Phase 3: VQE for the Heisenberg Model

In this phase, the goal is to estimate the ground-state energy of a small Heisenberg spin chain using the Variational Quantum Eigensolver (VQE). Unlike Phases 1 and 2, we are not studying time evolution anymore. The task now is to prepare different quantum states, measure their energy, and use a classical optimizer to search for the lowest energy the circuit can reach. This lets us approximate the ground state without diagonalizing the full Hamiltonian, which becomes impossible for larger systems.

We work with the Heisenberg model because it includes interactions in all three spatial directions (X, Y, and Z), making it more representative of real spin physics. Even though the general model can describe many qubits, we will focus on small chains (e.g., 2–4 qubits) so the circuits remain shallow enough for simulation and potential hardware runs.

Heisenberg Hamiltonian

In the literature, the standard nearest-neighbor Heisenberg Hamiltonian is written as

$$H = J \sum_{\langle i,j \rangle} \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z \right)$$

where the notation $\langle i, j \rangle$ means "neighboring sites" in the chain. Here each σ_k^α means we apply the Pauli matrix σ_α to qubit (site) k. The constant J controls the strength of the coupling.

This Hamiltonian is already a sum of Pauli operators, which is important for VQE because the algorithm measures the expectation value of each term separately. Every product like $\sigma_i^x \sigma_j^x$ is called a Pauli string.

Why We Expand H in Pauli Terms (and What the Terms Mean)

VQE estimates the energy of a trial state $|\psi(\theta)\rangle$ by computing

$$E(\theta) = \langle \psi(\theta) | \, H \, | \psi(\theta) \rangle$$

To make this measurable, we rewrite the Hamiltonian as a sum of Pauli strings:

$$H = \sum_k h_k P_k$$

where:

- P_k is a Pauli string
- h_k is the coefficient. Representing weight of each Pauli string. For the Heisenberg model, these coefficients are essentially copies of J.

Once H is expressed in this form, the energy splits cleanly into

$$E(\theta) = \sum_k h_k \, \langle\psi(\theta)| \, P_k \, |\psi(\theta)\rangle$$

This decomposition matters because a quantum computer cannot measure the full Hamiltonian in one shot. It can only measure single-qubit observables in a chosen basis. Pauli strings are exactly the operators that match the natural measurement bases of the hardware. So rewriting H as a sum of these terms lets us evaluate the energy using repeated measurements of the same circuit in different bases.

Variational Principle

VQE is based on the variational principle, which states that for any normalized state:

$$\langle\psi| \, H \, |\psi\rangle \geq E_0$$

where E_0 is the true ground-state energy. That means if we can minimize $\langle\psi(\theta)| \, H \, |\psi(\theta)\rangle$ over some parameter set θ, the lowest value we reach is an approximation of E_0.

We prepare trial states using a parameterized circuit:

$$|\psi(\theta)\rangle = U(\theta) \, |0 \cdots 0\rangle$$

and let a classical optimizer update the parameters to push the energy downward.

Ansatz Circuit

The circuit $U(\theta)$ is called an *ansatz*. It must be expressive enough to represent a variety of states but also shallow enough to run on hardware. A simple and commonly used structure for a 1D chain is:

- Apply single-qubit rotations (e.g., R_y or R_z) to each qubit.
- Add entangling gates (e.g., CNOTs) between neighboring qubits.
- Repeat this pattern for a few layers to increase expressiveness.

Even with only a few layers, the circuit can represent many possible spin configurations, making it workable for small-scale VQE experiments.

Measuring the Energy

Since $H = \sum_k h_k P_k$, the energy estimate becomes

$$E(\theta) = \sum_k h_k \langle P_k \rangle$$

where each expectation value is computed from measurement statistics. To measure the different Pauli terms:

- For $Z \otimes Z$, measure in the computational (Z) basis.
- For $X \otimes X$, apply a Hadamard to each qubit before measuring.
- For $Y \otimes Y$, apply $S^\dagger$ then Hadamard before measuring.

Repeating the process many times (shots) gives empirical averages for each Pauli string. Summing these values with the coefficients h_k yields $E(\theta)$.

Classical Optimization Loop

The classical optimizer takes the current energy estimate and updates the parameters θ trying to reduce the energy. The loop is:

1. Prepare $|\psi(\theta)\rangle$ on the quantum device.

2. Measure all required Pauli strings to estimate $E(\theta)$.

3. Update θ using an optimizer (e.g., COBYLA, SPSA).

This continues until the energy stops decreasing or reaches a chosen tolerance.

Connection to Earlier Phases

- Phase 1 taught us how to express a Hamiltonian using Pauli matrices and how that determines physical behavior.
- Phase 2 introduced multi-qubit systems and interactions, and forced us to think about operators acting on specific qubits.
- Phase 3 now uses the same operator ideas, but instead of time evolution we focus on computing expectation values and performing energy minimization.

VQE brings together everything from the earlier phases: constructing operators, working with multi-qubit systems, measuring expectation values, and using these measurements to learn something physically meaningful about a Hamiltonian.