|\Phi_0\rangle$$

VQA

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, C(\boldsymbol{\theta})$$

Layers of rotation
and entangling gates

$$U(\boldsymbol{\theta}) =$$