Structure motifs in interpretable quantum algorithm design

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Background

Variational quantum eigensolver algorithm (VQE)

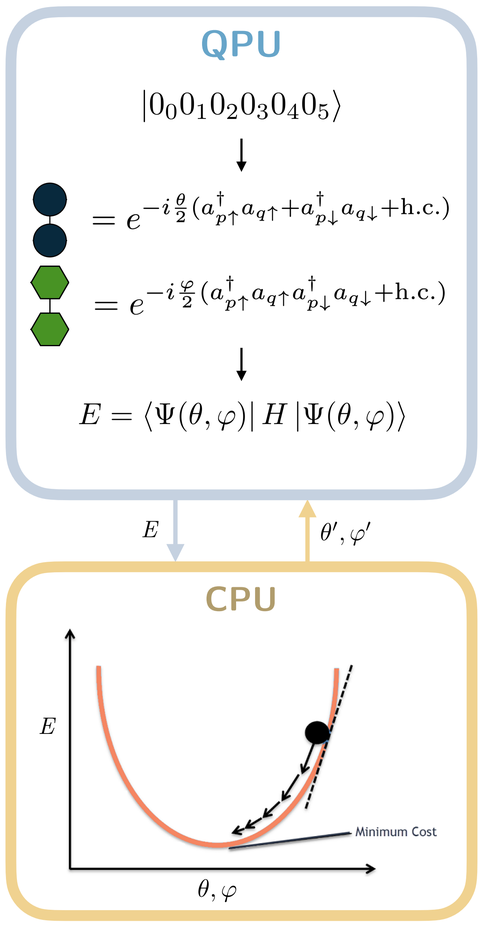
A **wave function**, or ansatz, is prepared on a quantum computer using:

- Qubits as information register
- Quantum gates as logical operations (e.g. single- and double-excitations)

Ansatz design is a complex task and State-of-the-Art circuits are often too expensive for today's hardware.

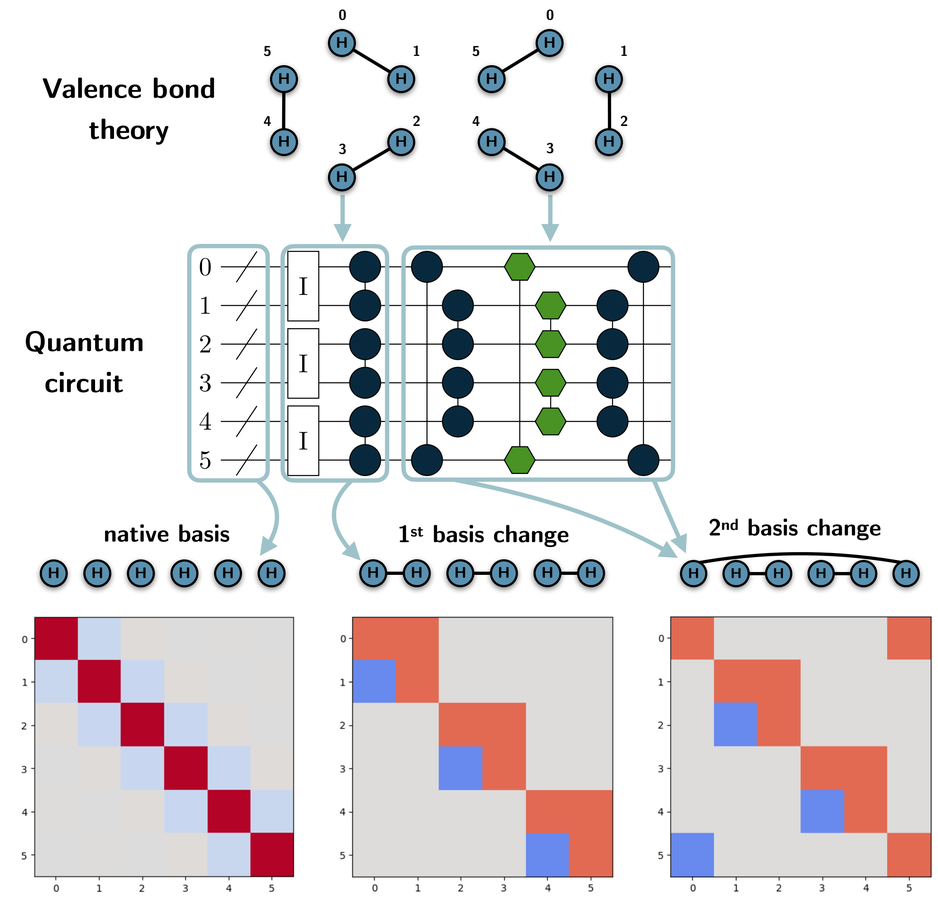
Energy is computed as the **expectation value** of the Hamiltonian and then passed to the classical computer.

Parameters are optimized through **gradient descent-like algorithm** and sent back to the quantum computer.
The process runs until convergence.



Basis change analysis

Original ansatz: Graph-based approach[1]

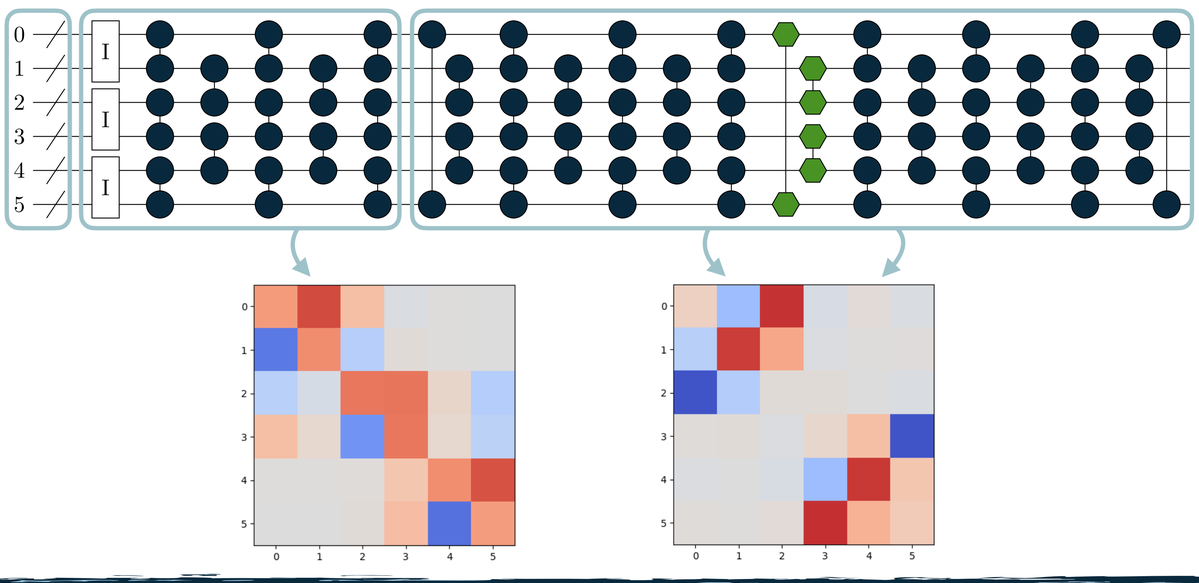


[1]: Quantum 7, 1073 (2023)

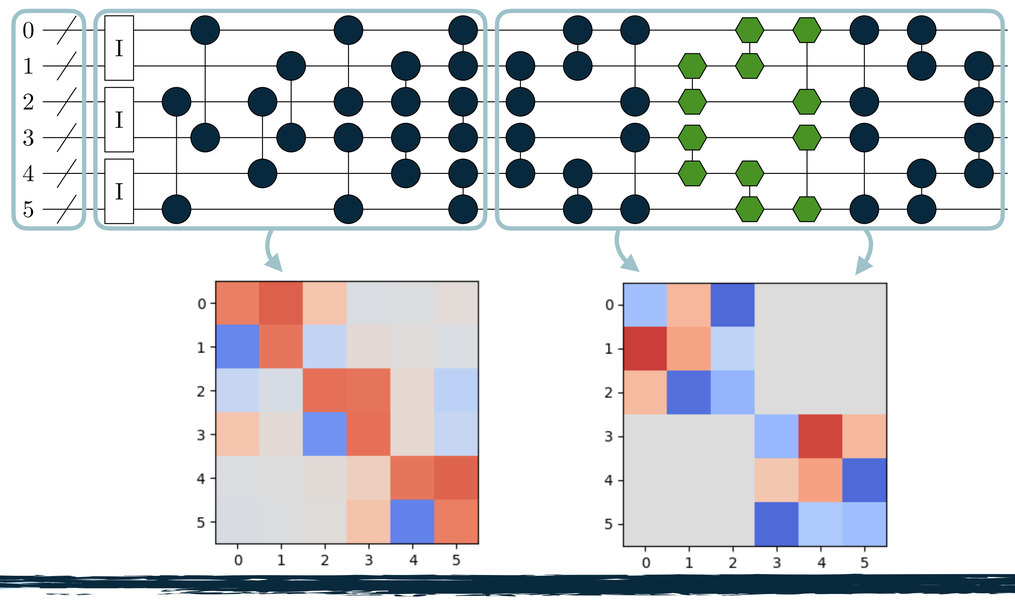
Ansatz extensions

New circuits apply more general basis change and provide orbitals that catch complex interactions.

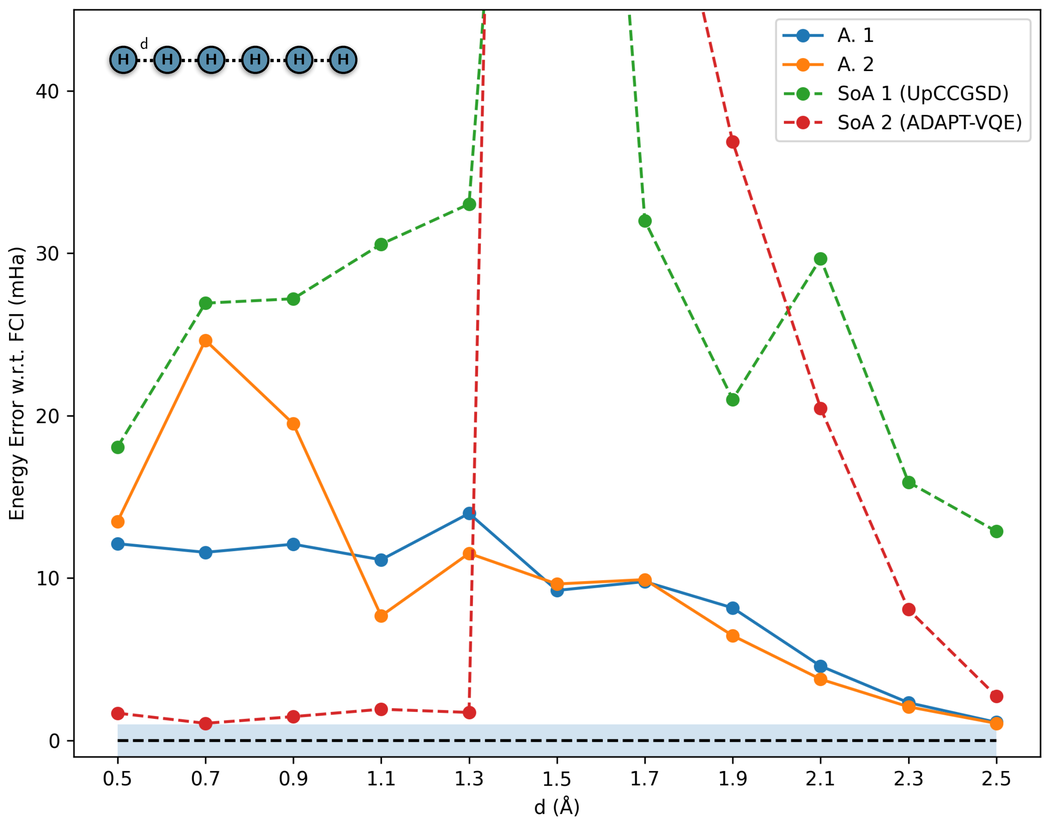
Ansatz 1: local dense layers



Ansatz 2: optimal connections



Results



A. = Ansatz, SoA = State-of-the-Art

Code with tequila-basic framework

```
import tequila as tq
mol = tq.Molecule(geometry=linear_h6.xyz, basis_set="sto-3g")

reference_state = mol.make_ansatz("spa", edges=[(0,1),(2,3),(4,5)])
basis_change_1 = mol.UR(0,1,"r01") + mol.UR(2,3,"r23")
                 + mol.UR(4,5,"r45")

basis_change_2 = mol.UR(0,5,"r05") + mol.UR(1,2,"r12")
                 + mol.UR(3,4,"r34")
correlation = mol.UC(0,5,"c05") + mol.UC(1,2,"c12")
              + mol.UC(3,4,"c34")

ansatz = reference_state + basis_change_1.dagger()
     + basis_change_2 + correlation + basis_change_2.dagger()

E = tq.ExpectationValue(U=ansatz, H=mol.make_hamiltonian())
result = tq.minimize(E)
```

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