

XXIII B. VQE Algorithm - Python Program - (GCP)

The VQE algorithm finds the lowest energy state of the 4-qubit transverse-field Ising model

The VQE algorithm guesses a quantum state

- Computes energy
- Updates parameters
- Energy moves downward
- Eventually converges to the TFIM ground-state energy

Read Results of Python VQE Algorithm

```
Energy := READPRN("./VQE/energy_data.txt")
Prob := READPRN("./VQE/probability_data.txt")
Initial_State := READPRN("./VQE/initial_state.txt")
```

It defines the 4-qubit transverse-field Ising Hamiltonian

The TFIM Hamiltonian (open boundary)

$$H = -J \sum_{i=0}^2 Z_i Z_{i+1} - h \sum_{i=0}^3 X_i,$$

where

- J = coupling strength
- h = transverse-field strength
- $Z_i Z_{i+1}$ = interaction of neighboring qubits
- X_i = field term flipping spins

VQE is used in quantum research and engineering.

It is used during the optimization loop where the program repeatedly updates the circuit parameters to minimize the energy of the 4-qubit TFIM Hamiltonian.

This Hamiltonian creates quantum correlations and possible entanglement.

The program builds this Hamiltonian in matrix or operator form.

For each iteration:

1. Prepare trial state $|\psi(\theta)\rangle$
2. Compute expected energy $E(\theta) = \langle \psi | H | \psi \rangle$
3. Update parameters θ
4. Repeat until convergence

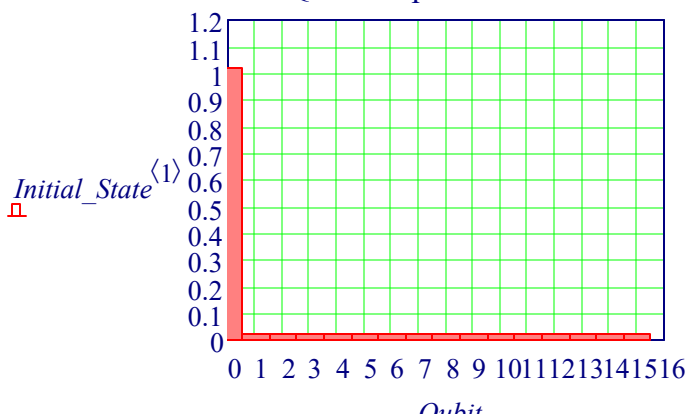
It runs the Variational Quantum Eigensolver (Python - VQE)

The program uses a parameterized circuit (ansatz) and a classical optimizer.

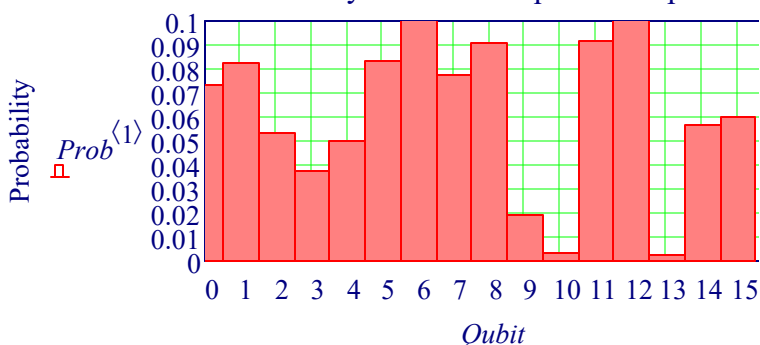
Created the Python Program for VQE:

VQE for a 4-qubit transverse-field Ising model.py

VQE Example: Initial States



Probability of States - Squared Amplitude



VQE is used in real quantum research and engineering.

It can find the ground-state energies of molecules

Some Applicationszz:

Determine the

- Chemical reactivity
- Bond lengths
- Reaction pathways
- Catalyst effectiveness of Molecules.

VQE Convergence - Min Energy Solution

