QAMP Fall 21 Final Checkpoint: Constraint-Specific VQE Entanglers

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Qiskit

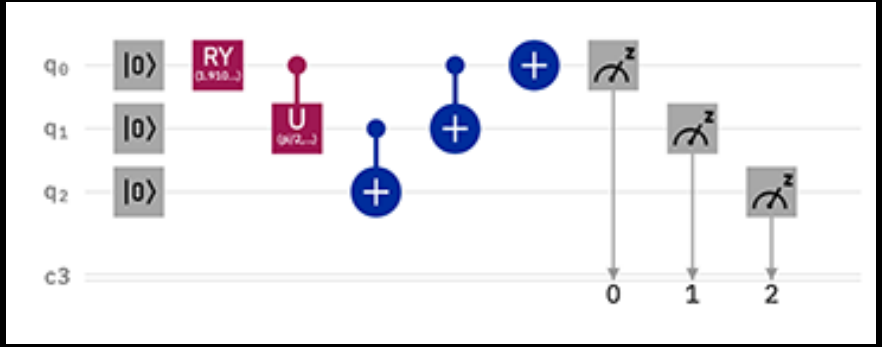
Project Ideas

- VQE – ground state energy estimation
- Entanglers/Variational Forms/PQCs – Tunable unitary operation on “n” qubits applied to a reference state
- Current limitations
  - Few entangler types with general static structures
  - Lack feasibility consideration
- Solution: Dynamic entanglers that reflect constraints

W-states

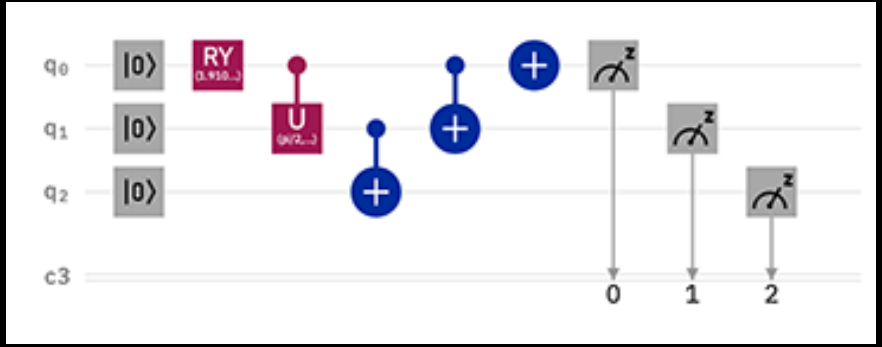
- W-states: Multi-qubit superposition state of where exactly 1 qubit is in state |1>
- Satisfies the following constraint for each base:

$$\sum_{v=1}^{N} x_{v,p} = 1$$



W-states

- Qiskit doesn’t have a circuit library for W-states or any similar multi-qubit ansatz.
- Created W-state circuit library for “n” qubits.



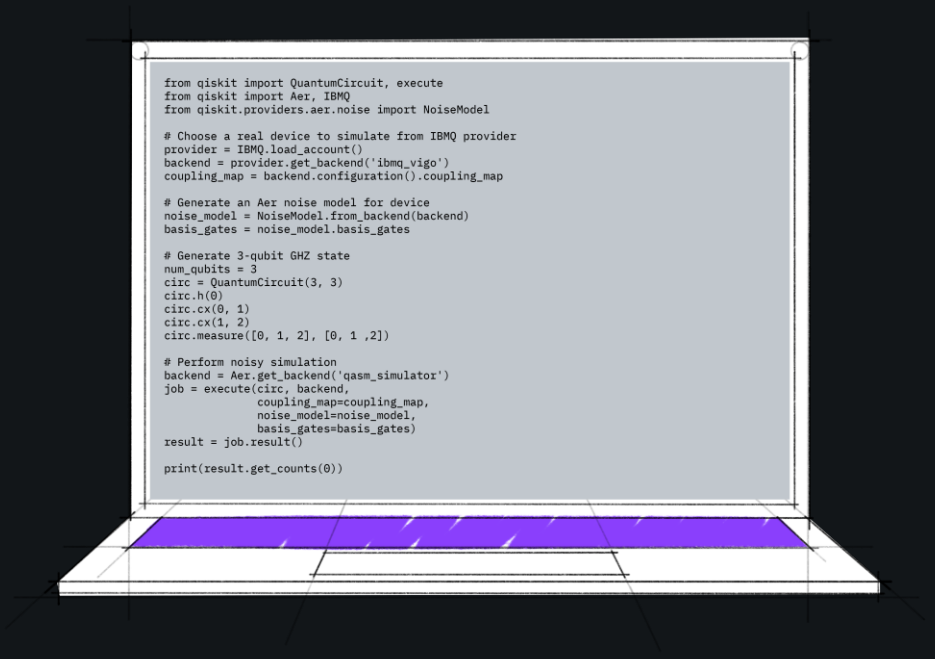
Solution Strategy

Each circuit library deals with specific constraint.

Create multiple libraries for different kinds of constraints.

Combine into single circuit library.

Check for each constraint class when running VQE.



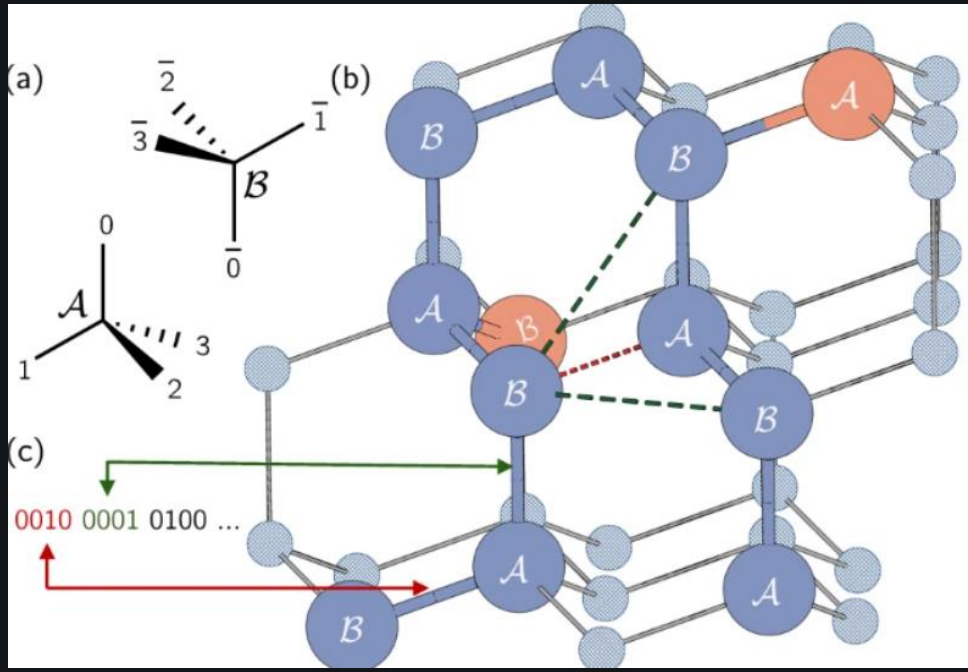
```
from qiskit import QuantumCircuit, execute
from qiskit import Aer, IBMQ
from qiskit.providers.aer.noise import NoiseModel

# Choose a real device to simulate from IBMQ provider
provider = IBMQ.load_account()
backend = provider.get_backend('ibmq_vigo')
coupling_map = backend.configuration().coupling_map

# Generate an Aer noise model for device
noise_model = NoiseModel.from_backend(backend)
basis_gates = noise_model.basis_gates

# Generate 3-qubit GHZ state
num_qubits = 3
circ = QuantumCircuit(3, 3)
circ.h(0)
circ.cx(0, 1)
circ.cx(1, 2)
circ.measure([0, 1, 2], [0, 1 ,2])

# Perform noisy simulation
backend = Aer.get_backend('qasm_simulator')
job = execute(circ, backend,
              coupling_map=coupling_map,
              noise_model=noise_model,
              basis_gates=basis_gates)
result = job.result()

print(result.get_counts(0))
```

Test case problem

Protein Folding:

Problem: Find a folded structure of linear amino acid chain in a regular lattice (scales exponentially with number).

Solution: Assign binary variables to different orientations (constraints) and minimize string using hybrid algorithm.



Challenges

Qiskit

Long term strategy for updating library

Deciding problem cases and catching up with literature.

Updates since deprecation of Qiskit Aqua.

Next steps

Represent all different constraint parameters as circuit libraries and benchmark over existing solution.

Generalize and update for unique constraints from more problems.

PRs for each circuit state library to be submitted.

Technical Report coming later...