QUBO Formulation of Vehicle Routing as a Spin Glass Hamiltonian

1 Problem Formulation

Given:

- A set of delivery points $i \in \{1, \ldots, N\}$ with known coordinates.
- A distance or travel-time matrix d_{ij}.
- Vehicles $k \in \{1, \ldots, M\}$ with capacity constraints Q_k, starting and ending at specific locations.
- Additional constraints such as time windows, fuel costs, and penalties.

We define binary variables:

$$x_{i,j,k} \in \{0, 1\}, \quad \text{where } x_{i,j,k} = 1 \text{ if vehicle } k \text{ travels from } i \text{ to } j. \tag{1}$$

Here, (i, j, k) represents a specific site in the problem, meaning a qubit that encodes whether vehicle k travels from node i to node j.

2 Spin Glass Hamiltonian Formulation

The problem can be mapped into a quadratic unconstrained binary optimization (QUBO) Hamiltonian of the form:

$$H = H_{\text{cost}} + \lambda_1 H_{\text{visit}} + \lambda_2 H_{\text{capacity}} + \lambda_3 H_{\text{subtour}} \tag{2}$$

where the terms encode the optimization objective and constraints:

2.1 Cost Function

Minimizing the total travel cost:

$$H_{\text{cost}} = \sum_{i,j,k} d_{ij} x_{i,j,k} + \sum_{i,j,k} C_{ij} x_{i,j,k} \tag{3}$$

where C_{ij} represents additional cost factors (fuel, penalties, etc.).

2.2 Constraints as Penalty Terms

Each location is visited exactly once:

$$H_{\text{visit}} = \sum_i \left(\sum_{j,k} x_{i,j,k} - 1 \right)^2 \tag{4}$$

Each vehicle starts and ends at the designated locations:

$$H_{\text{start/end}} = \sum_k \left(\sum_j x_{s,j,k} - 1 \right)^2 + \sum_k \left(\sum_i x_{i,e,k} - 1 \right)^2 \tag{5}$$

Vehicle capacity constraints:

$$H_{\text{capacity}} = \sum_k \left(\sum_i d_i x_{i,j,k} - Q_k \right)^2 \tag{6}$$

Subtour elimination: To prevent disjoint loops in the solution:

$$H_{\text{subtour}} = \sum_{i,j,k} x_{i,j,k} x_{j,i,k} \tag{7}$$

3 Quantum Hamiltonian Construction

We map the binary variables $x_{i,j,k}$ into spin variables $s_{i,j,k} \in \{-1, 1\}$ using:

$$x_{i,j,k} = \frac{1 + s_{i,j,k}}{2} \tag{8}$$

Rewriting the Hamiltonian in terms of spin variables:

$$H = H_0 + H_1 = \sum_{(i,j,k)} h_{i,j,k} Z_{i,j,k} + \sum_{(i,j,k),(l,m,n)} J_{i,j,k,l,m,n} Z_{i,j,k} \otimes Z_{l,m,n} \tag{9}$$

where:

- $Z_{i,j,k}$ is the Pauli-Z operator acting on qubit (i, j, k).
- $h_{i,j,k}$ represents local field coefficients, related to travel cost:

$$h_{i,j,k} = \frac{1}{2}(d_{ij} + C_{ij}) \tag{10}$$

- $J_{i,j,k,l,m,n}$ are interaction terms enforcing constraints:

$$J_{i,j,k,l,m,n} = \lambda_1 \delta_{i,l} \delta_{j,m} + \lambda_2 \delta_{k,n} + \lambda_3 \text{subtour penalty} \tag{11}$$

The term site (i, j, k) site (i, j, k) now refers to the qubit representing the decision of whether vehicle k travels from node i to node j.

4 Annealing

WE then preparer the initial state in the ground state of H_0 (easy since diagonal) and then drive it under $H(t) = H_0 + tH_1$.