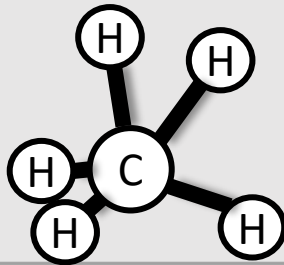


1) Molecular geometry

(xyz)



2) Hamiltonian representation

(second quantization)

$$\hat{H} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$



3) Fermion-qubit Transformation

(encoding fermionic operators to Pauli operators)

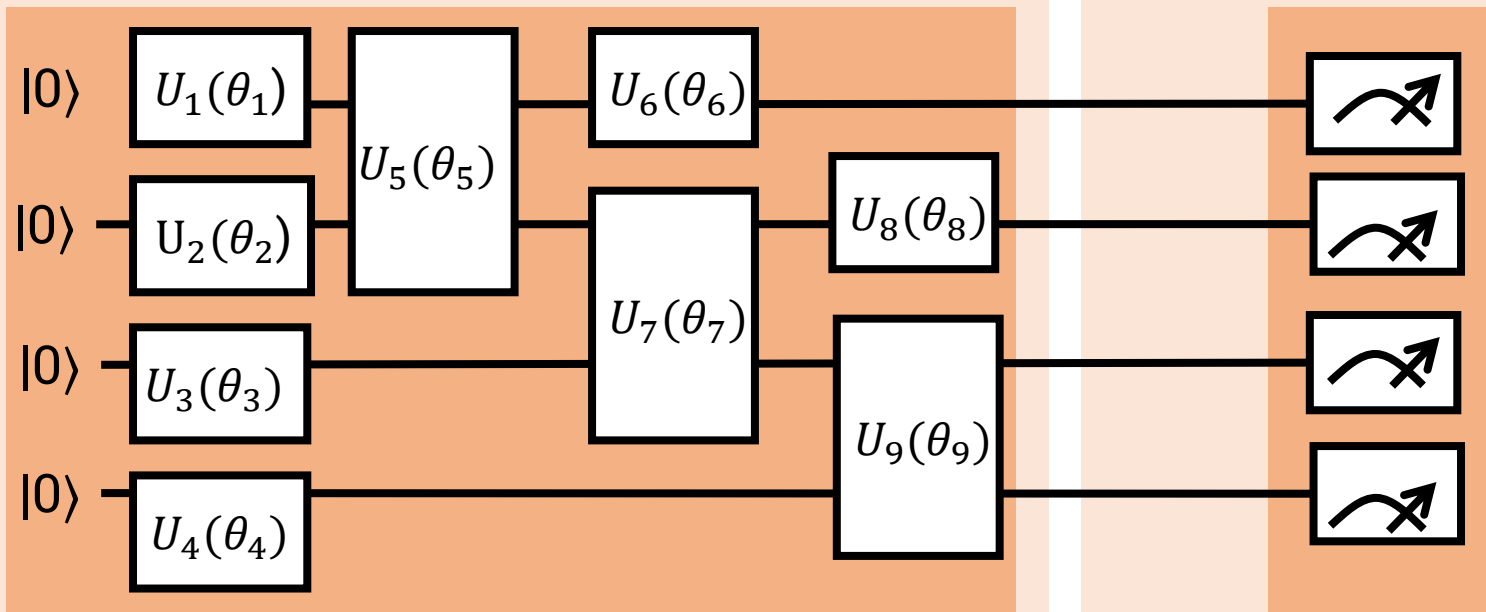
$$\hat{H}_{el} = \sum_j \alpha_j P_j = \sum_j \alpha_j \prod_i \sigma_i^j$$



4) Ansatz parameterized quantum circuit (U_k)

(preparation of trial state)

$$|\psi(\vec{\theta}_k)\rangle = U(\vec{\theta}_k) |\psi_{HF}\rangle$$



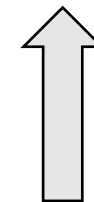
6) Parameter optimization

(adjusting the parameters, $\vec{\theta}_k$, with a classical optimizer)

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

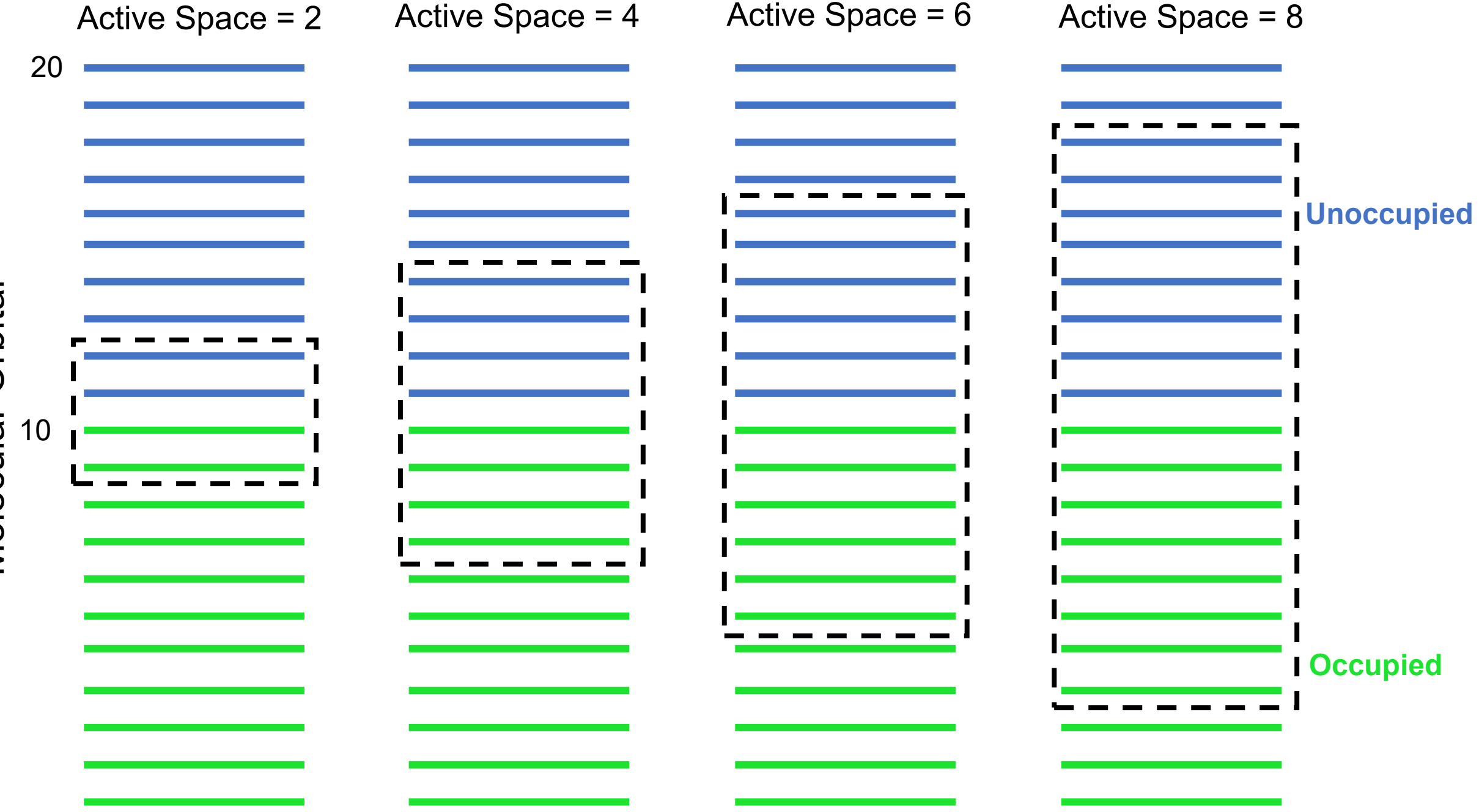


$E(\vec{\theta}_k)$

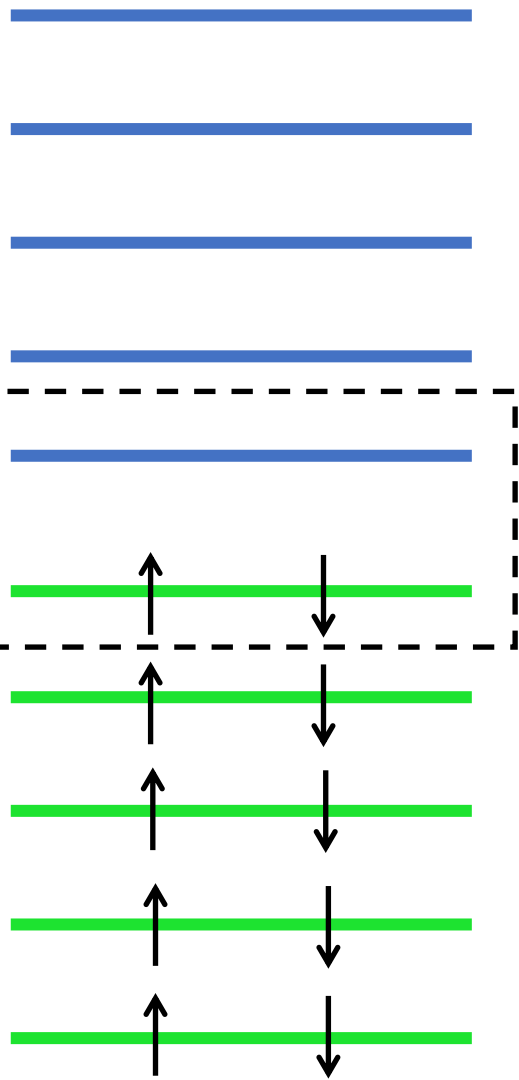


5) energy measurement

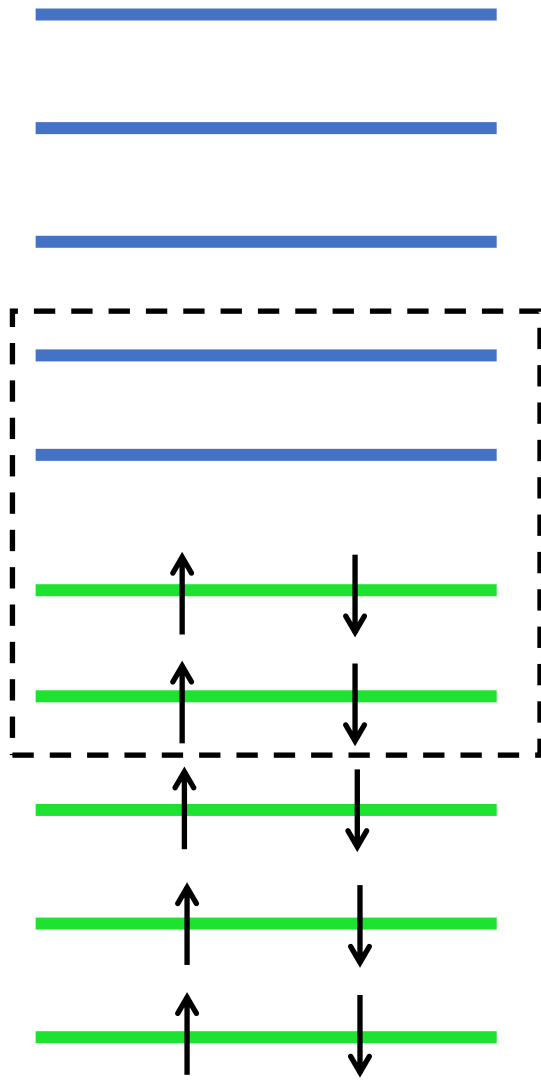
$$E(\vec{\theta}_k) = \sum_j \alpha_j \langle \psi(\vec{\theta}_k) | P_j | \psi(\vec{\theta}_k) \rangle$$



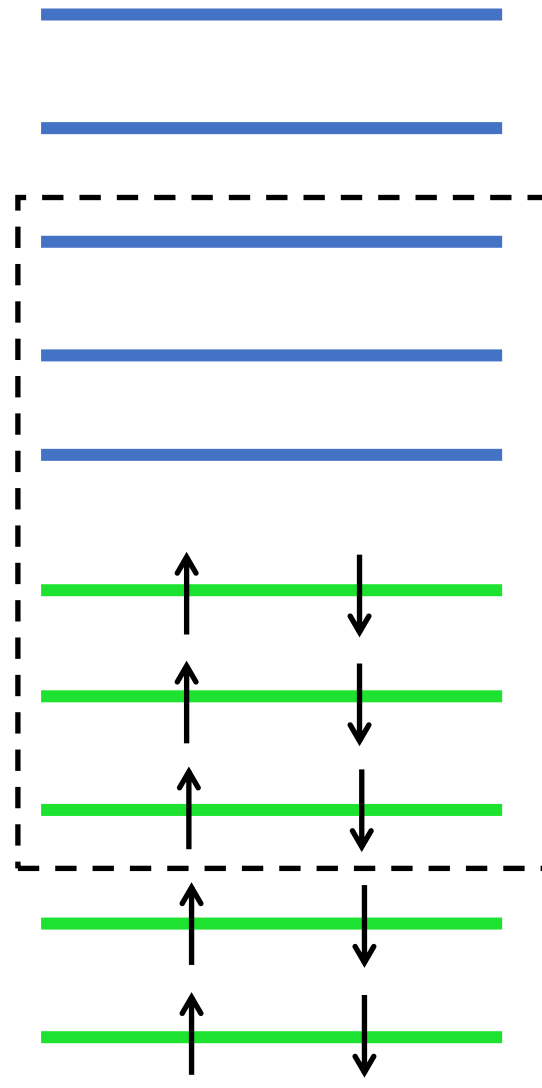
AS2

 $N_{\text{qubits}} = 4$

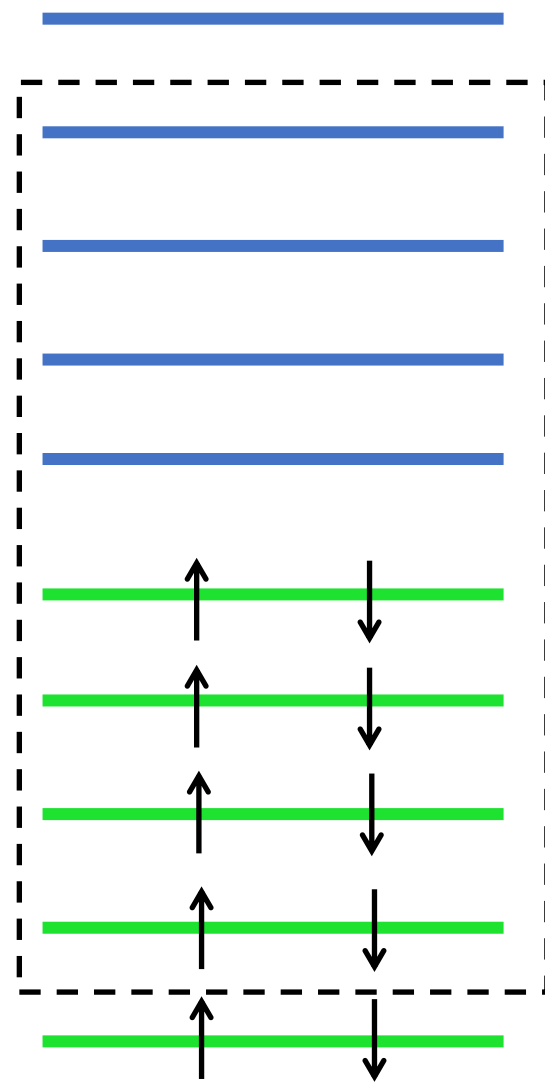
AS4

 $N_{\text{qubits}} = 8$

AS6

 $N_{\text{qubits}} = 12$

AS8

 $N_{\text{qubits}} = 16$

Molecular Orbital

1) Dissociation Profiles of H_2 and CH_5^+

H_2 : 0.6 to 2.7 Å between hydrogen atoms.

CH_5^+ : 1.3, 1.5, 1.7 and 2.0 Å between the C and the H_2 that leaves.

Base Set: CISD/STO-3G.

Program: Gaussian 09.

2) Classical Computing Methods

Calculation of energies with CISD.

Base Set: CISD/STO-3G.

Program: Gaussian 09.

3) Quantum computing methods

Obtaining the energy of dissociation structures using VQE.

Base Set: STO-3G.

Program: PennyLane.

Ansätze

UCCSD, GateFabric, GRSD, HE-A, HE-B, HE-C and EHA.

4) Active Spaces for CH_5^+

CH_5^+ has 10 electrons.

Active space analyzed: 2, 4, 6 and 8 electrons.

Comparison between VQE and CISD.

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