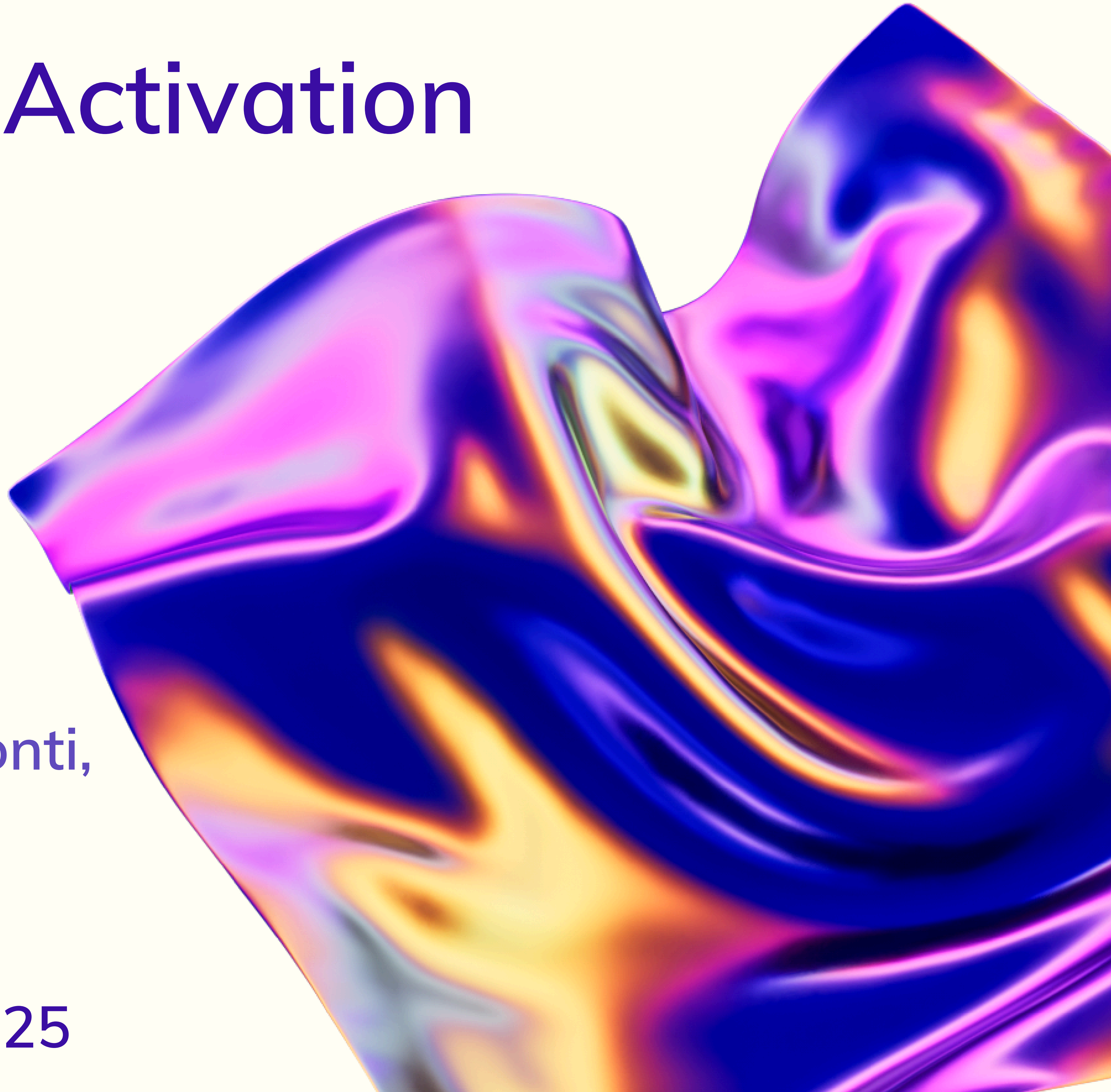
From Quantum Principles to Biomechanics

A Case Study on Muscular Activation



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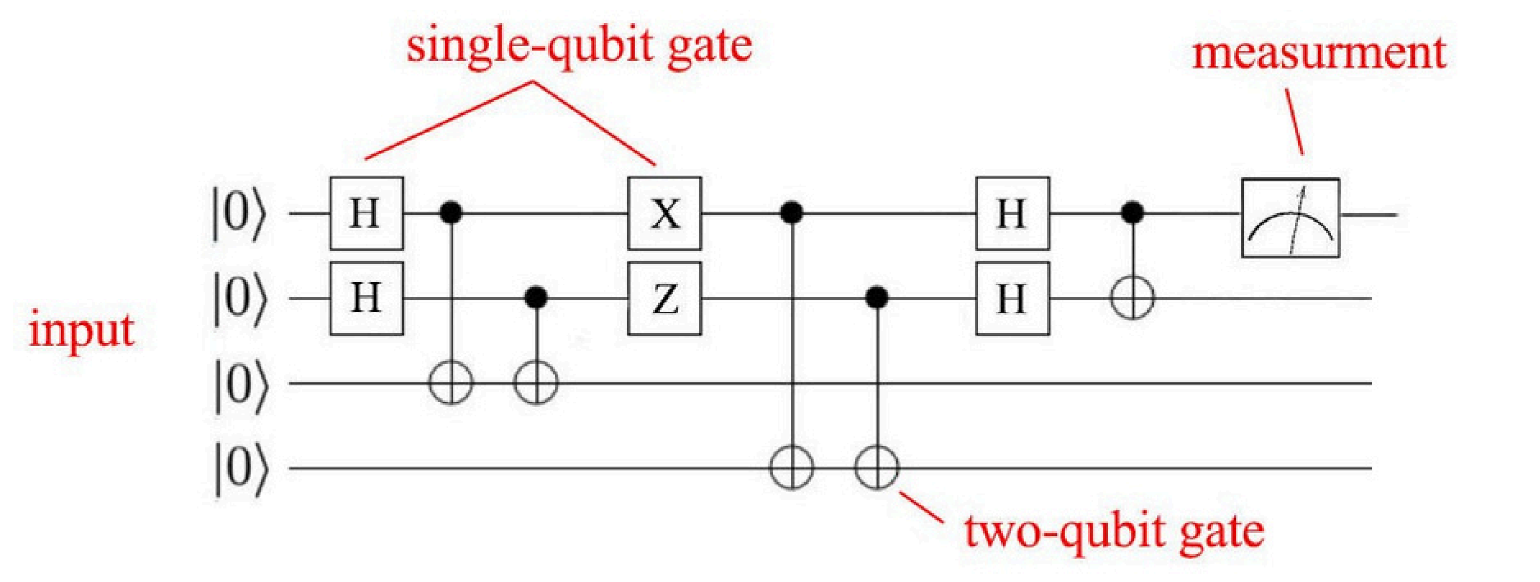
INFN-CNAF

31 Gen 2025

Introduction

The **gate model** is a general-purpose approach to quantum computing that uses **quantum gates**, similar to classical logic gates, to manipulate **qubits** for solving complex problems.
It supports a wide range of applications, including **cryptography, chemistry simulations and machine learning**.
Their construction is challenging due to **qubit coherence** and **error correction** requirements.



Quantum annealing is a specialized optimization technique designed for solving combinatorial problems by leveraging **quantum adiabatic theorem** to find the lowest energy state, representing the optimal solution. It is particularly effective for **optimization** tasks in logistics, finance, and machine learning. Implemented in hardware like D-Wave quantum processors, it is **less versatile** than gate-based quantum computing but **highly efficient** for specific problem types.

PART 1: QUANTUM INTRODUCTION

Quantum superposition

Quantum entanglement

Hamiltonian operator

Quantum adiabatic theorem

Quantum tunneling

Quantum superposition

Imagine you have a coin in your hand. If you hold it still, it is either heads or tails. This is similar to a classical bit, which can be in one of two states: **0** or **1**.

Now you spin the coin on a table. In that moment it's not just heads or tails, it's a combination of both of them at the same time. You can think of it as existing in a **superposition** of both states until you stop it and observe whether it lands on heads or tails.
The bits that can be put in a superposition state of 0 and 1 are called **qubits**

The general state of a single qubits can be written as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where $|\alpha|^2$ is the probabilty to observe the state $|0\rangle$ after the measurement
and $|\beta|^2$ the probability to observe $|1\rangle$.
It follows that $|\alpha|^2 + |\beta|^2 = 1$

Quantum superposition

For two qubits we have:

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

We can decide to measure one qubit at a time. Suppose that we measure the first qubit and we get the state $|0\rangle$, the state becames:

$$|\psi\prime\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{01}|01\rangle}{\sqrt[2]{\alpha_{00} + \alpha_{01}}}$$

Quantum entanglement

Now you have a special pair of coins that are **strongly related:** if you spin both coins and stop one of them, the other one will stop also and they will fall on the same face.

It works indipendently from the coins distance.

In this case we say that the coins are **entangled.**

Quantum entanglement is the phenomenon of a group of particles being generated, interacting, or sharing spatial proximity in such a way that the quantum state of each particle of the group cannot be described independently of the state of the others, including when the particles are separated by a large distance.

An example are the Bell states:

$$|\psi\rangle = \frac{1}{\sqrt[2]{2}}(|00\rangle + |11\rangle)$$

Hamiltonian operator

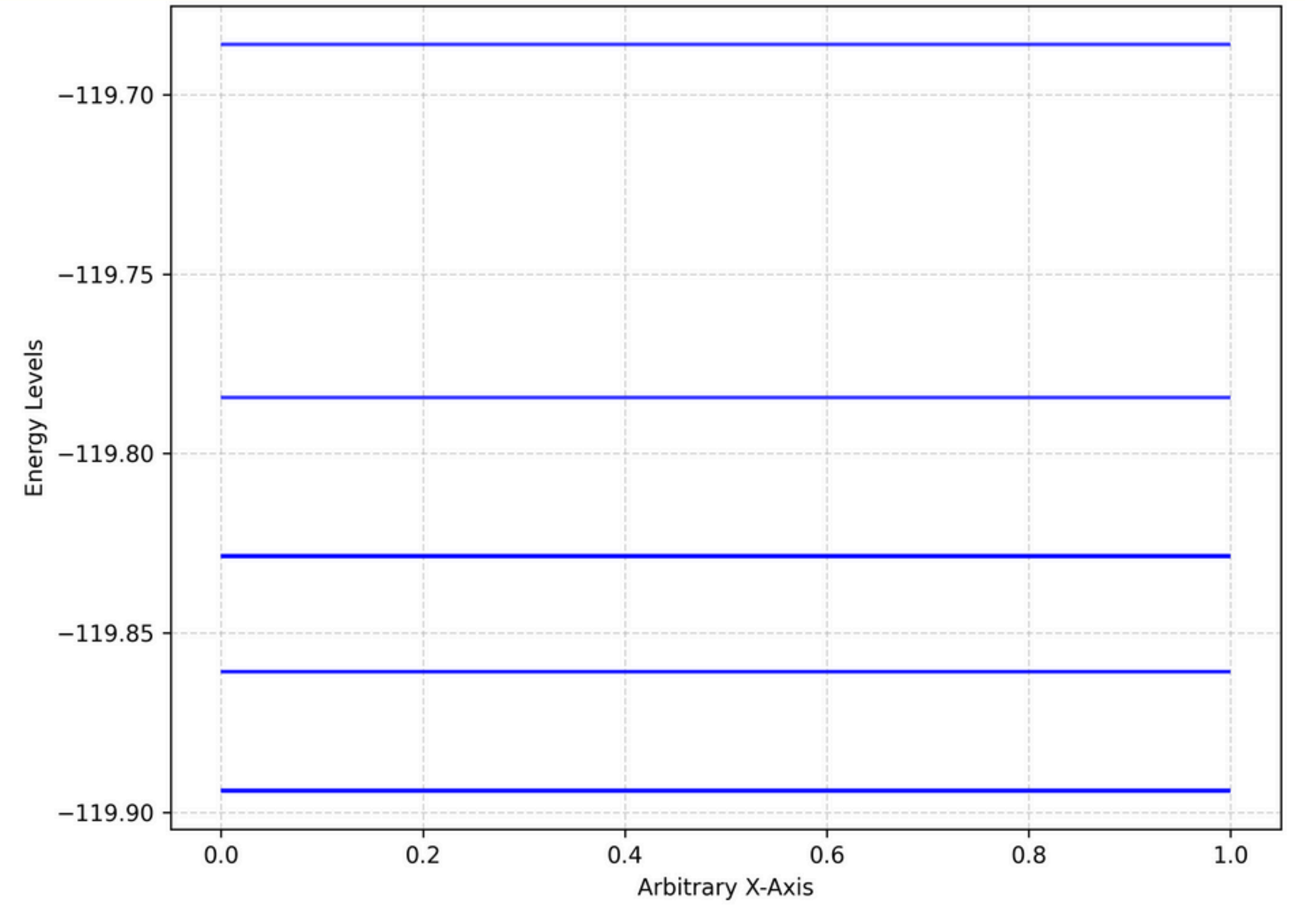
As we know, we can change our potential energy increasing the height of our position.
If we are moving on a ramp we can occupy any position and our energy change **continously**.
If we are on a staircase, we can only occupy certain strairs and have only specific energy values.
In this case our energy is **quantized.**

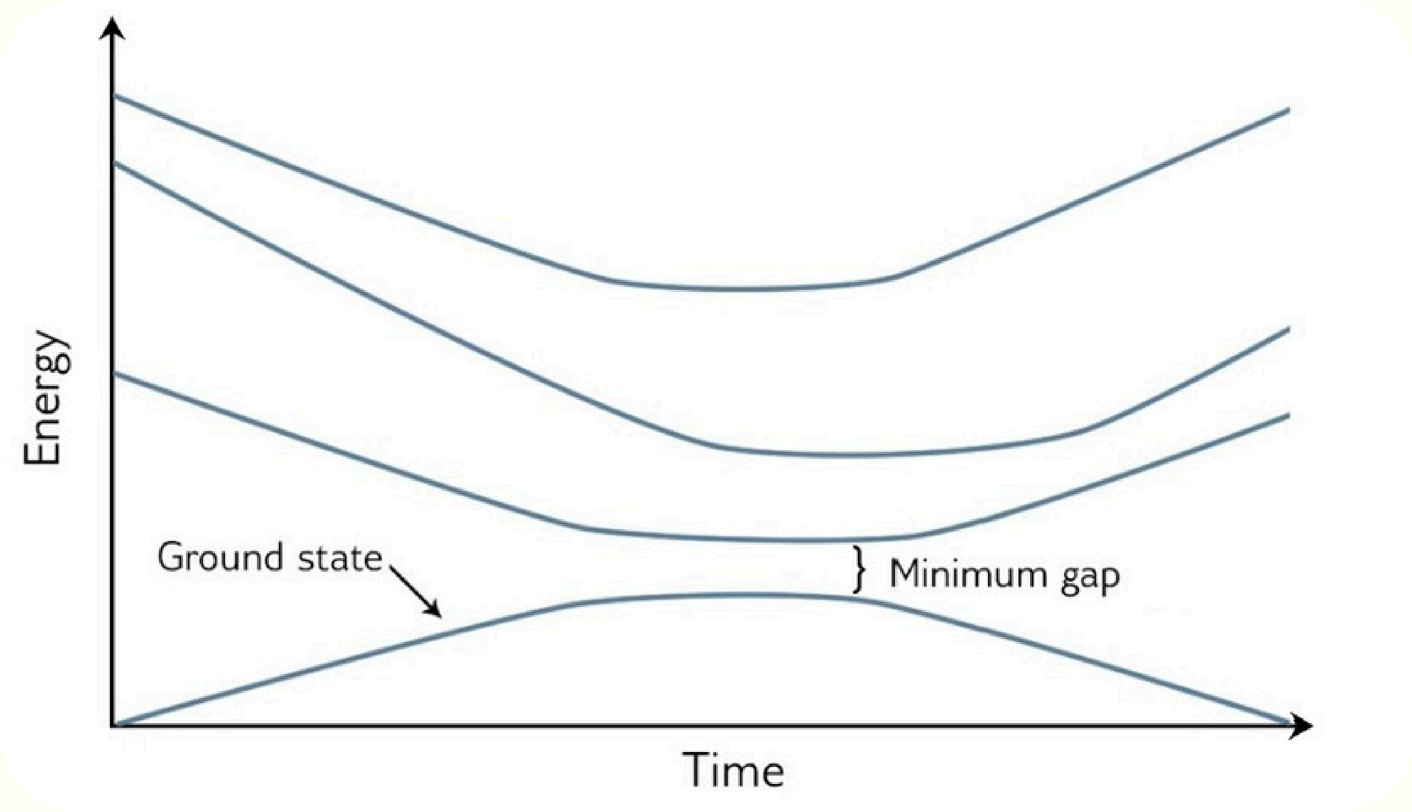
In classical physics the **Hamiltonian** is a function that associates to coordinates and momenta components of the elements in the system to the energy of the system.

In quantum mechanics exists its analogous which is the **Hamiltonian operator.**
It maps certain states, called **eigenstates**, to energies. Only when the system is in an eigenstate of the Hamiltonian, its energy is well defined and called the **eigenenergy**. When the system is in any other state, its energy is uncertain. The collection of eigenstates with defined eigenenergies make up the **eigenspectrum**.

Quantum adiabatic theorem

Imagine yourself on a staircase that's not static but is slowly reshaping its steps. If it **changes slowly** enough, you can adjust your balance and stay on the same step without jumping to another.



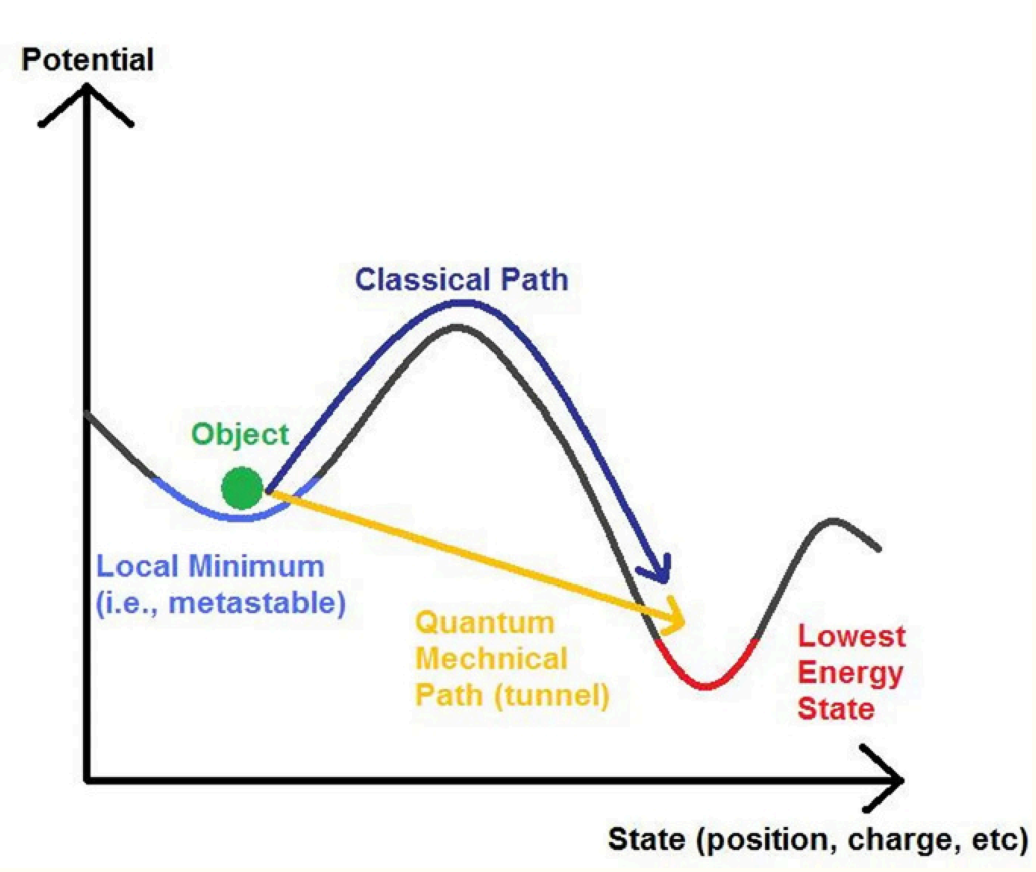


Quantum adiabatic theorem states:

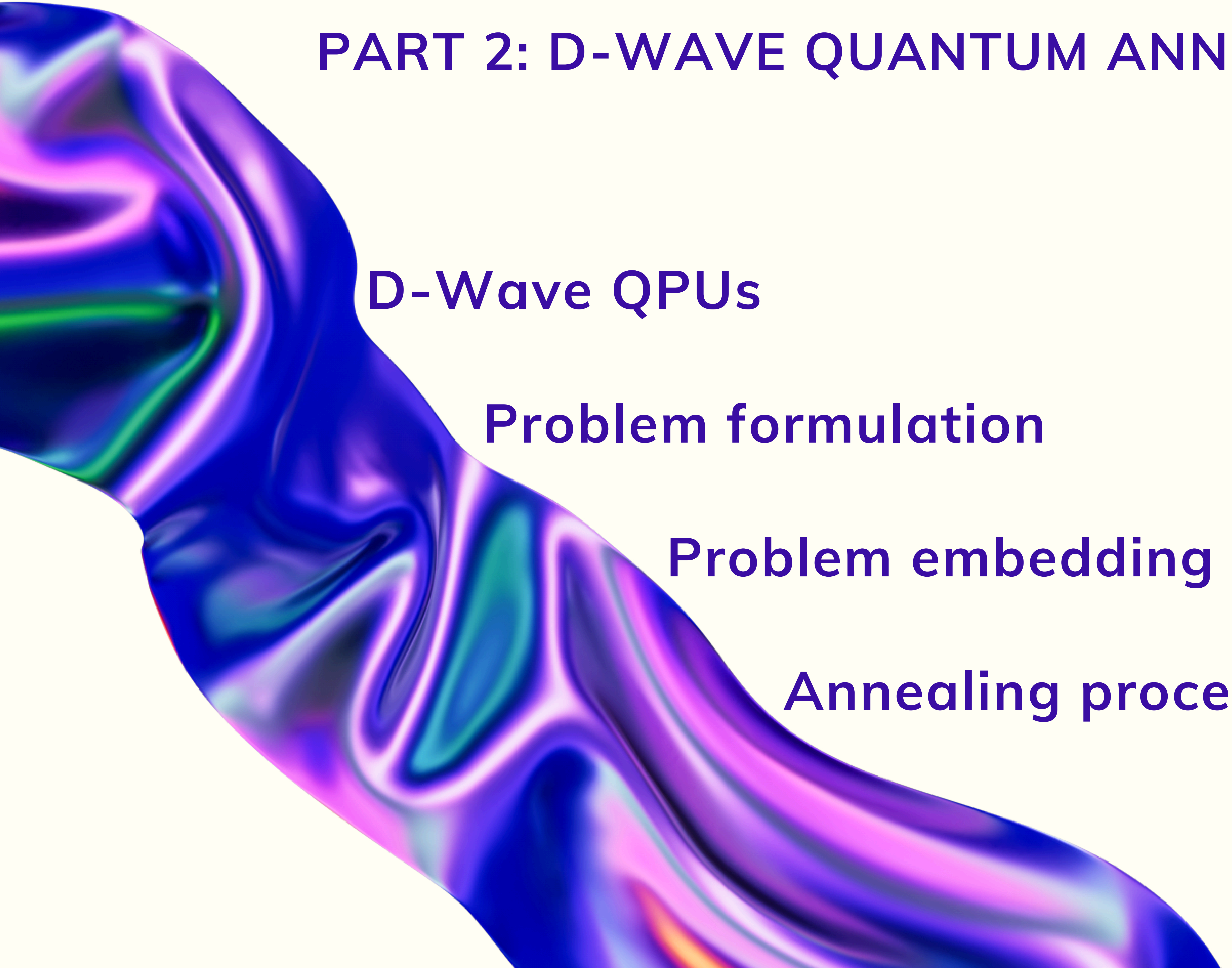
A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum.

Quantum tunneling

In an optimization problem, the goal is to find a solution that minimizes a given cost function. Classical algorithms search through the solution space to locate the absolute minimum. However, they are susceptible to **getting trapped in local minima**, where a solution appears optimal within a limited region but is not the best overall.



Quantum tunneling plays a crucial role in quantum annealing by allowing the system to move through energy barriers rather than going over them.



PART 2: D-WAVE QUANTUM ANNEALING

D-Wave QPUs

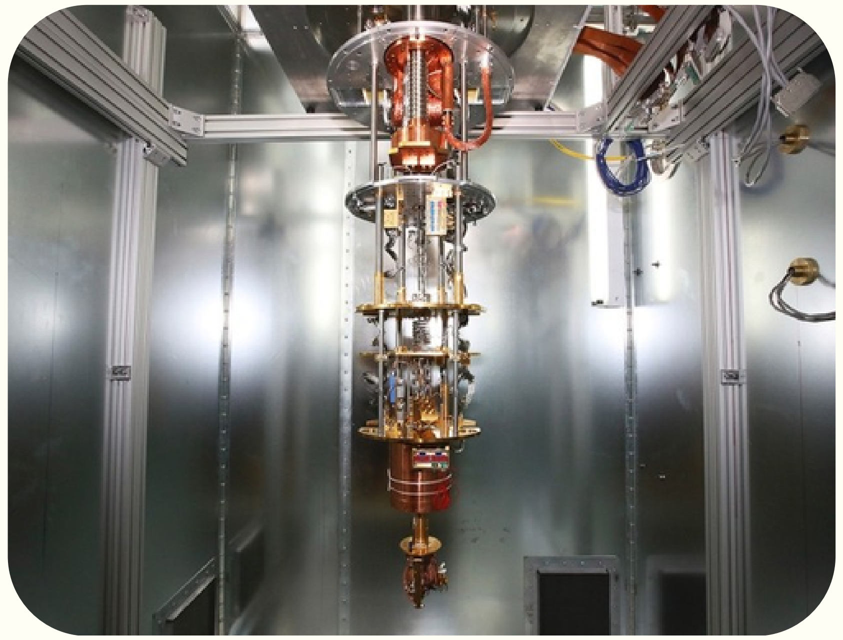
Problem formulation

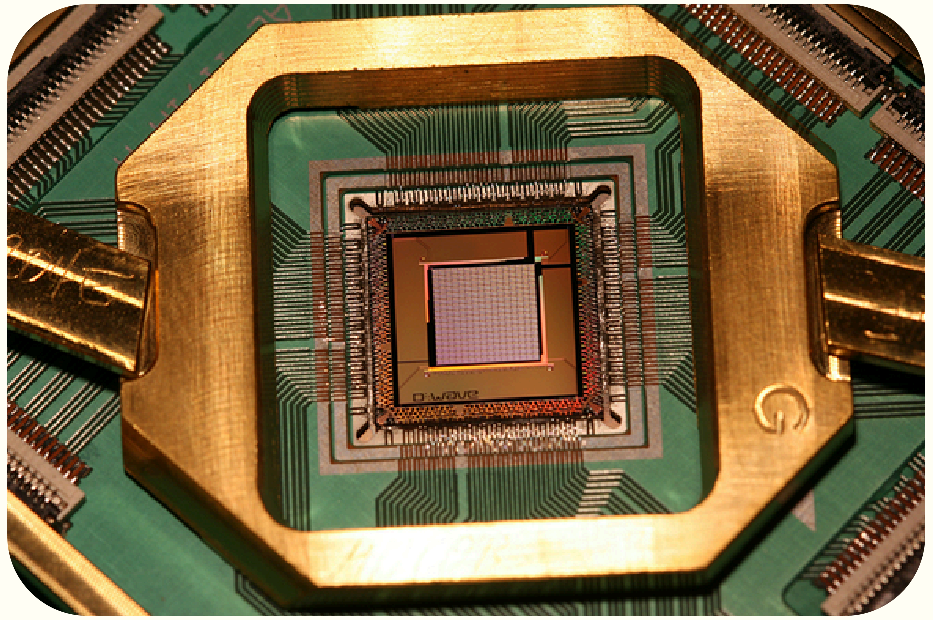
Problem embedding

Annealing process

D-wave QPU

The D-Wave **Quantum Processing Unit (QPU)** is the core computational component of quantum computers developed by D-Wave Systems.
The qubit consists of a small **superconducting loop** made of **niobium**, which has nearly zero electrical resistance at ultra-low temperatures.
The loop includes one or more **Josephson junctions**, which are thin insulating barriers between superconducting regions.
These Josephson junctions allow **quantum tunneling** of Cooper pairs, enabling **superposition** and quantum coherence.

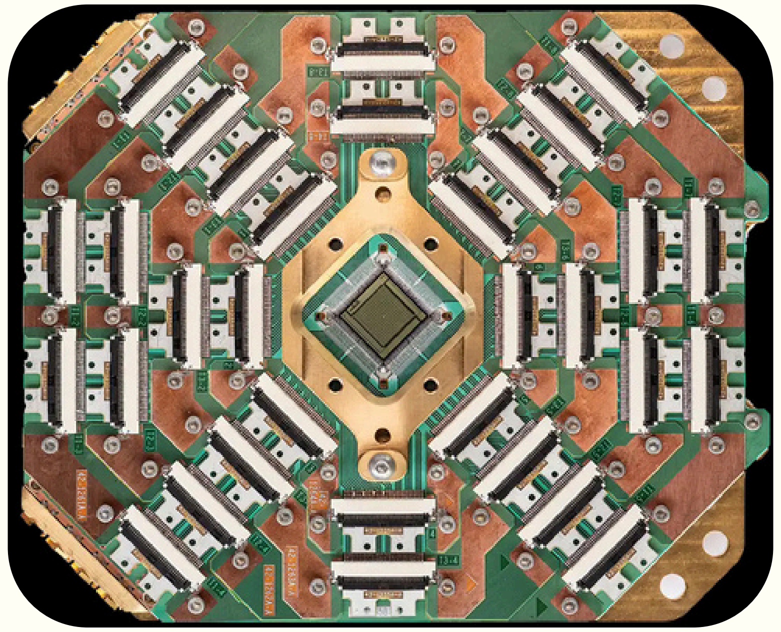




D-wave QPU

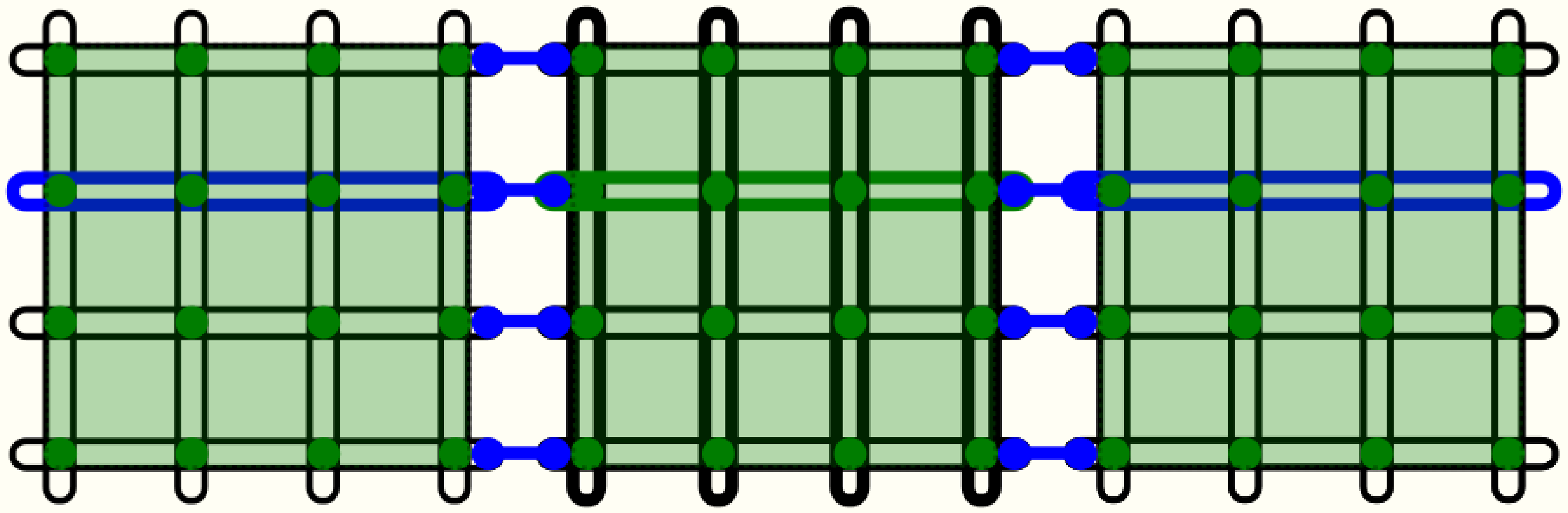
Timeline of QPU Releases

- D-Wave One → 2011 (128 qubits)
- D-Wave Two → 2013 (512 qubits, **Chimera topology**)
- D-Wave 2X → 2015 (1,152 qubits)
- D-Wave 2000Q → 2017 (2,048 qubits)
- D-Wave Advantage → 2020 (5,000+ qubits, **Pegasus topology**)
- D-Wave Advantage2 (Prototype) → 2023 (Prototype with 1,200+ qubits, testing new **Zephyr topology**)
- D-Wave Advantage2 (Full System) → Expected 2024-2025 (~7,000 qubits)



D-wave QPU

QPU Topologies: Chimera graph



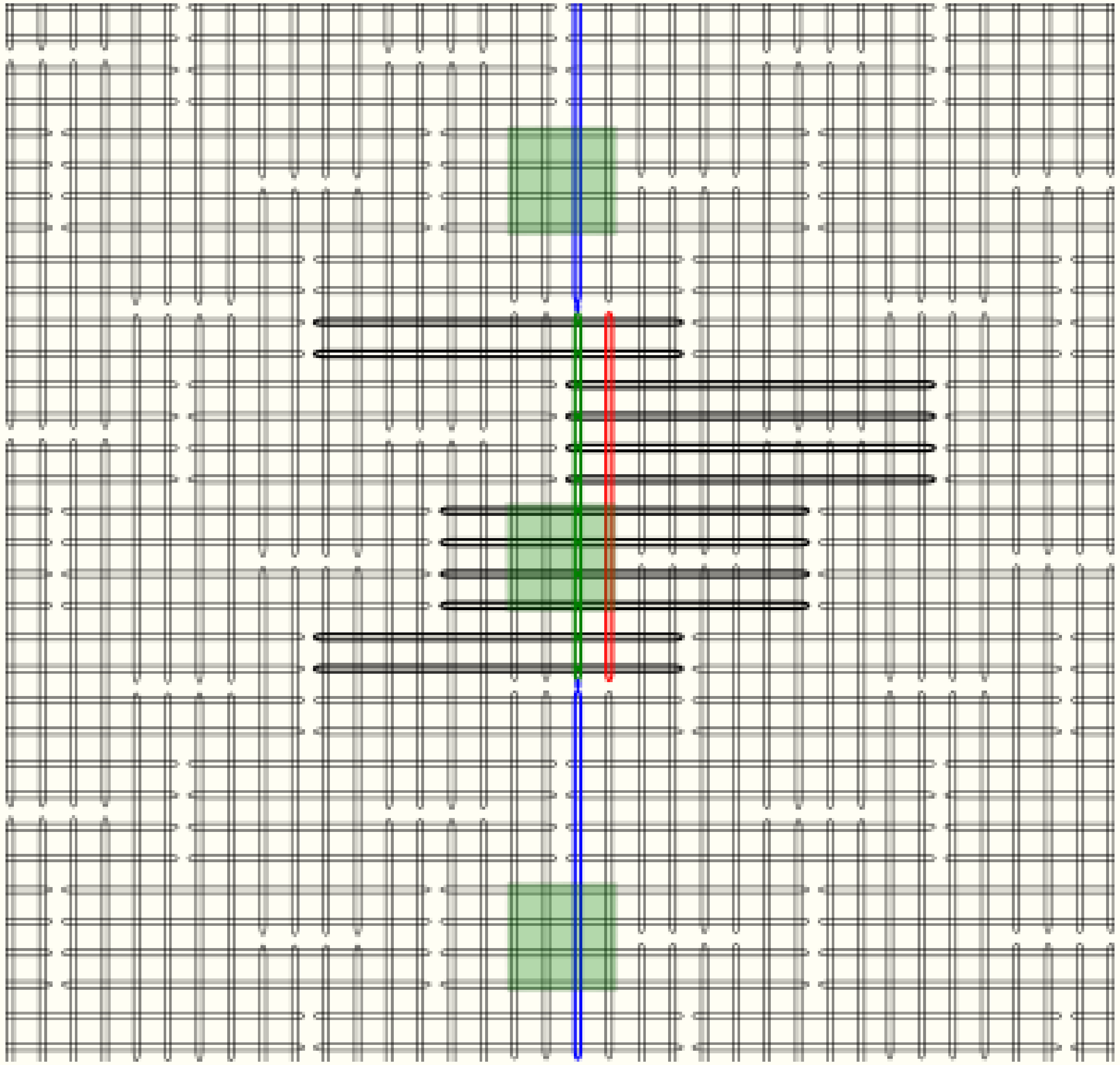
Three unit cells in the Chimera topology. Each of the three green squares contains 8 qubits, 4 horizontal and 4 vertical. External couplers couple horizontal qubits to adjacent horizontal qubits (shown as connected blue circles) and vertical qubits to adjacent vertical qubits (not shown). Internal couplers, shown in green, couple horizontal to vertical qubits inside each unit cell

Internal couplers per qubit: 4
External Couplers per qubit: 2

D-wave QPU

QPU Topologies: Pegasus graph

Internal couplers connect pairs of orthogonal qubits (green qubit with black qubits)
External couplers connect consecutive qubits with the same orientation (green qubit with blue qubits)
Odd couplers connect similarly aligned "parallel" pairs of qubits (green qubit and red qubit)

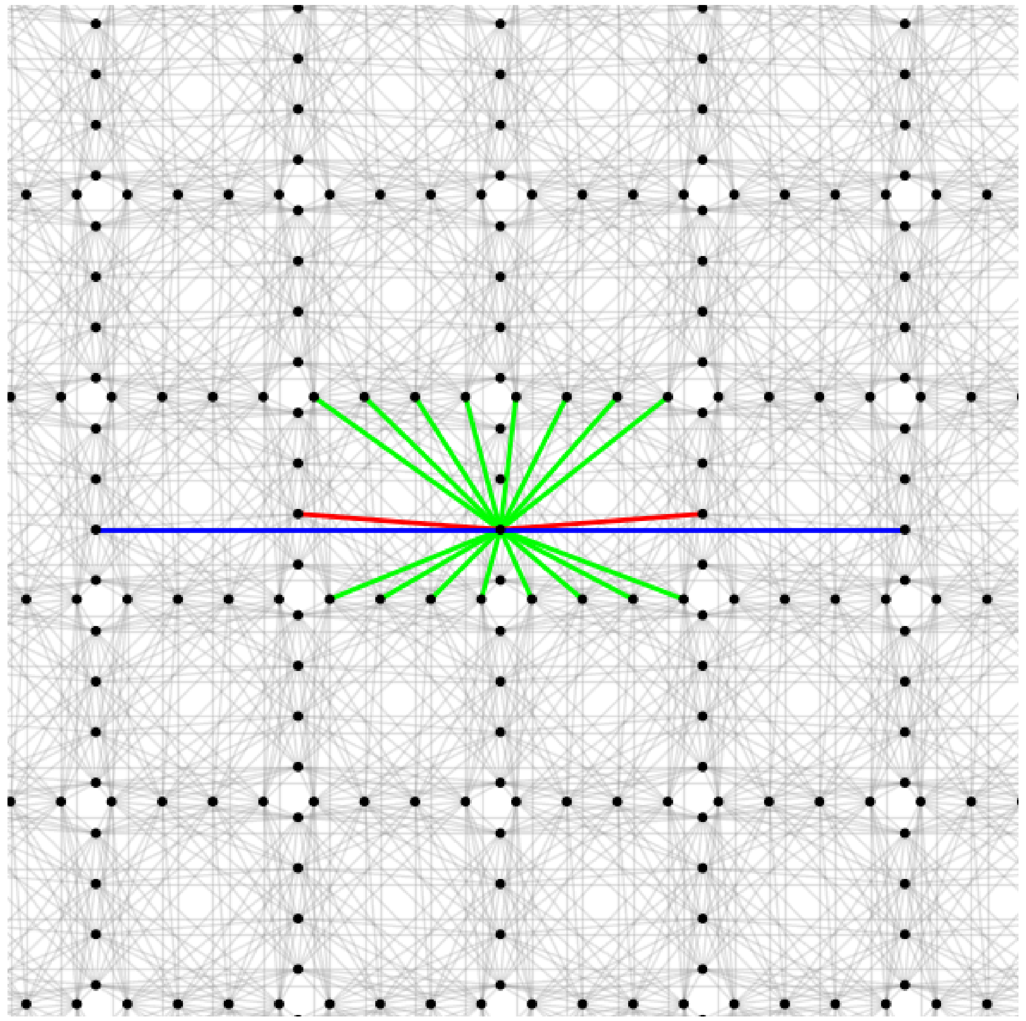


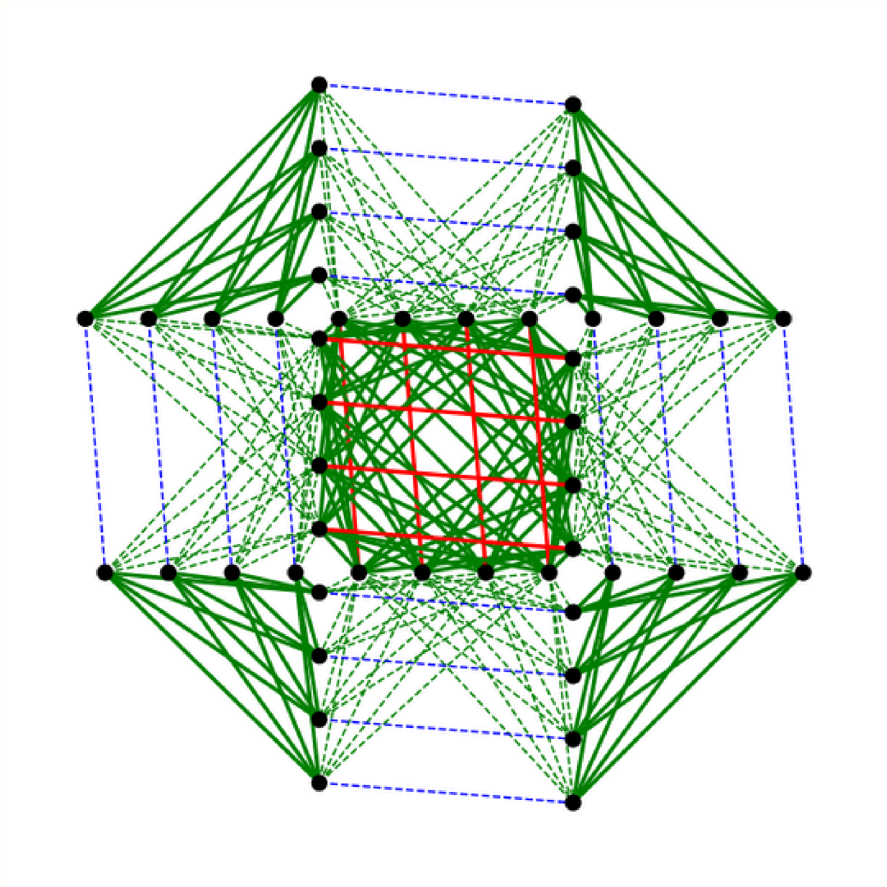
Internal couplers per qubit: 12
External couplers per qubit: 2
Odd couplers per qubit: 1

D-wave QPU

QPU Topologies: Zephyr graph

Internal couplers connect pairs of orthogonal qubits,
in green
External couplers connect consecutive qubits with the same orientation, in blue
Odd couplers connect similarly aligned "parallel" pairs of qubits, in red





Internal couplers per qubit: 16
External couplers per qubit: 2
Odd couplers per qubit: 2

Annealing process

Any optimization problem can be reformulated into the task of **minimizing** a function. In quantum annealing, this function is expressed as a **Hamiltonian**, which represents the total energy of a quantum system.
The **ground state** of this Hamiltonian (its state of lowest energy) encodes the solution to the optimization problem.

This Hamiltonian can be written using **Ising formulation** or **QUBO** (Quadratic unconstrained binary optimization) **formulation**.

Ising formulation

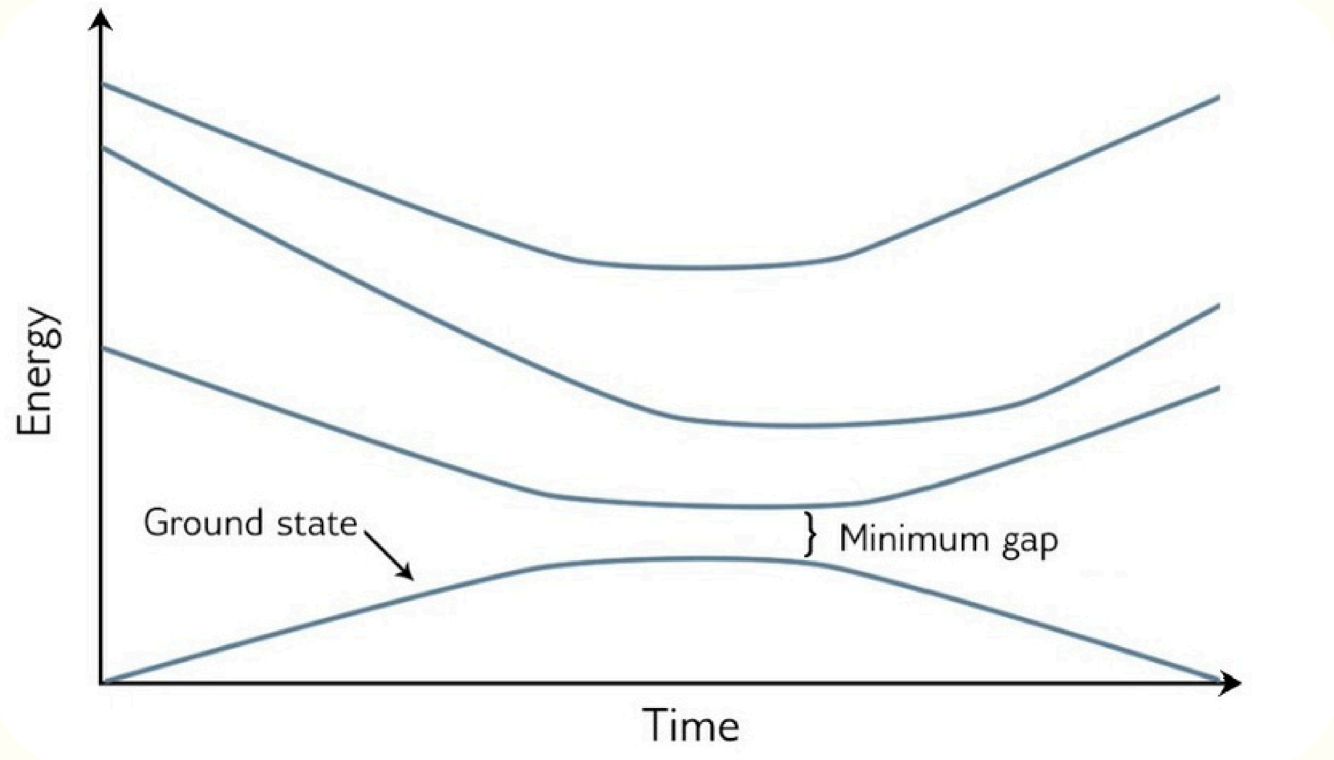
$$H = \Sigma_i h_i s_i + \Sigma_{i<j} J_{i,j} s_i s_j$$

QUBO formulation

$$H = \Sigma_i Q_{i,i} q_i + \Sigma_{i<j} Q_{i,j} q_i q_j$$

Annealing process

Taking advantage of the **quantum adiabatic theorem**, if we can create a system in the ground state of a specific Hamiltonian, we can transform it in the **Hamiltonian of our problem** so we will end up in its ground state and find our solutions!

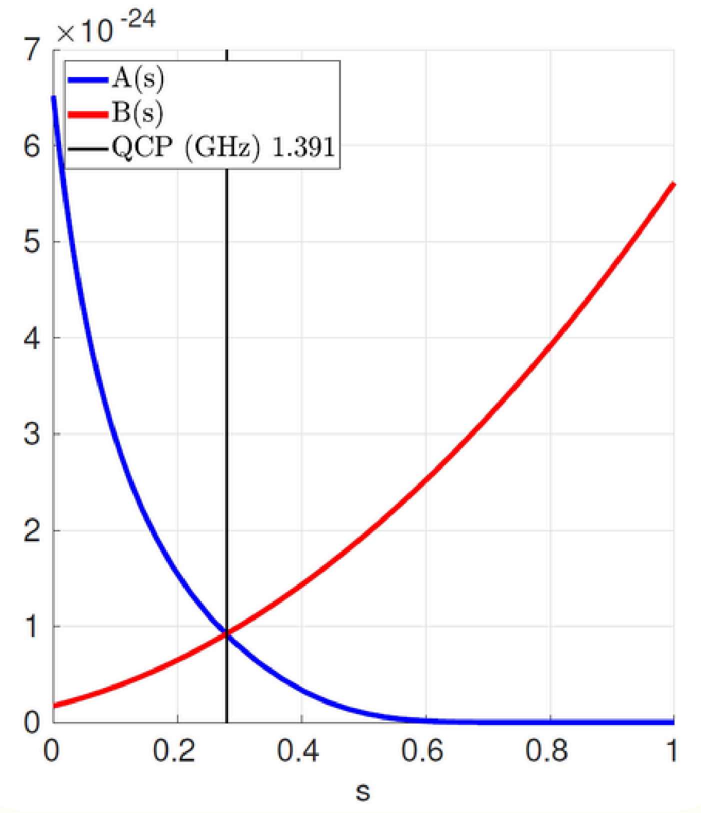


It is possible to set the **annealing time** and the **number of annealing** performed

$$H = A(t)H_{ini} + B(t)H_{fin}$$

$$H_{ini} = \Sigma_i q_i$$

$$H_{fin} = \Sigma_i Q_{i,i} q_i + \Sigma_{i<j} Q_{i,j} q_i q_j$$



Problem formulation

Case study: elbow flexion-extension

The elbow joint primarily involves one degree of freedom, meaning its motion can be described by a **single angular parameter**.
However, this movement is controlled by multiple muscles, in our case we have **three muscles** (1 flexor and 2 extensors).

$$\sum_{i=1}^{3} |B_i(t)||F_i(t)| f(\theta_i)(t) = M(t)$$

$$|B_i(t)| f(\theta_i)(t) = |B_i'(t)|$$

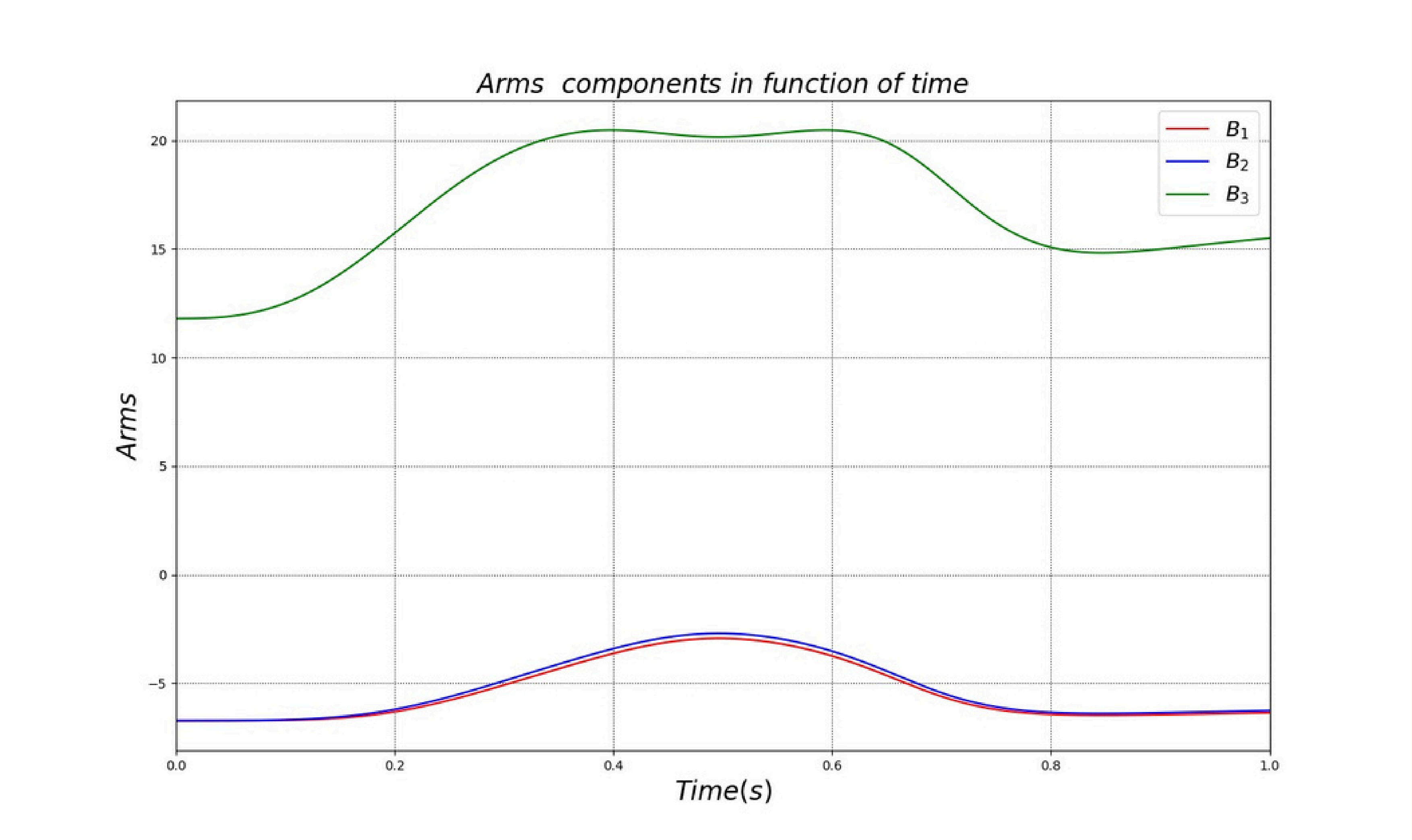
$$act_i(t) \in [0,1] \Rightarrow |F_i(t)| = |F_{i\_max}| act_i(t)$$

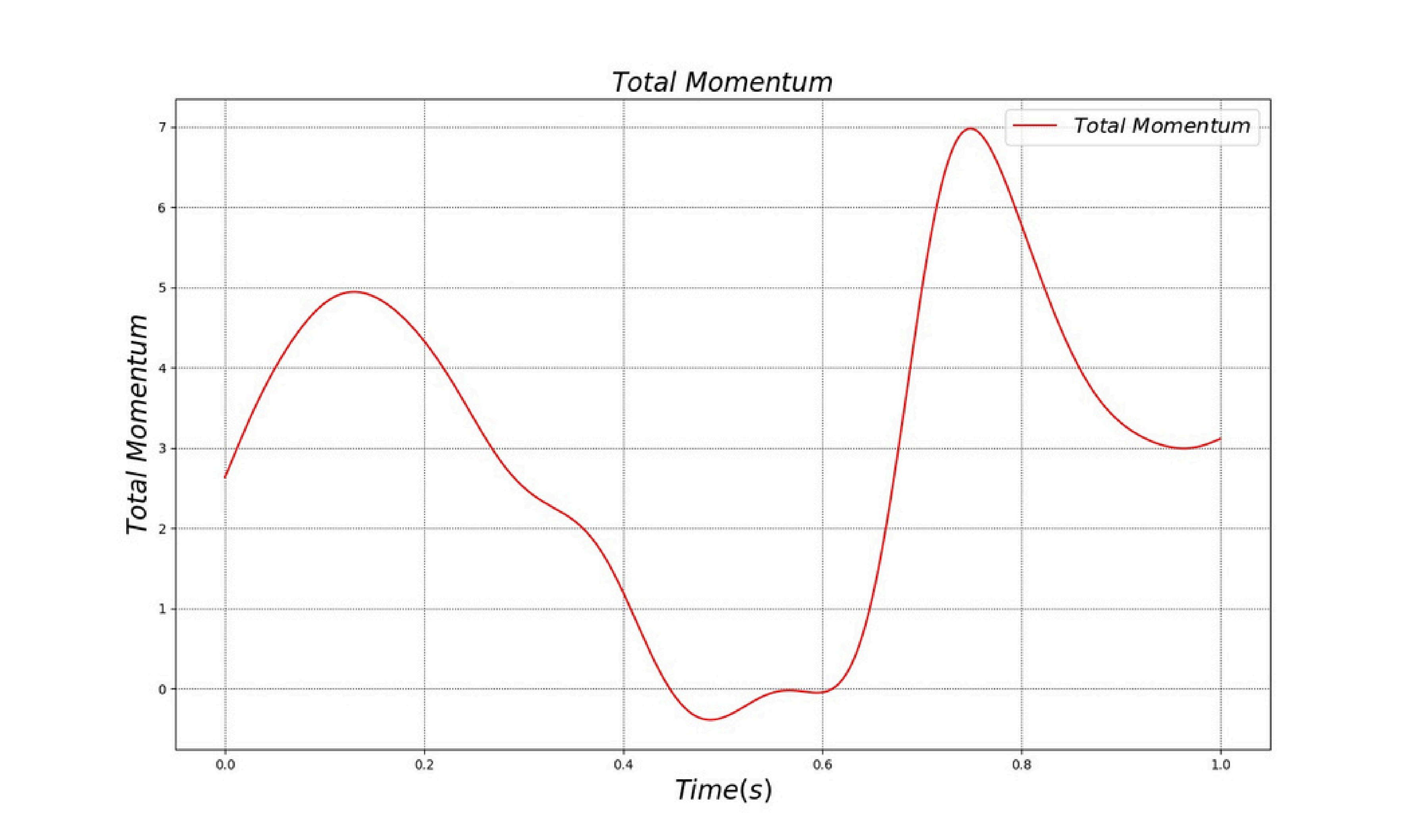
$$\sum_{i=1}^{3} |B_i'(t)||F_{i\_max}| act_i(t) = M(t)$$

Problem formulation

Case study: elbow flexion-extension

At each instant of time we know the value of Momentum, arms components, angles and the maximum force of each muscle. We want to find the activations value of each muscle





Data provided by Istituto Ortopedico Rizzoli

Problem formulation

Case study: elbow flexion-extension

With three muscles controlling one degree of freedom, the system is **redundant**. This means there are **infinitely** many ways to activate the muscles to produce the same net torque at the joint.

We need a criterion to select the **optimal** muscle activation pattern. Typically, this involves minimizing a physiological or biomechanical cost function. A common approach is to minimize the squared activations sum

$$min(\sum_{i=1}^{3} act_i^2)$$

Problem formulation

Case study: elbow flexion-extension

As we already said, we want to formulate the problem such that the optimal solution is associated with the minimun of the Hamiltonian, thus we have to rewrite the first equation as a function with the solutions in the minima:

$$\sum_{i=1}^{3} |B_i'(t)||F_{i\_max}|act_i(t) = M(t)$$

$$min\left(\sum_{i=1}^{3} |B_i'(t)||F_{i\_max}|act_i(t) - M(t)\right)^2$$

$$min(\sum_{i=1}^{3} act_i^2)$$

$$|B_i'(t)||F_{i\_max}| = |A_i(t)|$$

$$min\left(\sum_{i=1}^{3} |A_i(t)|act_i(t) - M(t)\right)^2$$

Problem formulation

Case study: elbow flexion-extension

Putting everything together:

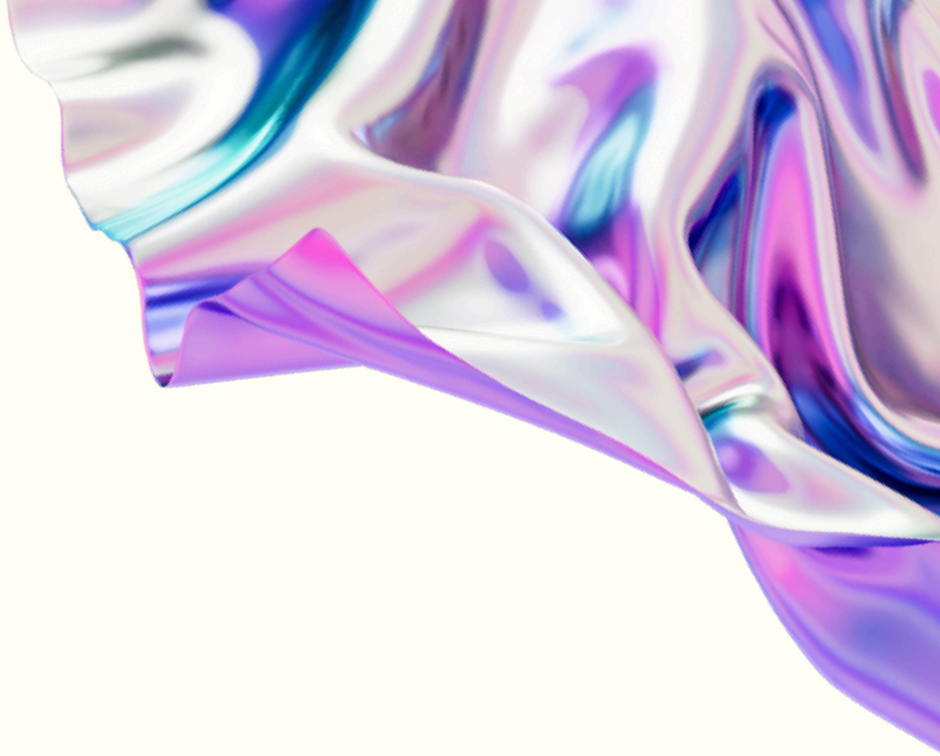
$$min\left[\left(\sum_{i=1}^{3}|A_i\left(t\right)|act_i\left(t\right)-M\left(t\right)\right)^2+\sum_{i=1}^{3}act_i^2\right]$$

so our Hamiltonian is:

$$H=\left[\left(\sum_{i=1}^{3}|A_i\left(t\right)|act_i\left(t\right)-M\left(t\right)\right)^2+\sum_{i=1}^{3}act_i^2\right]$$

But this is not the end of the story, we have to find the QUBO matrix to write it in the form:

$$H=\Sigma_i Q_{i,i}q_i+\Sigma_{i<j}Q_{i,j}q_iq_j$$



Problem formulation

Case study: elbow flexion-extension

To encode the activations we used a simple binary encoding:

$$act = s_i \sum_{i=1}^{n} (\frac{q_i}{2^i}) \quad \text{with} \quad q_i \in \{0, 1\} \quad \text{and} \quad s_i \quad \text{is a scaling factor}$$

Using 3 qubits we have

$$act_i = s_i(\frac{q_{3i-2}}{2} + \frac{q_{3i-1}}{4} + \frac{q_{3i}}{8})$$

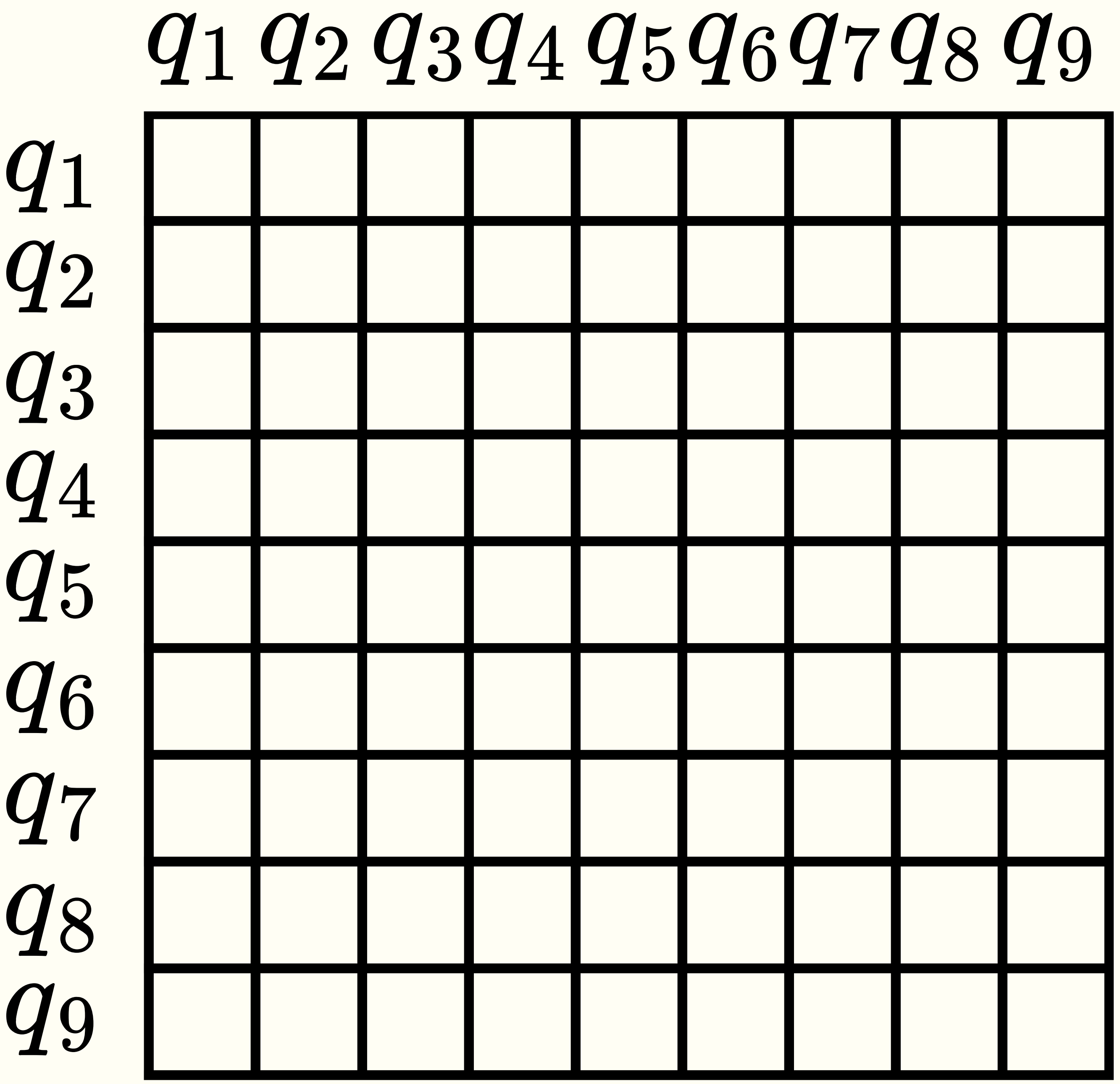
and substituting in the Hamiltonian

$$H = \left[\left(\sum_{i=1}^{3} |A_i\,(t)| s_i (\frac{q_{3i-2}}{2} + \frac{q_{3i-1}}{4} + \frac{q_{3i}}{8}) - M\,(t) \right)^2 + \sum_{i=1}^{3} \left[s_i (\frac{q_{3i-2}}{2} + \frac{q_{3i-1}}{4} + \frac{q_{3i}}{8}) \right]^2 \right]$$

Problem formulation

Case study: elbow flexion-extension

$$H = \left[\left(\sum_{i=1}^{3} |A_i(t)| s_i\left(\frac{q_{3i-2}}{2} + \frac{q_{3i-1}}{4} + \frac{q_{3i}}{8}\right) - M(t) \right)^2 + \sum_{i=1}^{3} \left[s_i\left(\frac{q_{3i-2}}{2} + \frac{q_{3i-1}}{4} + \frac{q_{3i}}{8}\right) \right]^2 \right]$$

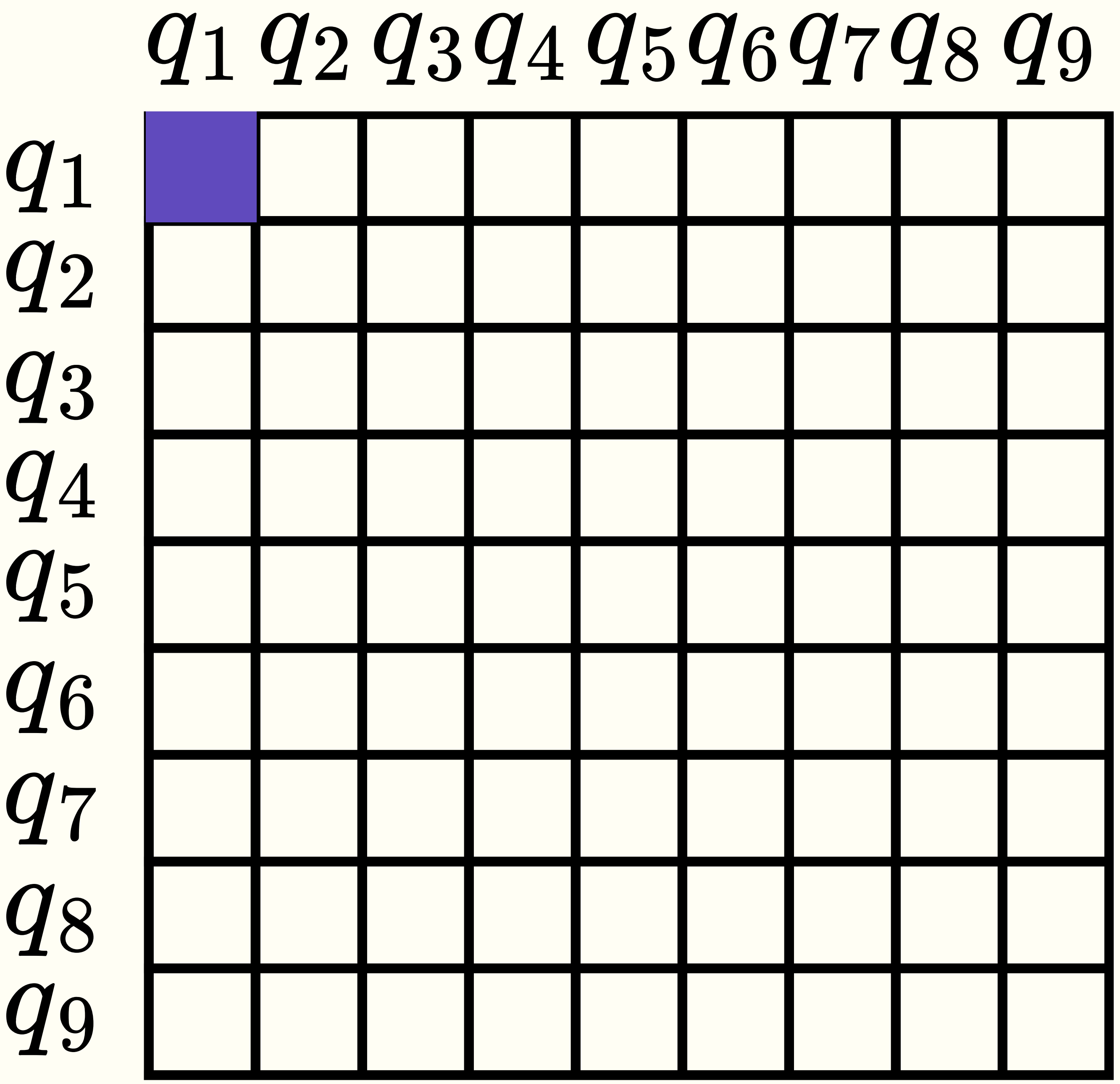


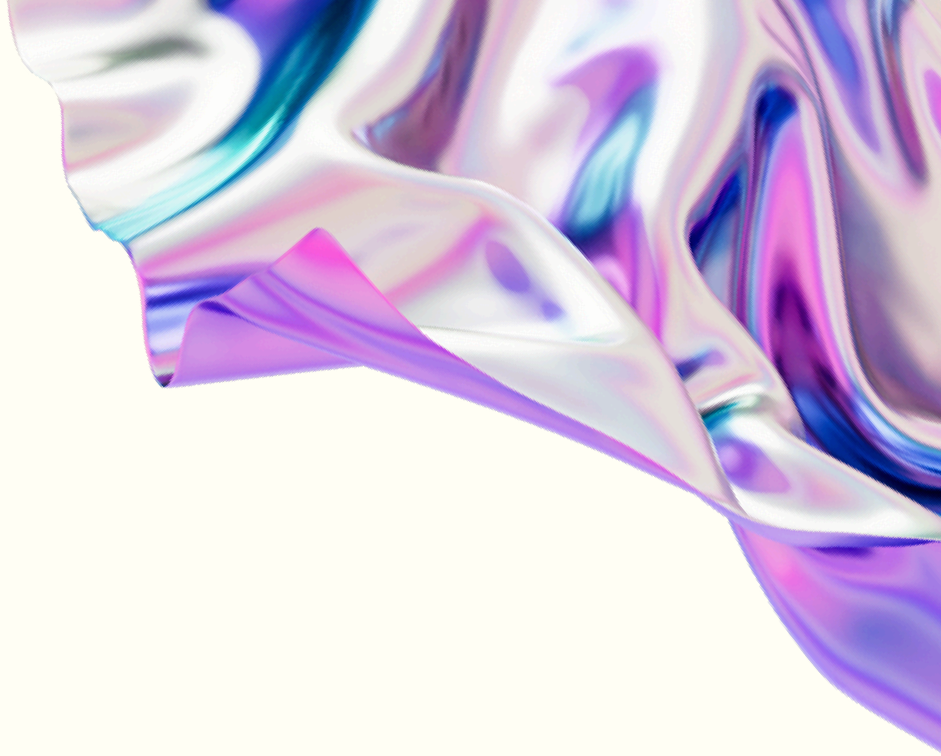
Problem formulation

Case study: elbow flexion-extension

$$H=\left[\left(\sum_{i=1}^{3}\left|A_i\left(t\right)\right|s_i\left(\frac{q_{3i-2}}{2}+\frac{q_{3i-1}}{4}+\frac{q_{3i}}{8}\right)-M\left(t\right)\right)^2+\sum_{i=1}^{3}\left[s_i\left(\frac{q_{3i-2}}{2}+\frac{q_{3i-1}}{4}+\frac{q_{3i}}{8}\right)\right]^2\right]$$

$$q_1\left[A_1^2\left(t\right)s_i^2\left(\frac{1}{4}\right)-2\left|A_1\left(t\right)\right|s_iM\left(t\right)\left(\frac{1}{2}\right)+s_i^2\frac{1}{4}\right]$$



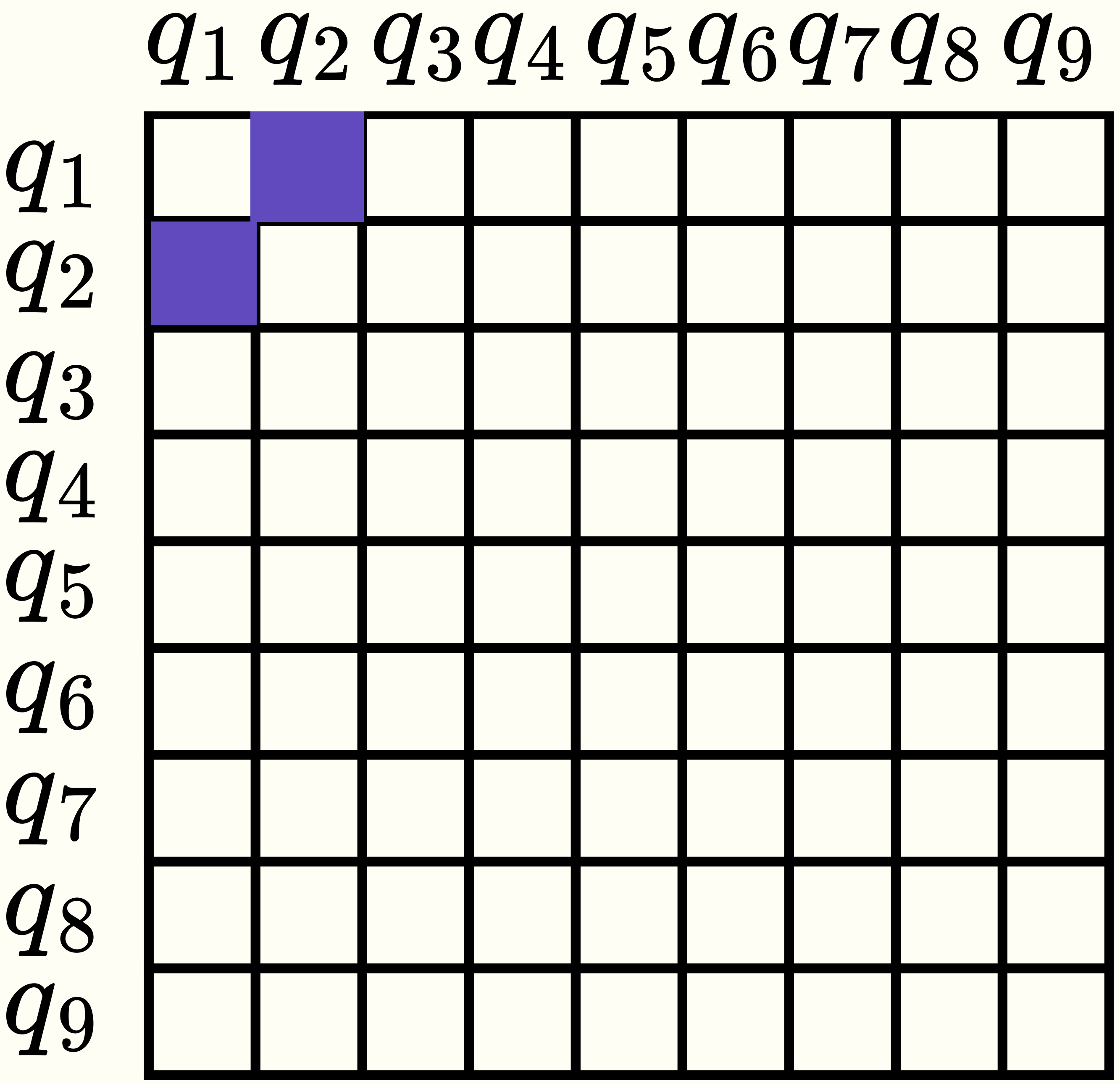


Problem formulation

Case study: elbow flexion-extension

$$H = \left[\left(\sum_{i=1}^{3} |A_i(t)| s_i\left(\frac{q_{3i-2}}{2} + \frac{q_{3i-1}}{4} + \frac{q_{3i}}{8}\right) - M(t)\right)^2 + \sum_{i=1}^{3}\left[s_i\left(\frac{q_{3i-2}}{2} + \frac{q_{3i-1}}{4} + \frac{q_{3i}}{8}\right)\right]^2\right]$$

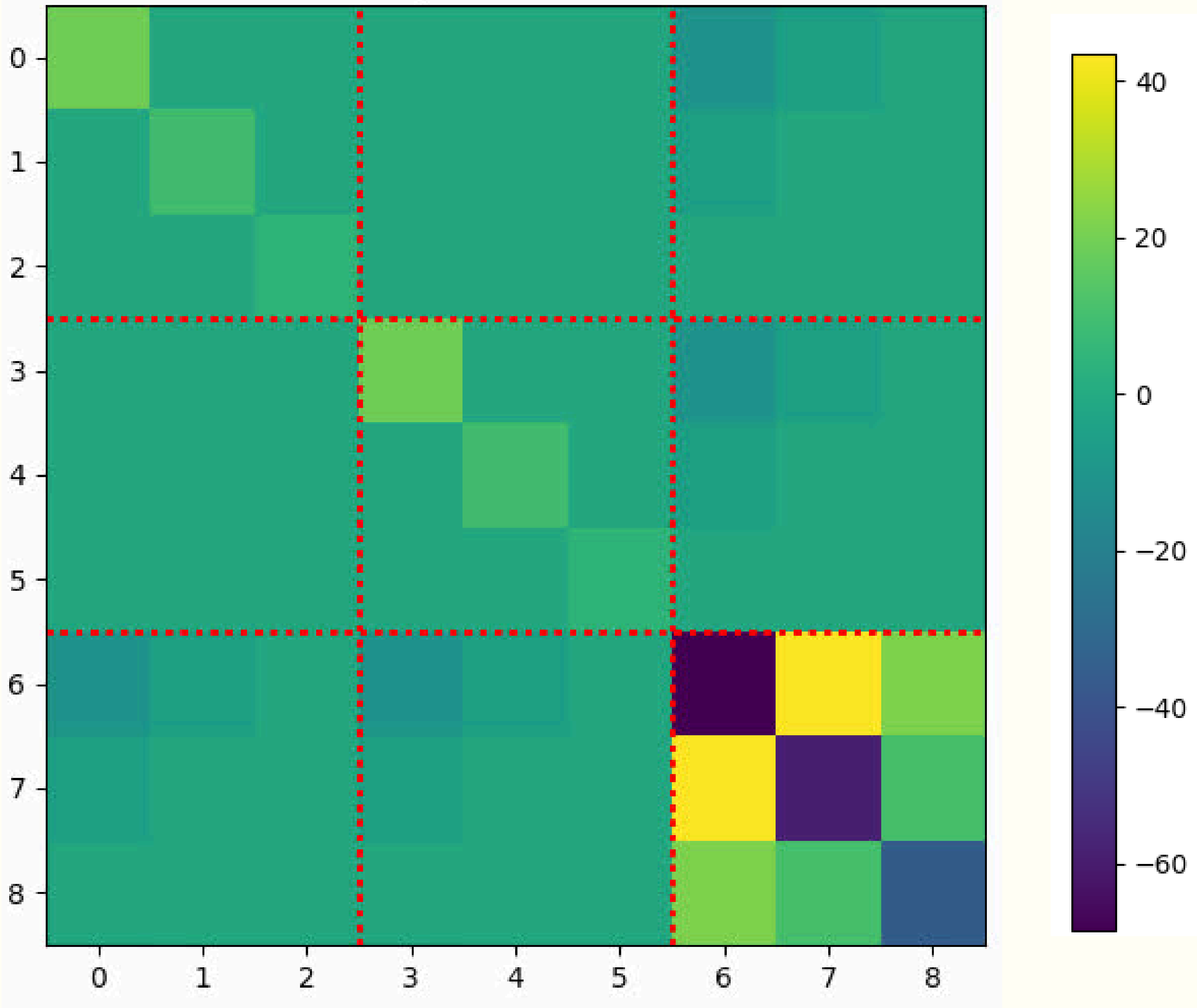
$$q_1 q_2 \left[2A_1^2(t) s_i^2 \left(\frac{1}{2} \times \frac{1}{4}\right) + 2 s_i^2 \left(\frac{1}{2} \times \frac{1}{4}\right)\right]$$



Problem formulation

Case study: elbow flexion-extension

QUBO matrix

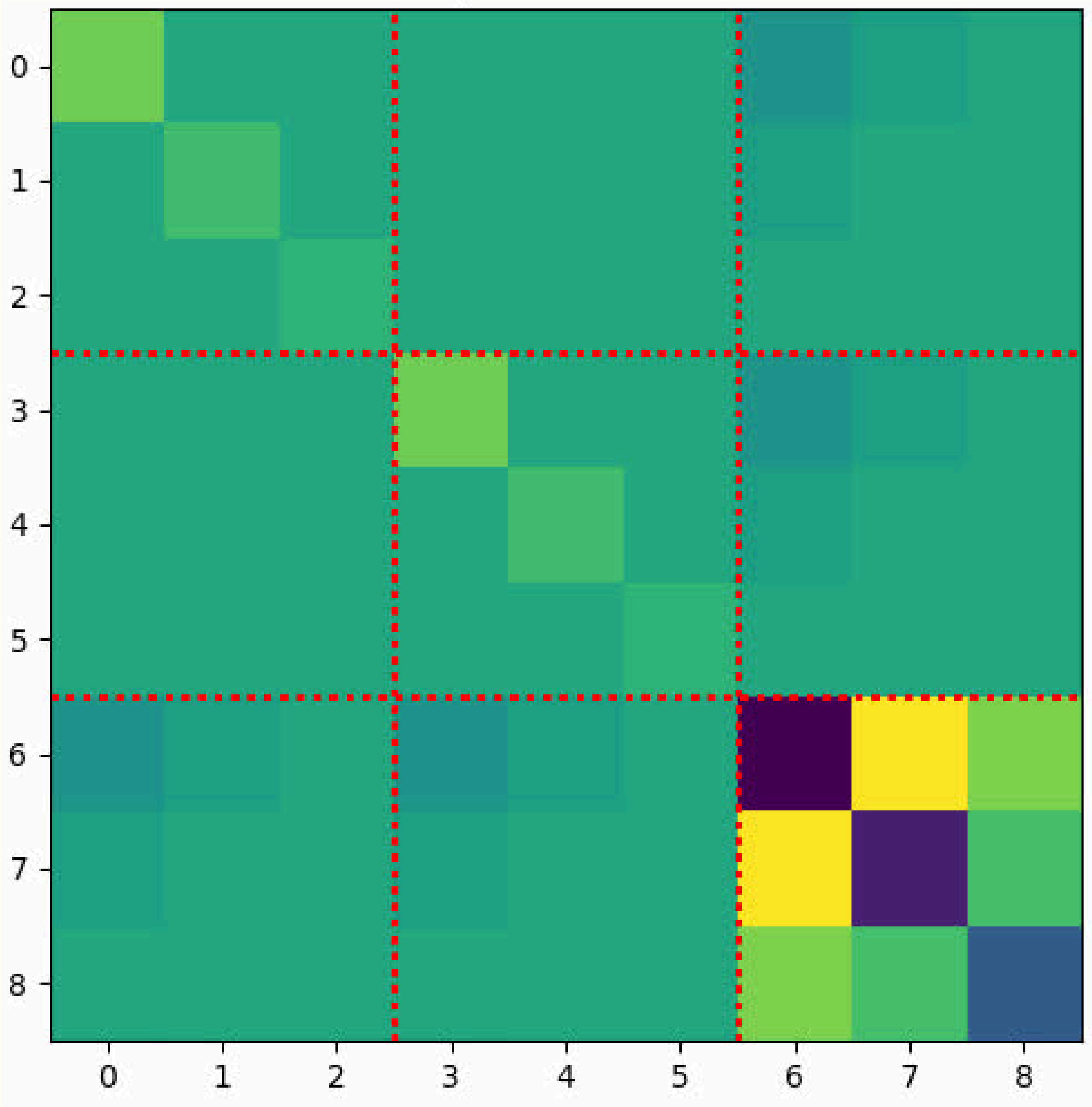


Problem formulation

Case study: elbow flexion-extension

We have a **symmetric sparse** matrix that can be decpomosed in a 3x3 block matrix.
Each block along the main diagonal is related with an activation while the off-diagonal block encode the information about **interaction** of different activations.

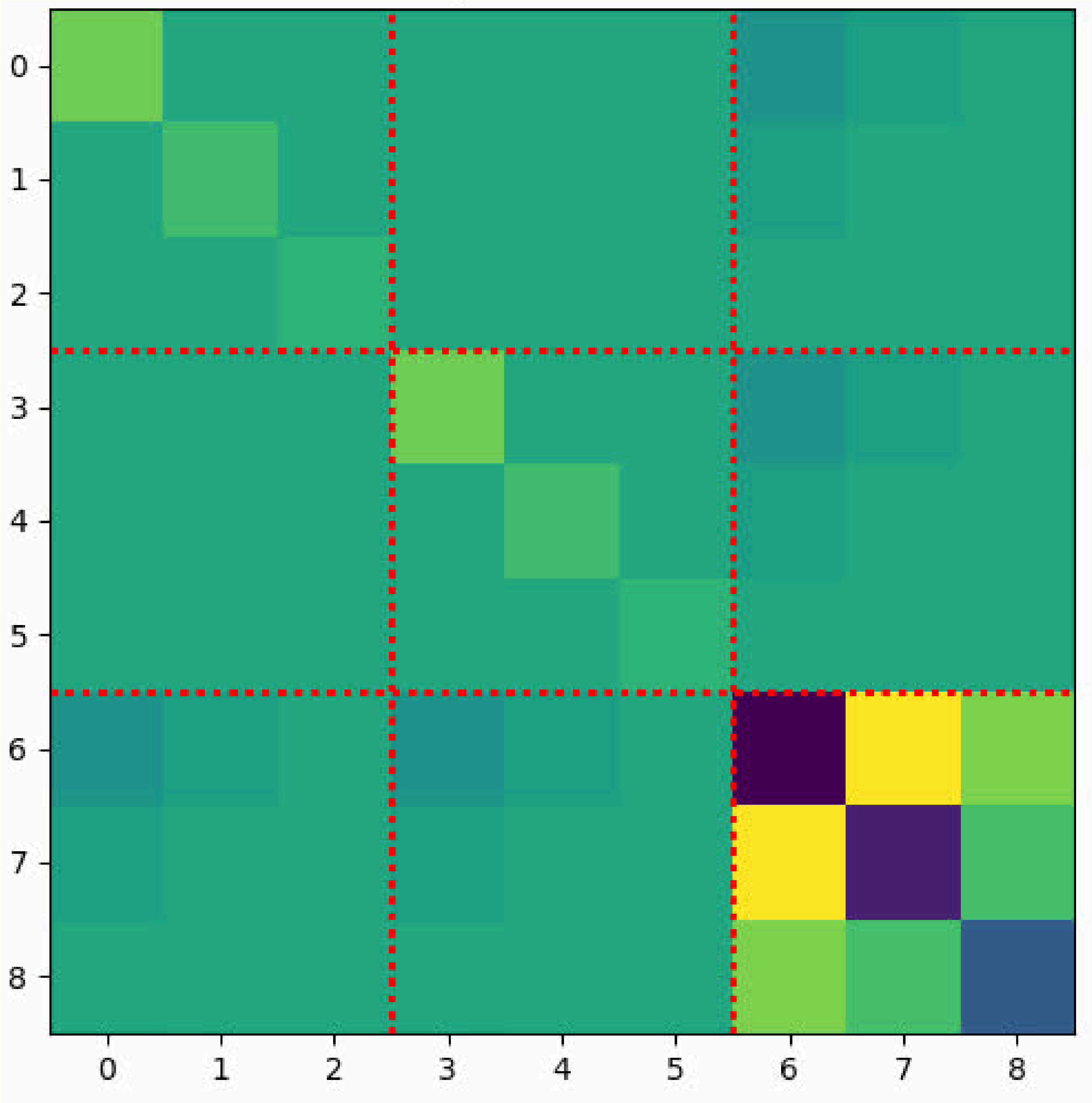
QUBO matrix



Problem formulation

Case study: elbow flexion-extension

QUBO matrix

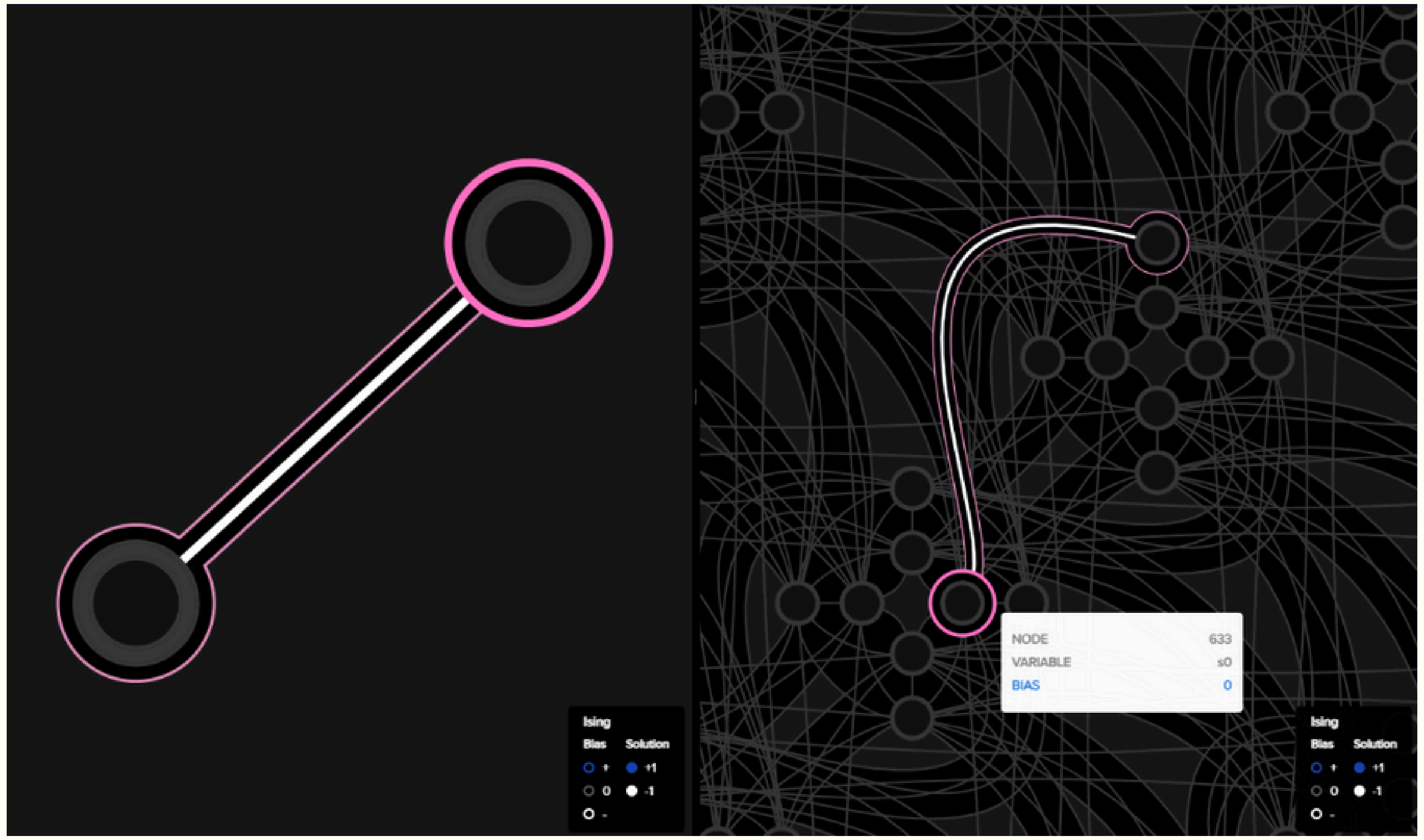


We can see the QUBO matrix as an **Adjiacency Matrix** of an undirected weighted graph. Each qubit is a node and the value in the cell i-j is the weight of the link between the qubit-i and qubit-j.
To apply the quantum annealing we have to map our graph in the **QPU topology** performing an **embedding**.

Problem embedding

Case study: elbow flexion-extension

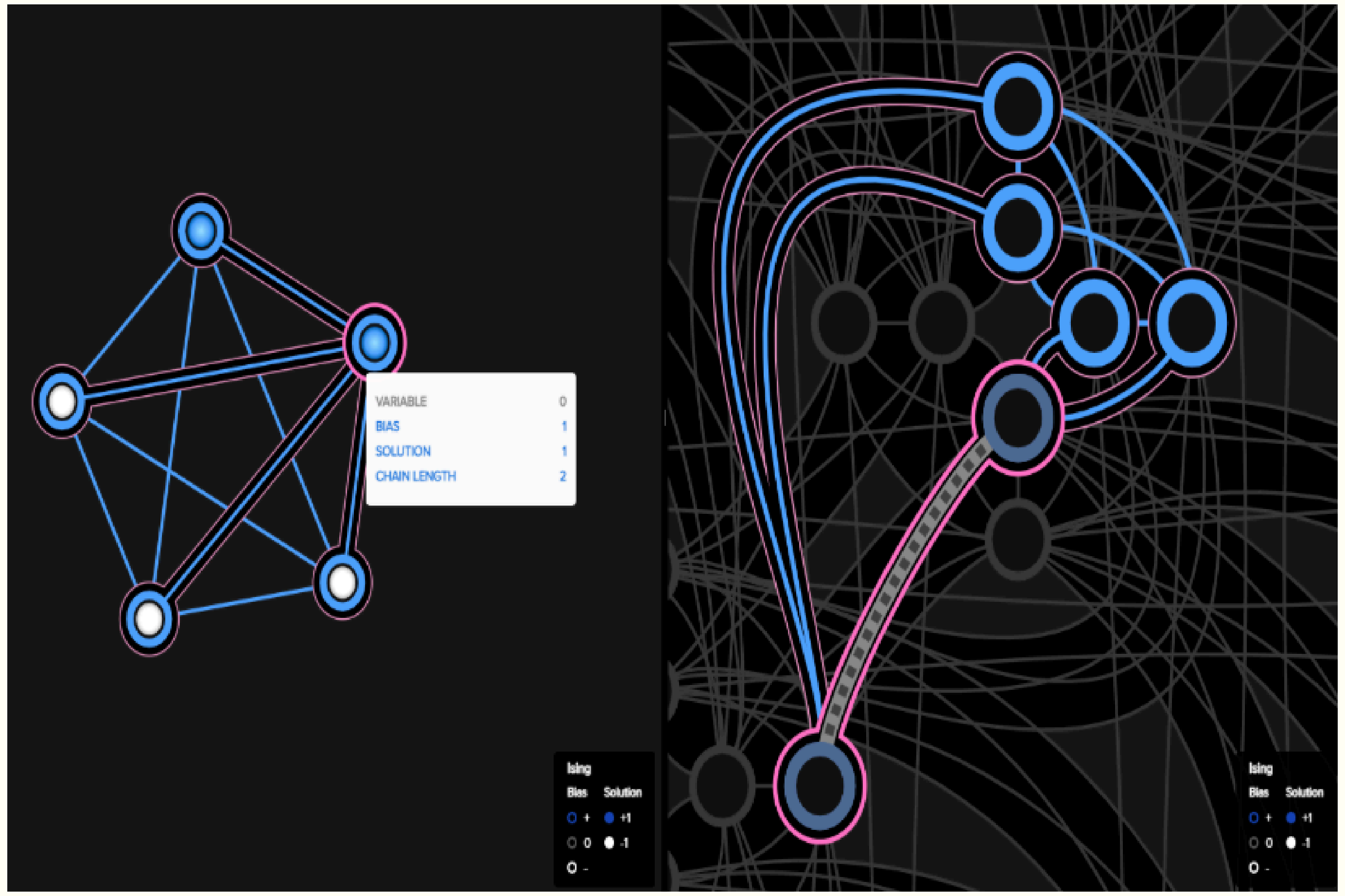
If we have only two qubits:



Problem embedding

Case study: elbow flexion-extension

Larger problems often require **chains** because the QPU topology is not fully connected.



On the left we have the **logical** qubits and on the right the **physical** qubits

Annealing process

To perform the annealing you can use the simulator installing D-wave ocean sdk

```
pip install dwave-ocean-sdk
```

```
import dimod
import neal

sampler = neal.SimulatedAnnealingSampler()
bqm = dimod.BinaryQuadraticModel.from_qubo(matrix)
Q = (bqm.to_qubo())[0]
results = sampler.sample_qubo(Q, num_reads=1000)
```

Annealing process

D-wave provides also cloud-based quantum computing platform named **Leap.**

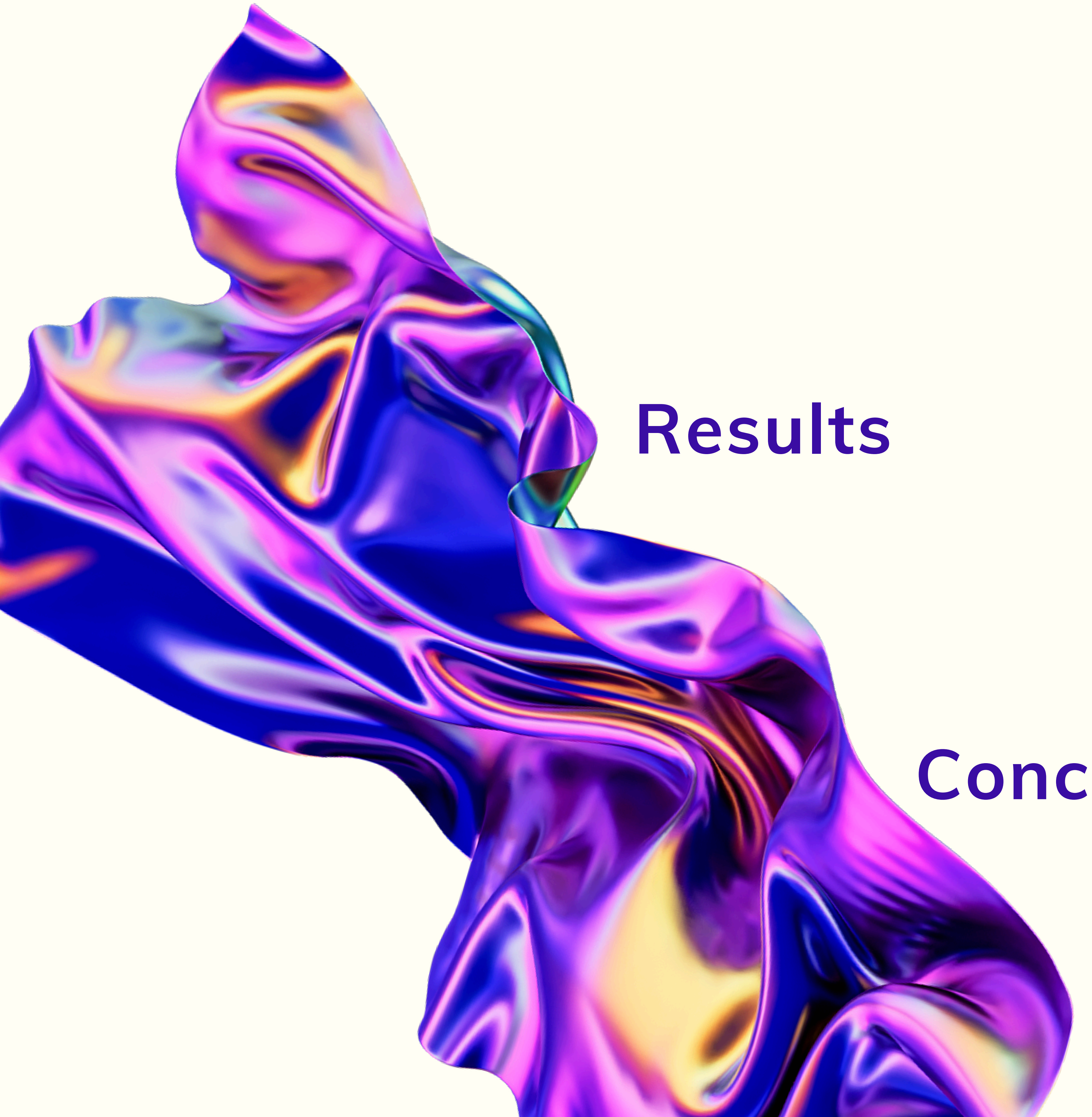
- Go to: D-Wave Leap
- Sign up for an account (you get for free one minute of quantum processing time every month).
- Once logged in, go to "My Account" > "Token" to find your API token.

```
import dwave.cloud
from dwave.system import DWaveSampler, EmbeddingComposite
from dimod import BinaryQuadraticModel


dwave.cloud.config.save_config(profile='dwave', token="YOUR-LEAP-API-TOKEN")


bqm = BinaryQuadraticModel.from_qubo(matrix)
sampler = EmbeddingComposite(DWaveSampler())
results = sampler.sample(bqm, num_reads=1000)
```

PART 3



Results

Conclusions

Results

Number of qubits per activations:3

TIME INSTANT	BITSTRING SOLUTION	ENERGY	NUM OCCURRENCES
57	(0, 1, 0, 0, 0, 1, 1, 0, 1)	-119.894	57
57	(0, 0, 1, 0, 1, 0, 1, 0, 1)	-119.894	62
57	(0, 1, 1, 0, 0, 0, 1, 0, 1)	-119.894	46
57	(0, 0, 0, 0, 1, 1, 1, 0, 1)	-119.894	56
57	(0, 0, 1, 0, 0, 1, 1, 0, 1)	-119.861	7
57	(0, 0, 0, 0, 1, 0, 1, 0, 1)	-119.861	4
57	(0, 1, 0, 0, 0, 0, 1, 0, 1)	-119.861	6

Results

Number of qubits per activations:3

TIME INSTANT	BITSTRING SOLUTION	ENERGY	NUM OCCURRENCES
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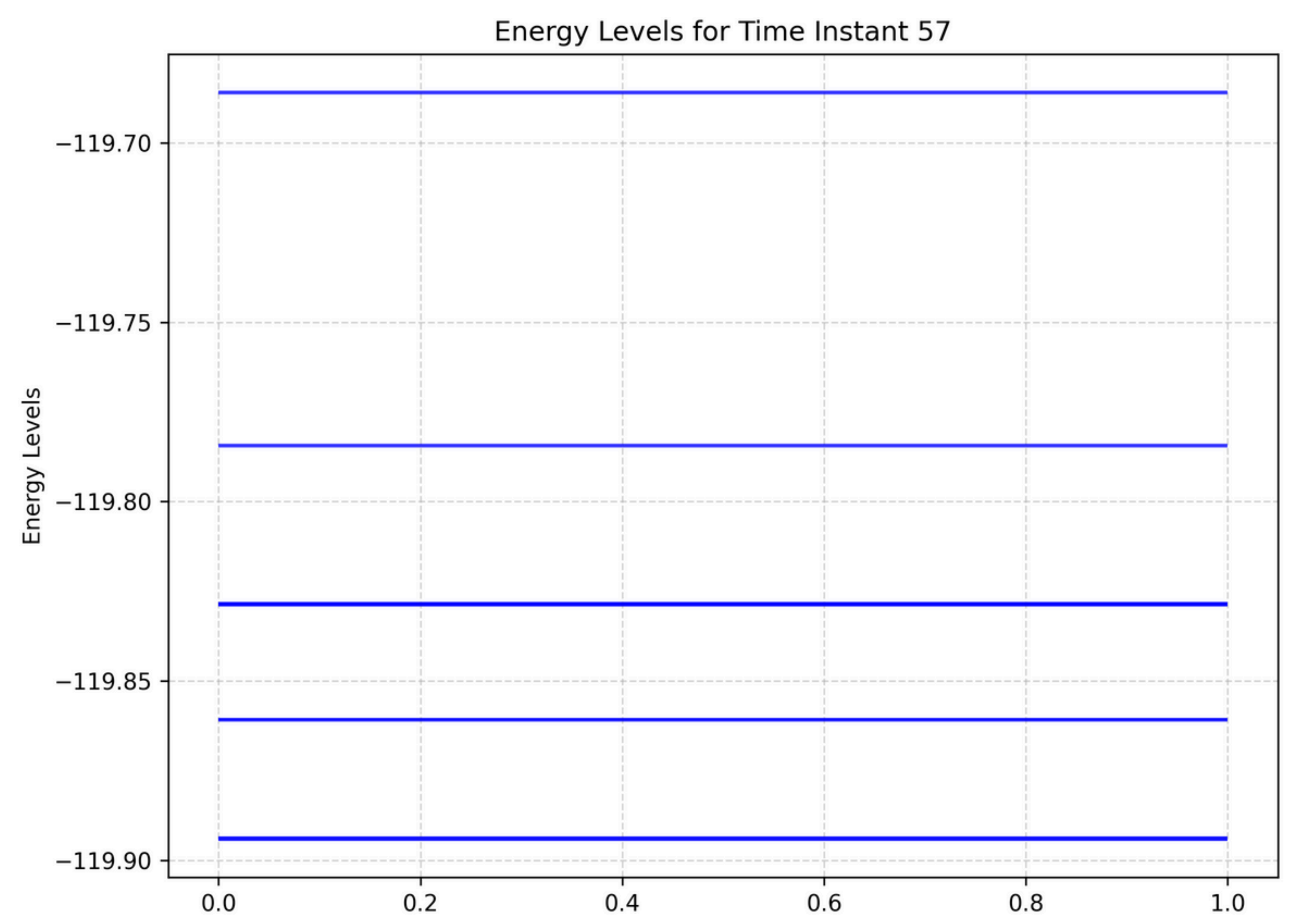
57	(0, 0, 0, 0, 1, 1, 1, 0, 1)	-119.894	56
57	(0, 0, 1, 0, 0, 1, 1, 0, 1)	-119.861	7
57	(0, 0, 0, 0, 1, 0, 1, 0, 1)	-119.861	4
57	(0, 1, 0, 0, 0, 0, 1, 0, 1)	-119.861	6



Results

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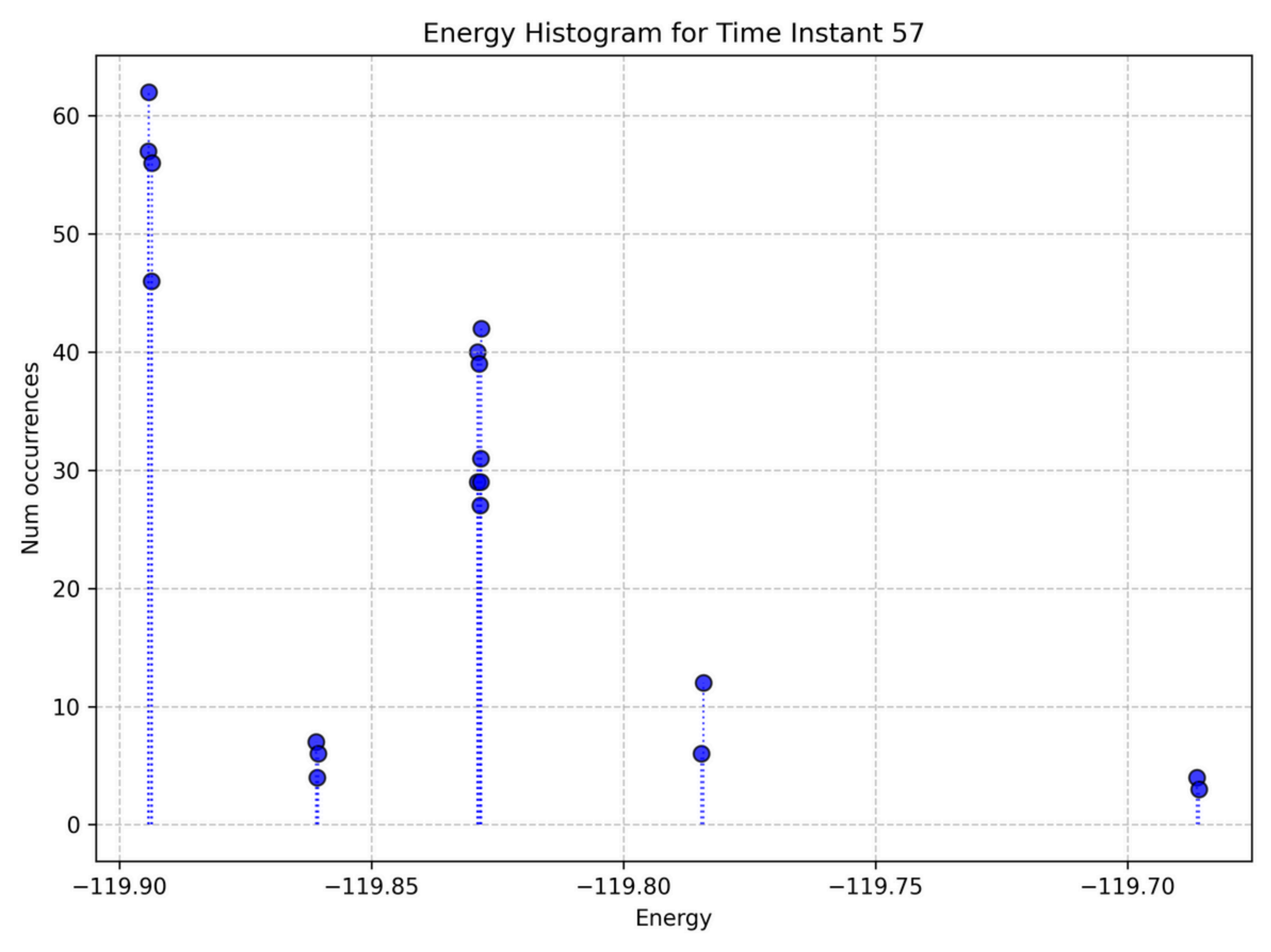
57	(0, 0, 1, 0, 1, 0, 1, 0, 1)	-119.894	62
57	(0, 1, 1, 0, 0, 0, 1, 0, 1)	-119.894	46
57	(0, 0, 0, 0, 1, 1, 1, 0, 1)	-119.894	56
57	(0, 0, 1, 0, 0, 1, 1, 0, 1)	-119.861	7
57	(0, 0, 0, 0, 1, 0, 1, 0, 1)	-119.861	4
57	(0, 1, 0, 0, 0, 0, 1, 0, 1)	-119.861	6



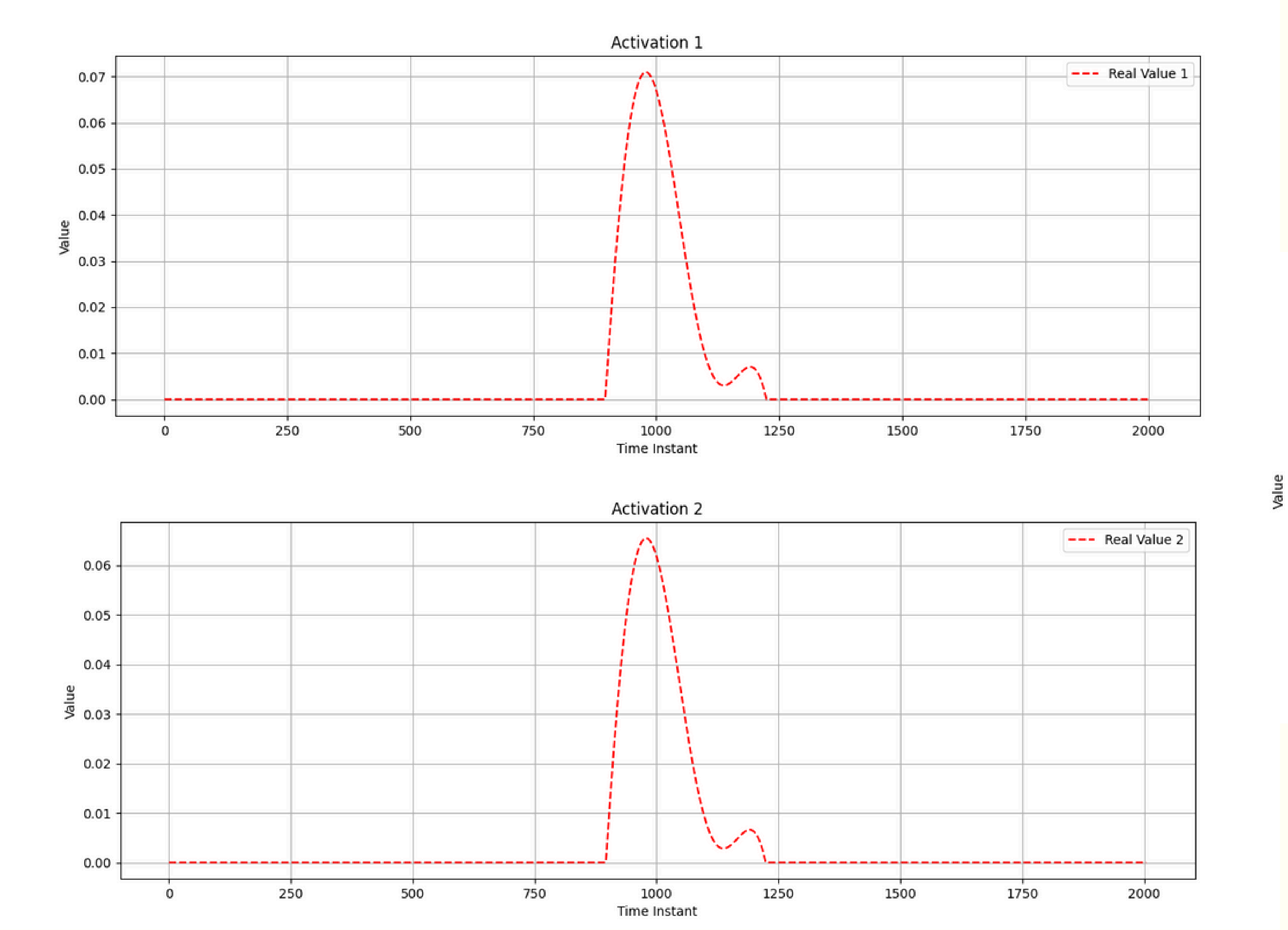
Results

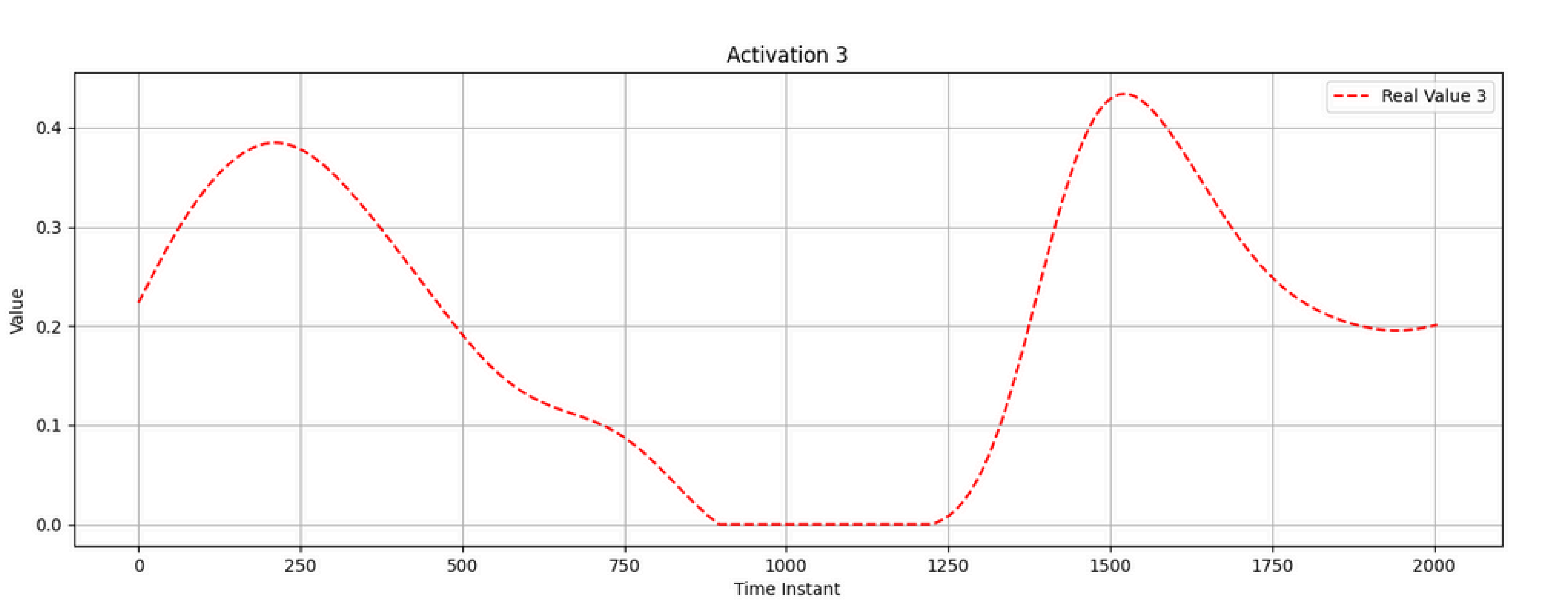
Number of qubits per activations:3

TIME INSTANT	BITSTRING SOLUTION	ENERGY	NUM OCCURRENCES
57	(0, 1, 0, 0, 0, 1, 1, 0, 1)	-119.894	57
57	(0, 0, 1, 0, 1, 0, 1, 0, 1)	-119.894	62
57	(0, 1, 1, 0, 0, 0, 1, 0, 1)	-119.894	46
57	(0, 0, 0, 0, 1, 1, 1, 0, 1)	-119.894	56
57	(0, 0, 1, 0, 0, 1, 1, 0, 1)	-119.861	7
57	(0, 0, 0, 0, 1, 0, 1, 0, 1)	-119.861	4
57	(0, 1, 0, 0, 0, 0, 1, 0, 1)	-119.861	6

$$act_i = s_i\left(\frac{q_{3i-2}}{2} + \frac{q_{3i-1}}{4} + \frac{q_{3i}}{8}\right)$$

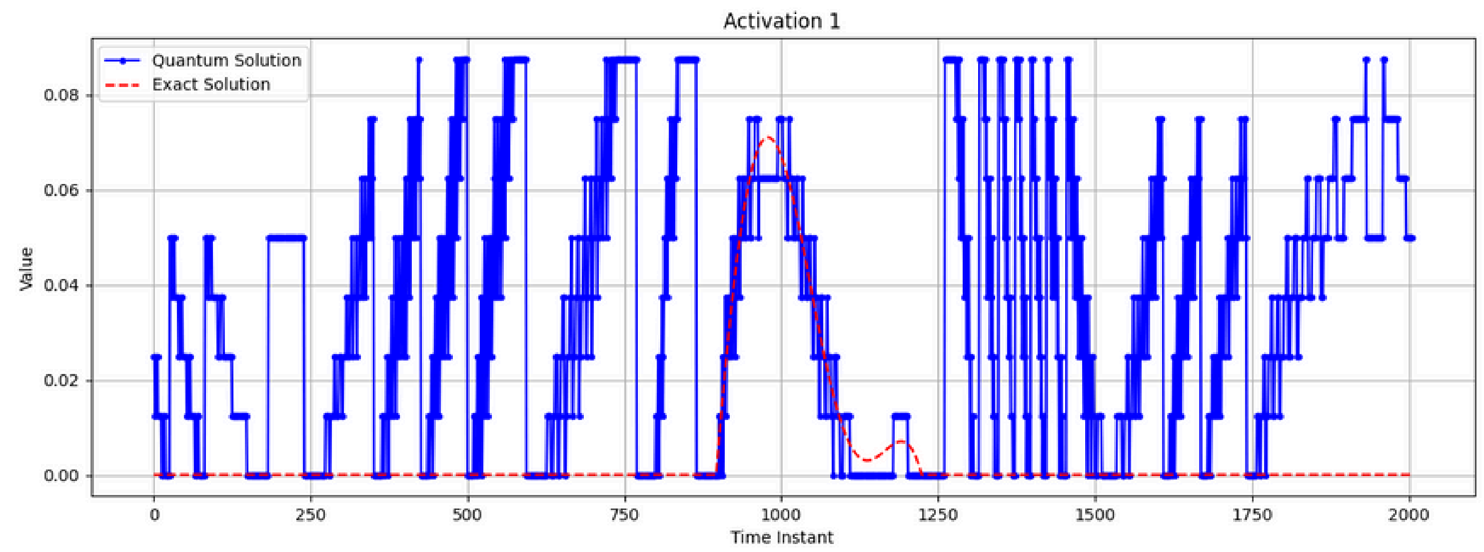
Results

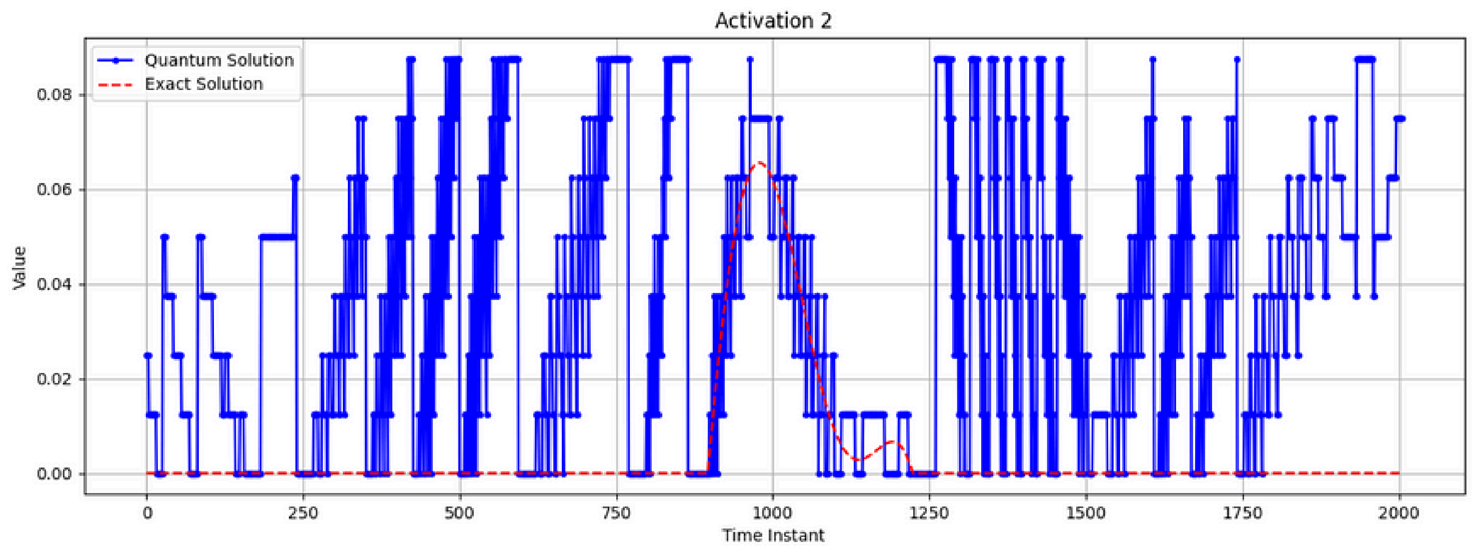

Activation 1
Real Value 1
Value
Time Instant
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
0
250
500
750
1000
1250
1500
1750
2000
Activation 2
Real Value 2
Value
Time Instant
0.06
0.05
0.04
0.03
0.02
0.01
0.00
0
250
500
750
1000
1250
1500
1750
2000

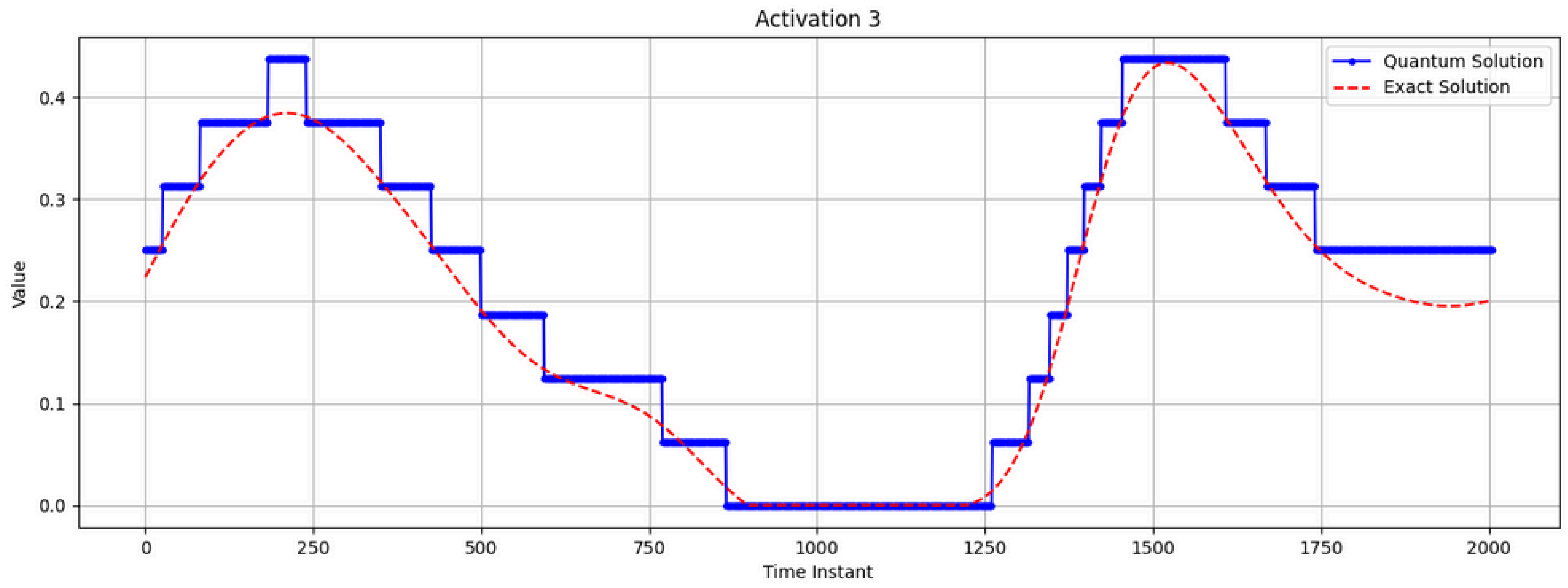

Activation 3
Real Value 3
Value
Time Instant
0.4
0.3
0.2
0.1
0.0
0
250
500
750
1000
1250
1500
1750
2000

Results

Number of qubits per activation: 3



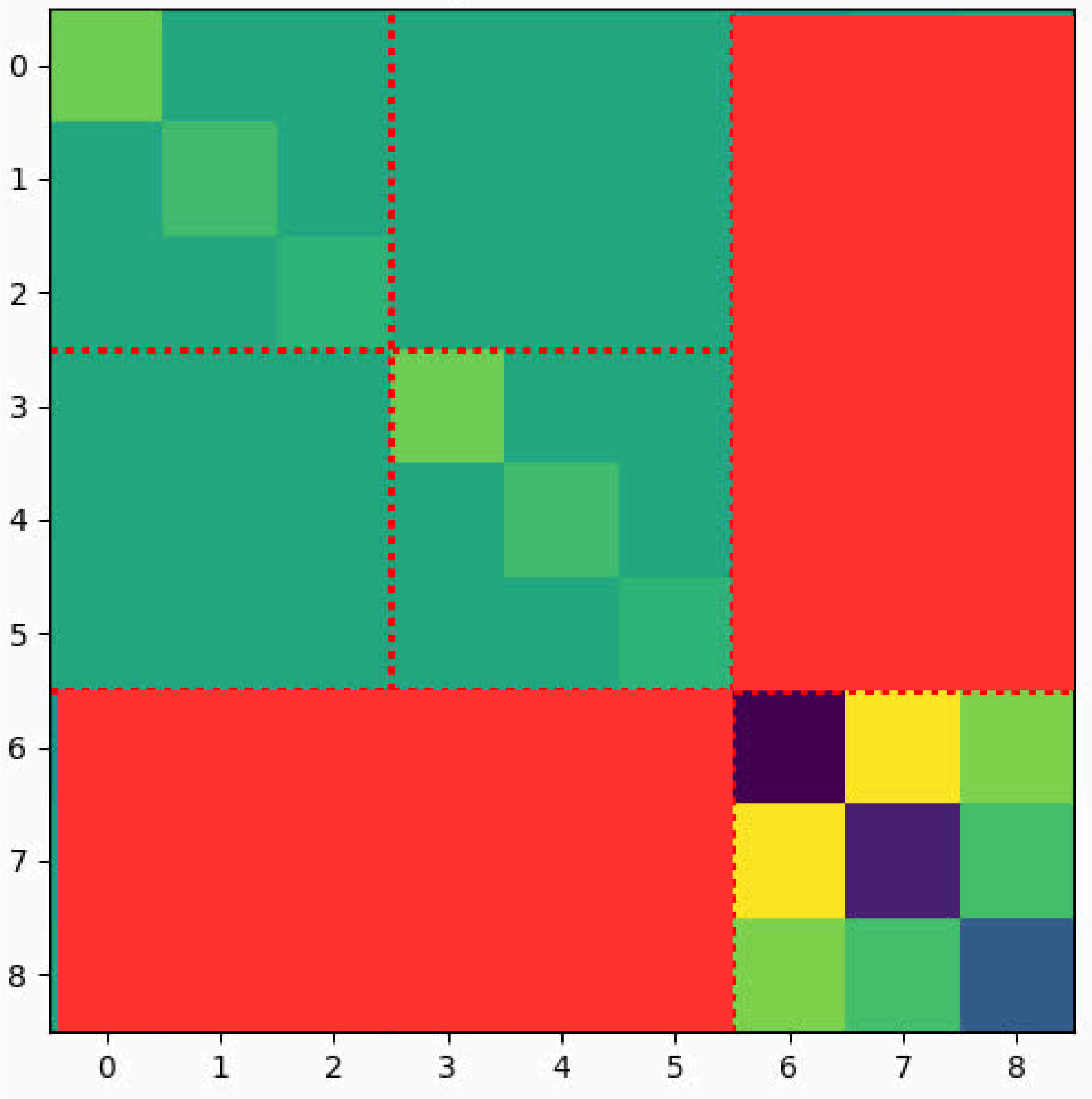




Results

Decoupling antagonists muscles

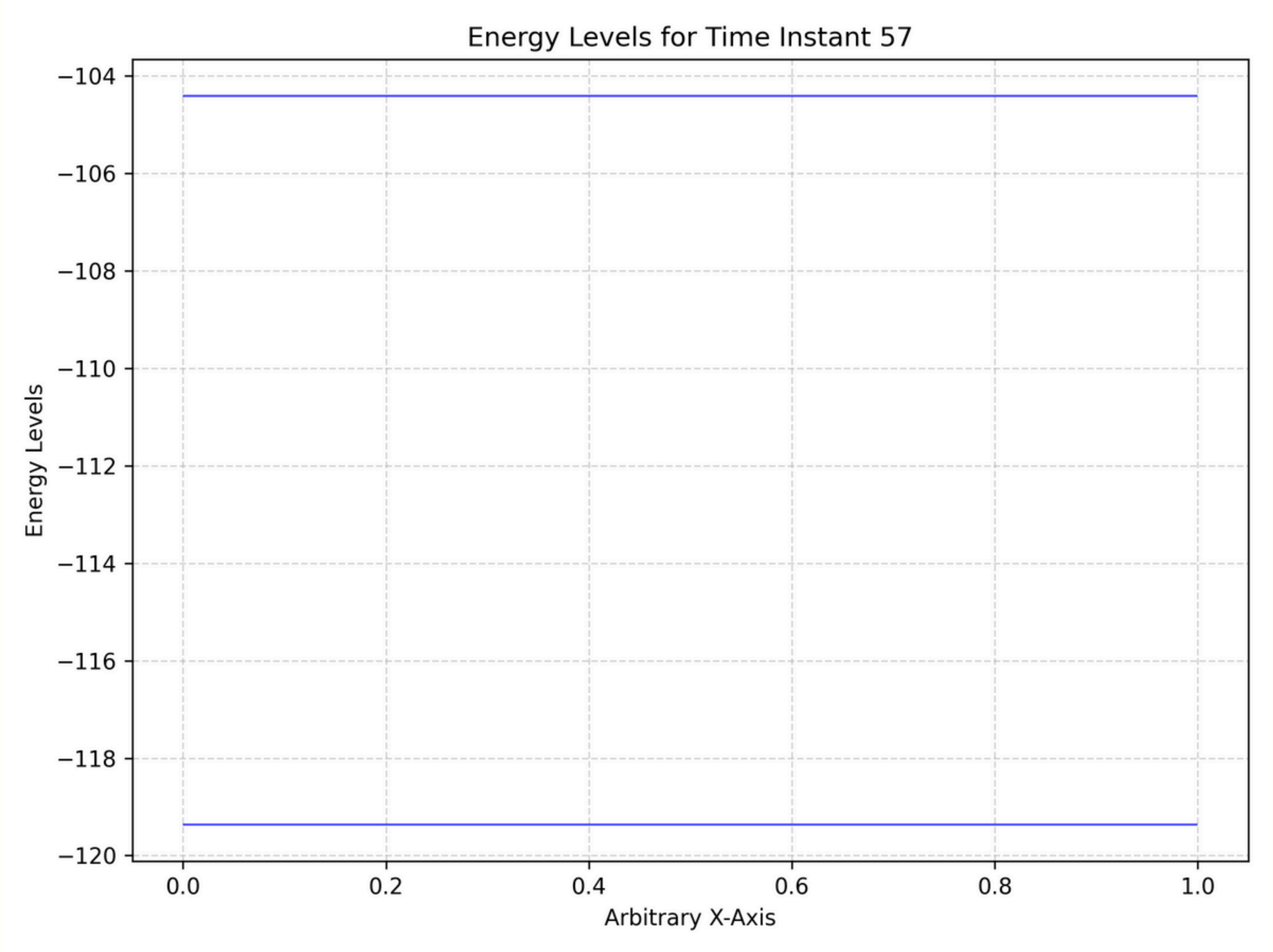
QUBO matrix

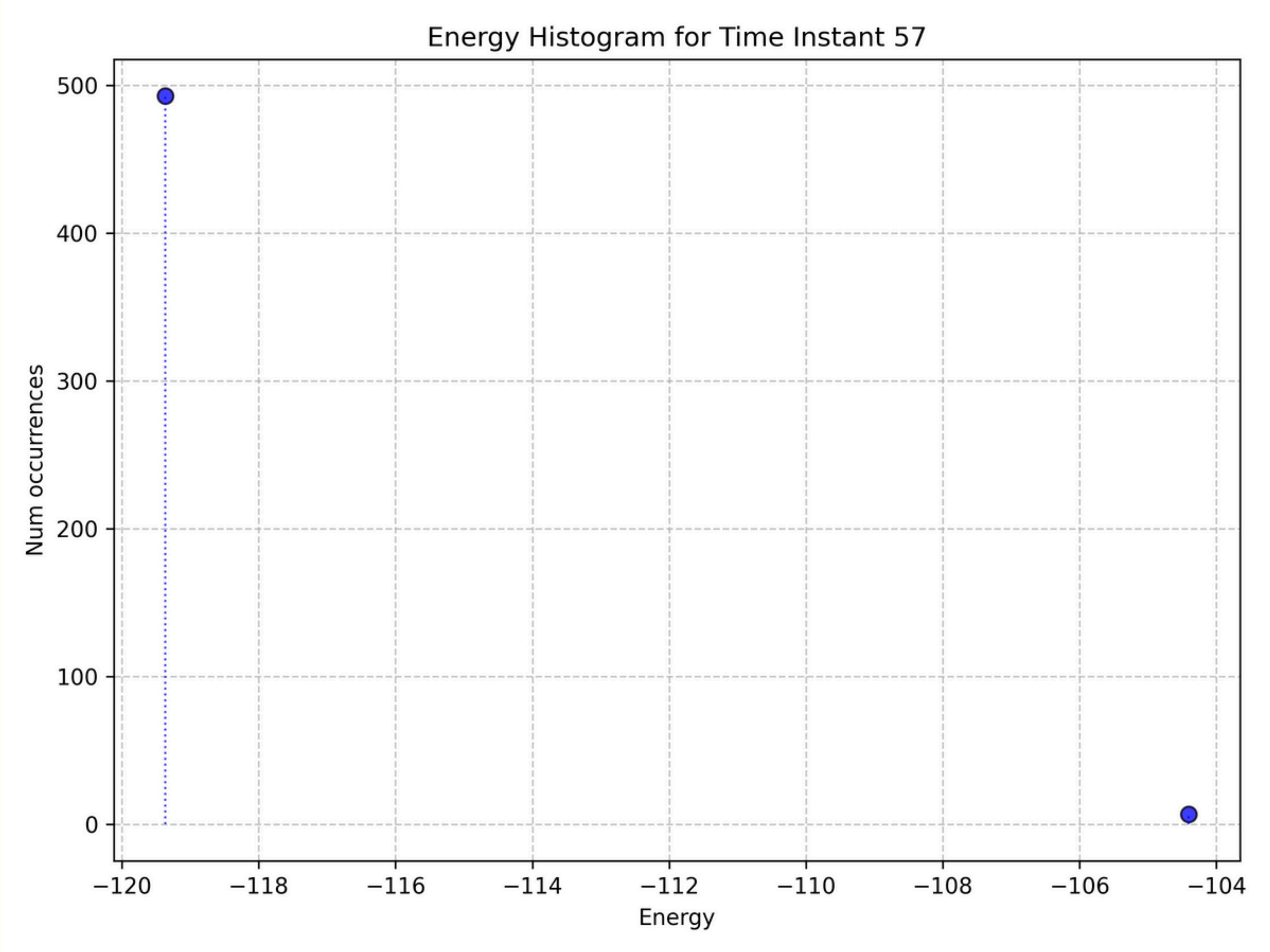


The highlighted blocks encode the interaction between flexor and extensors. We know that they are **antagonists** muscles so don't act in the same moment. They can be **decoupled** setting every entries equal to zero.

Results

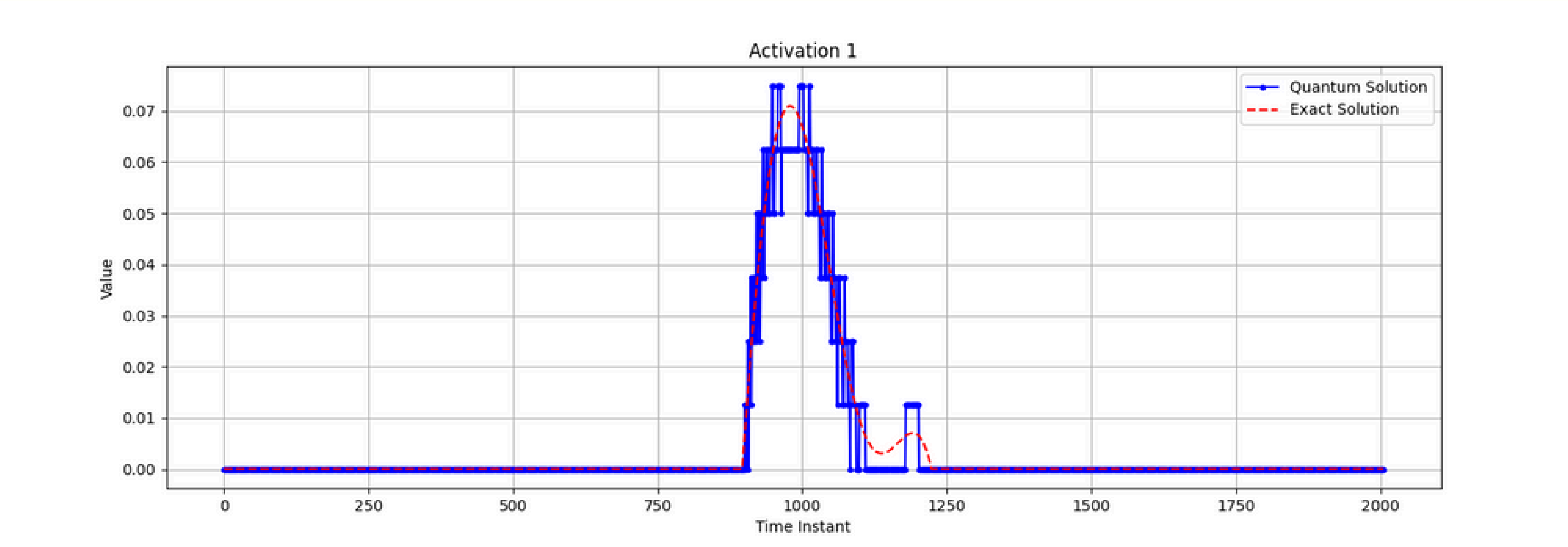
Number of qubit per activation: 3

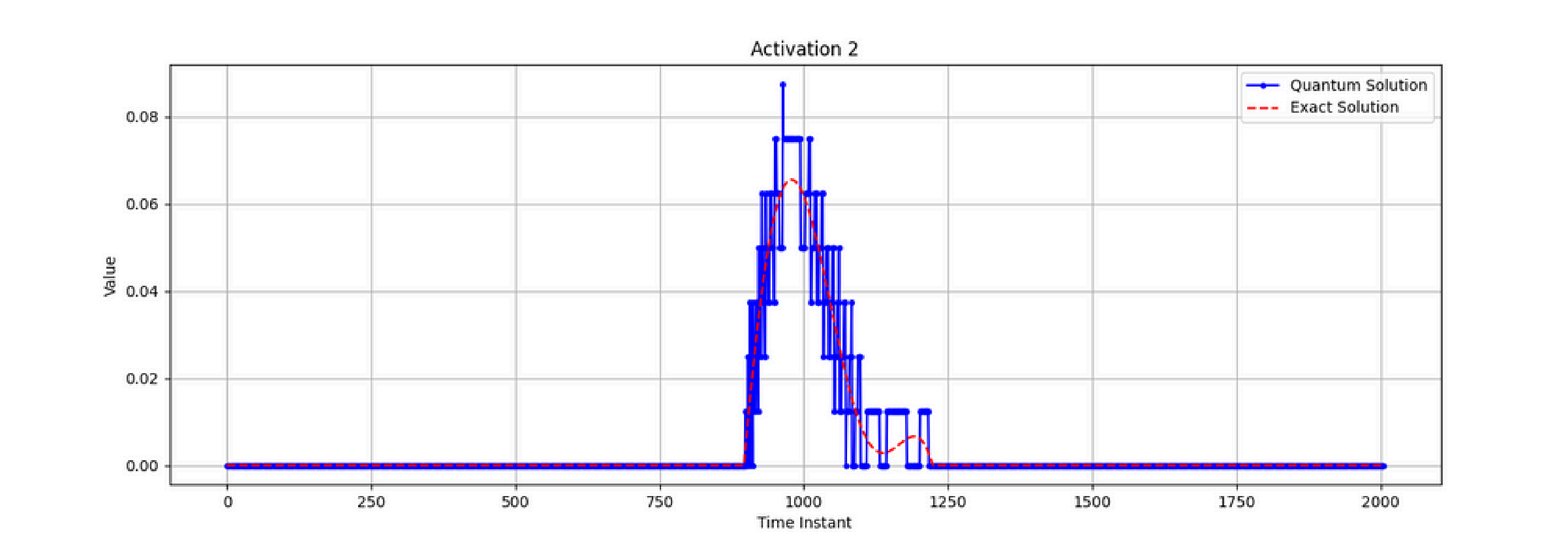


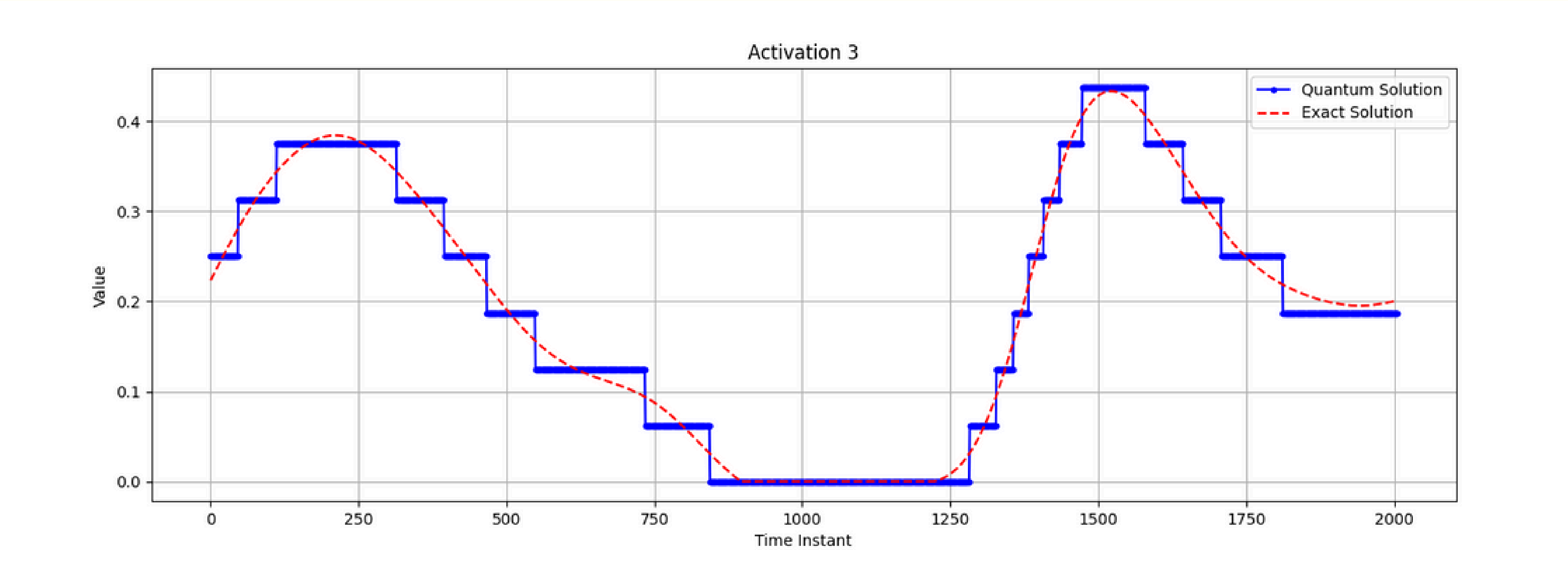


Results

Number of qubits per activation: 3

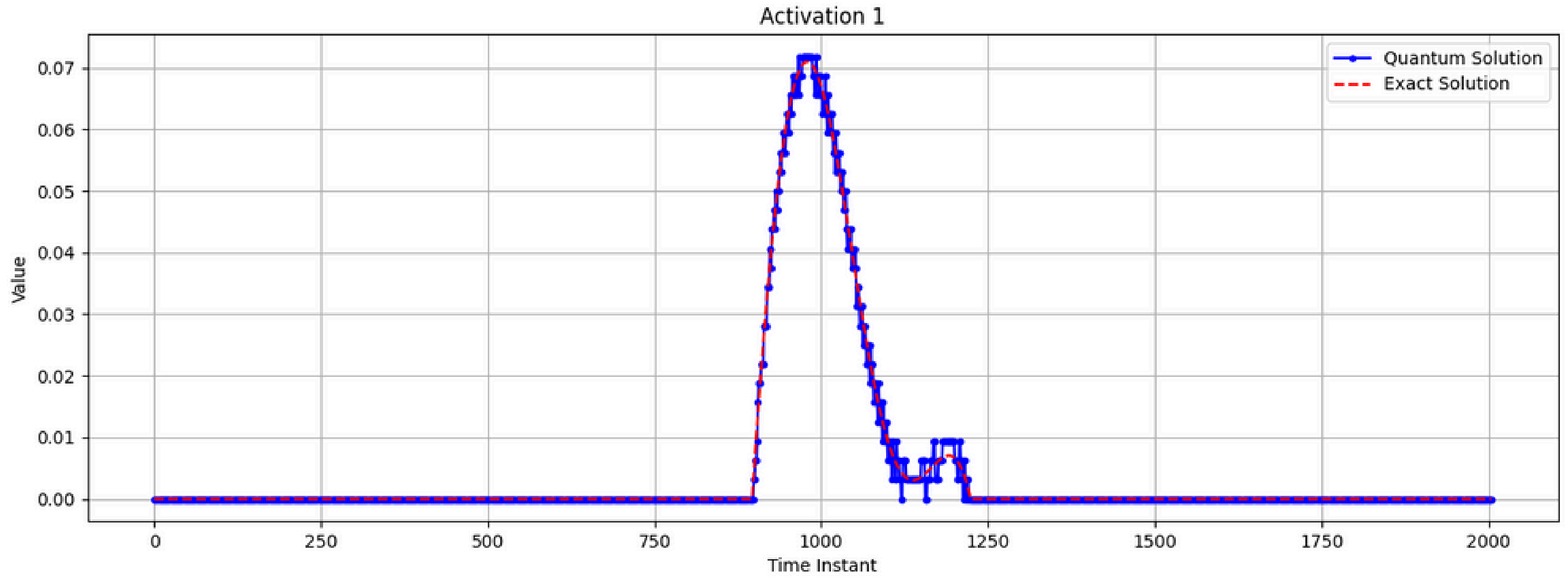


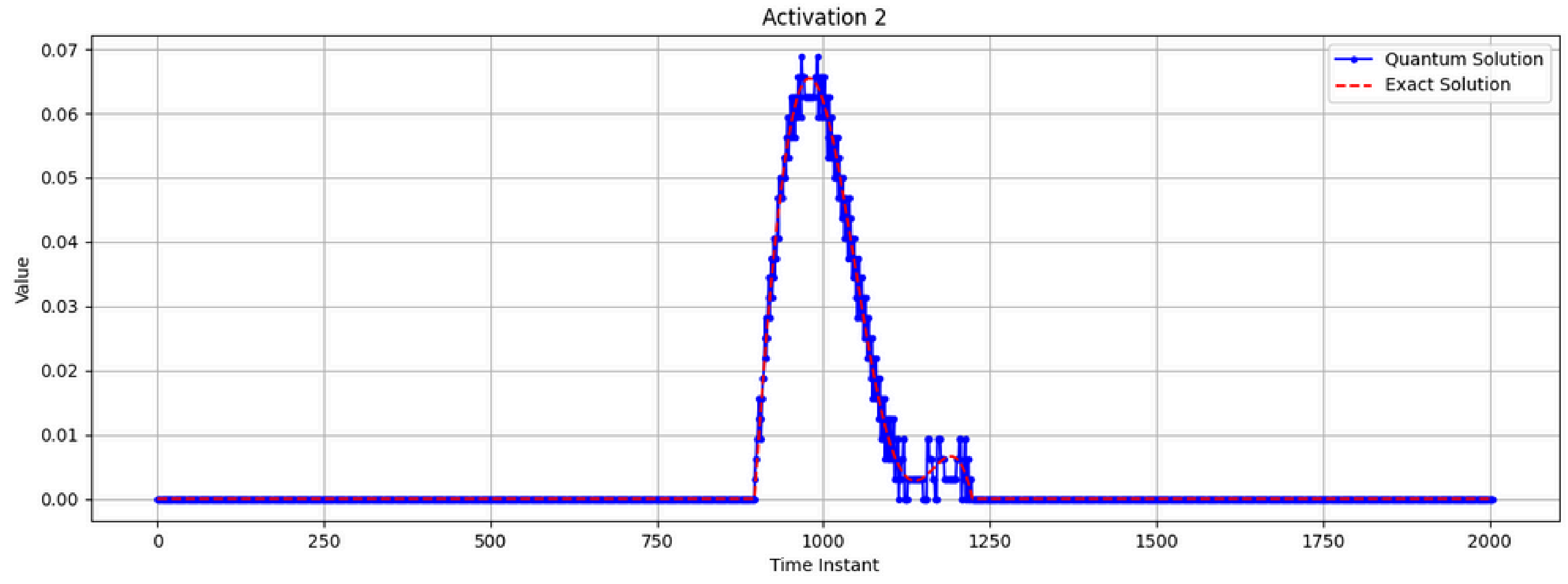


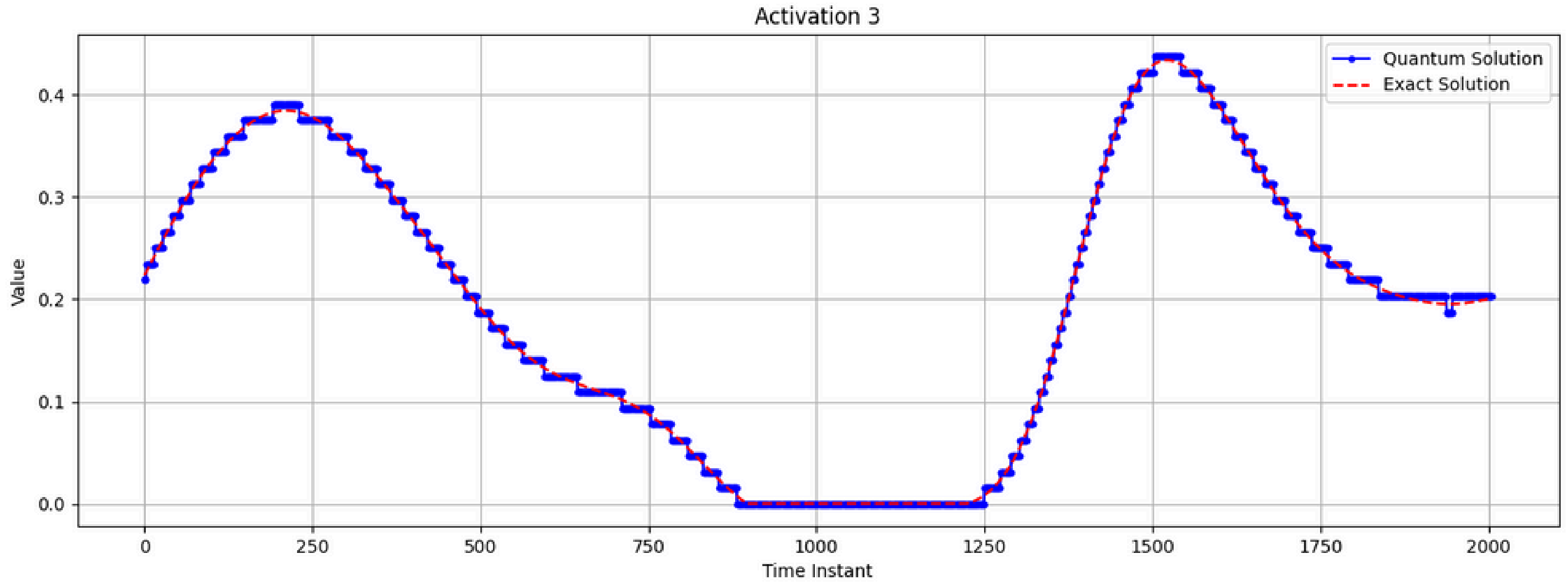


Results

Number of qubits per activation: 5

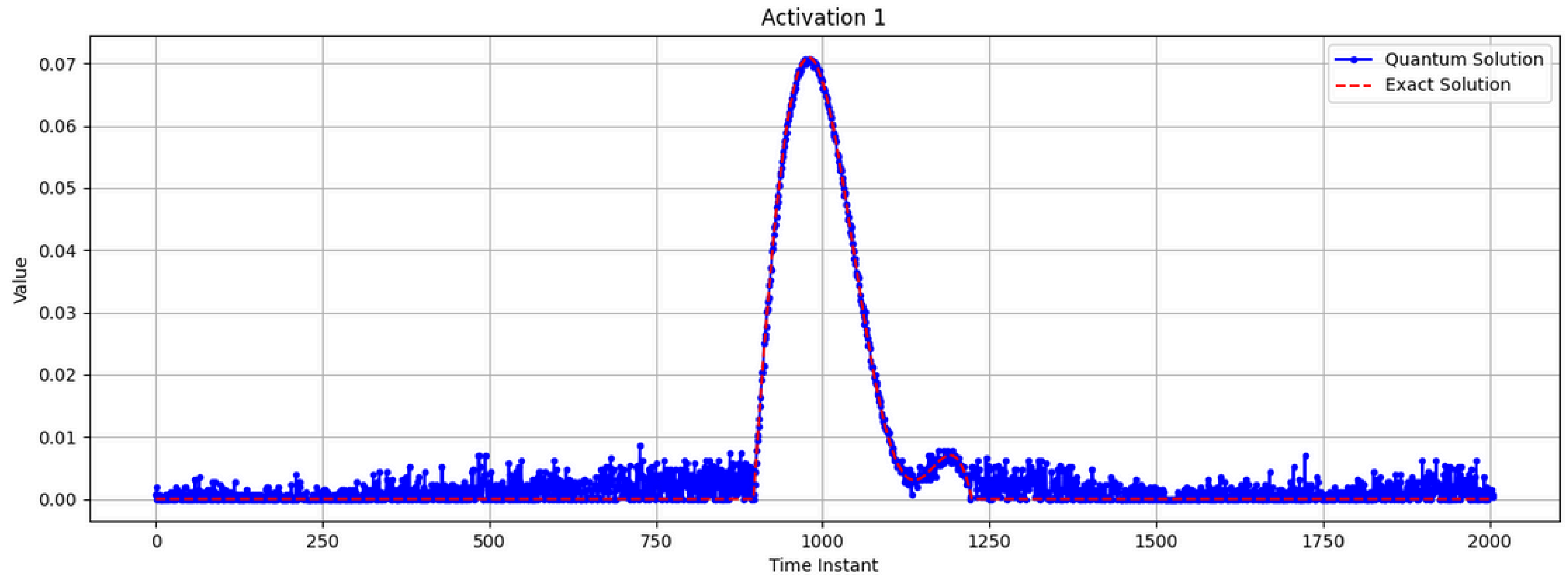


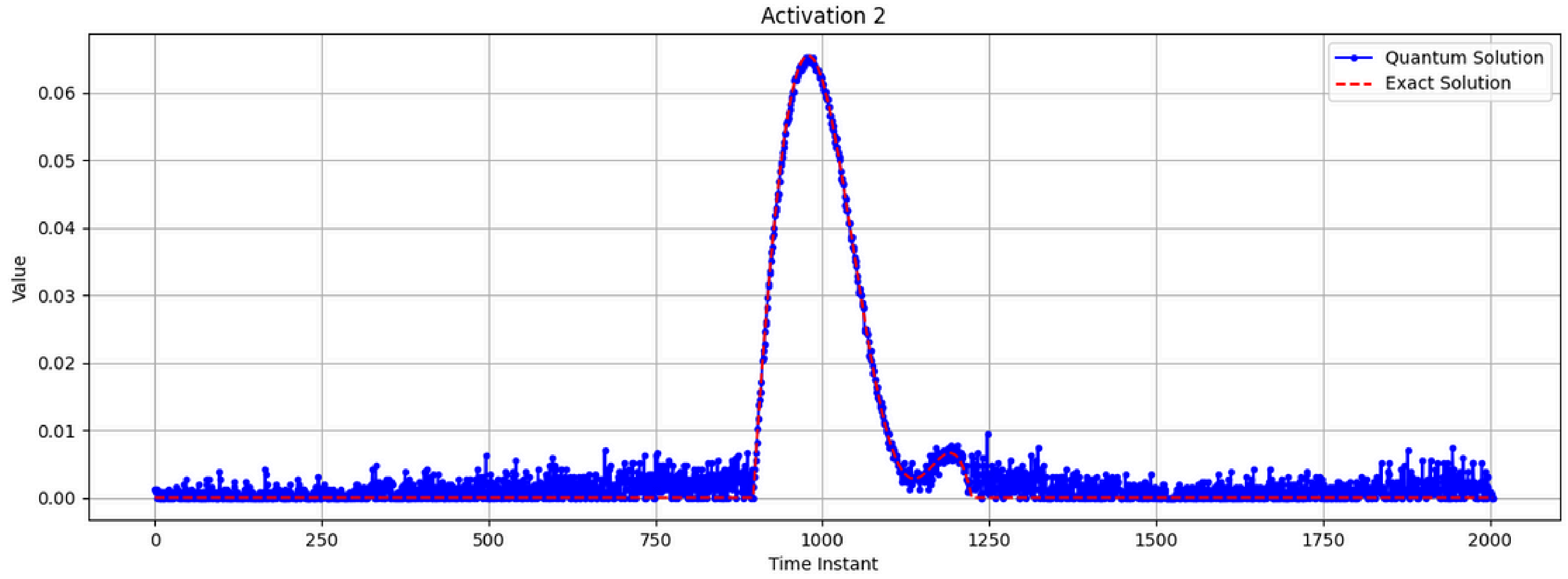


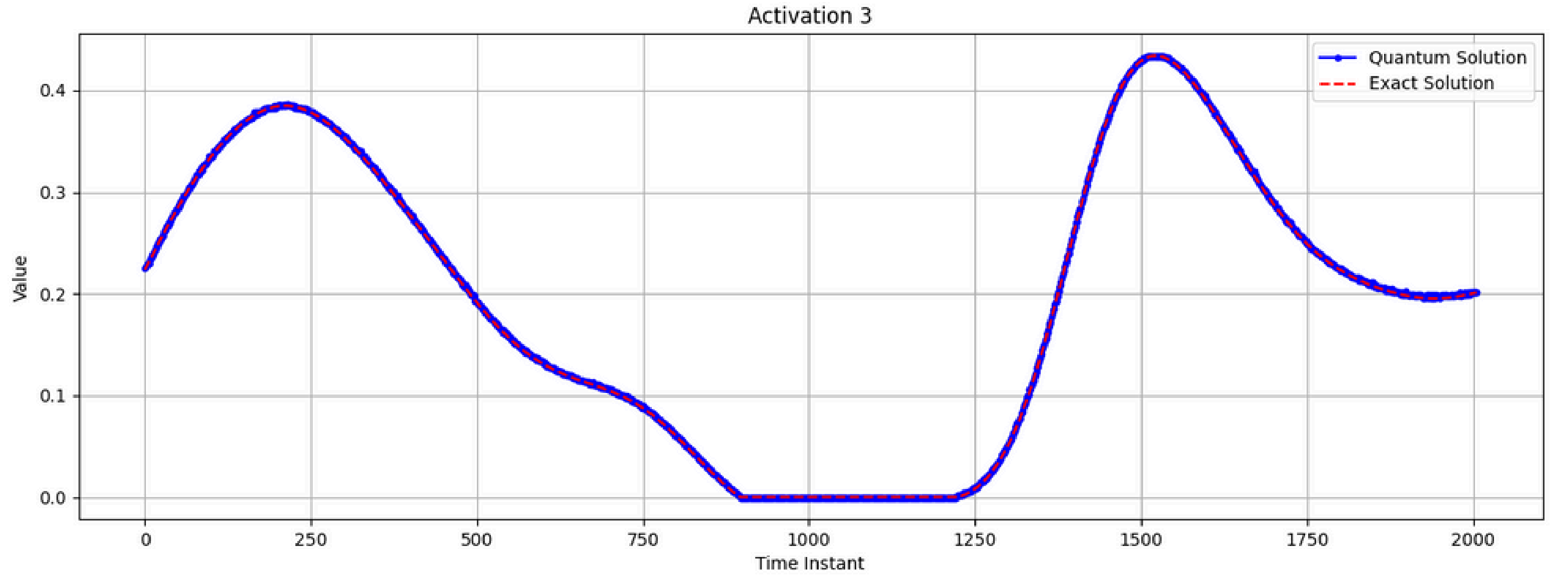


Results

Number of qubits per activation: 8

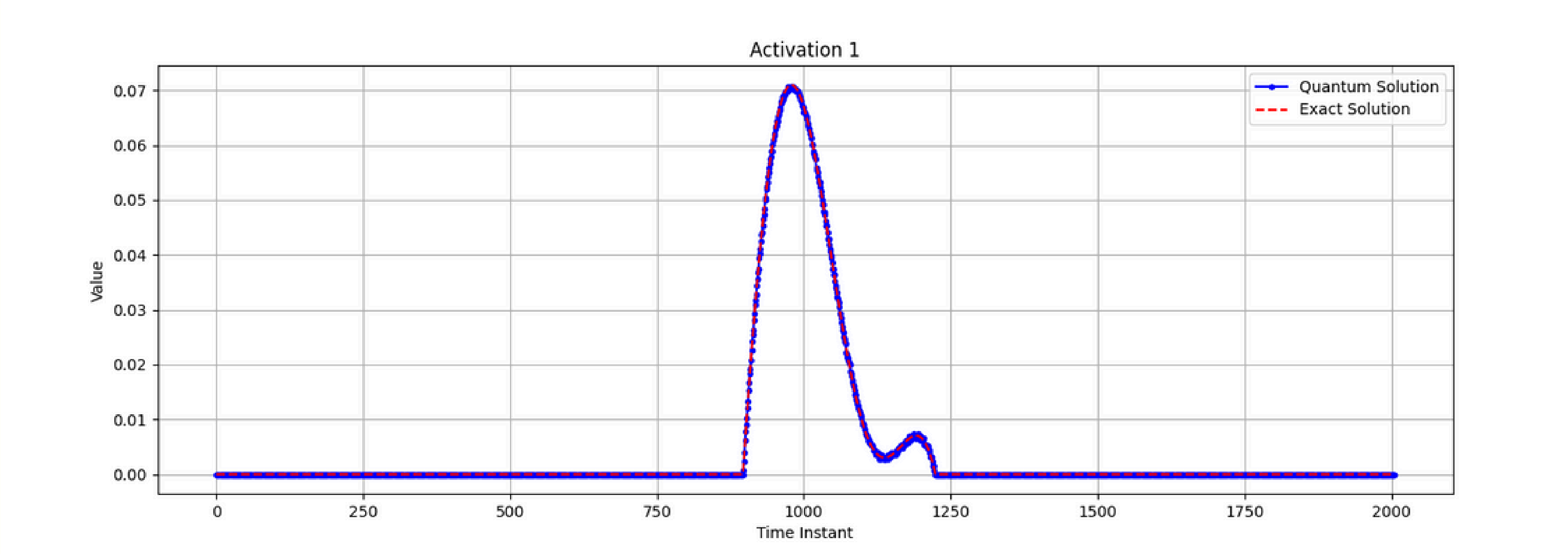


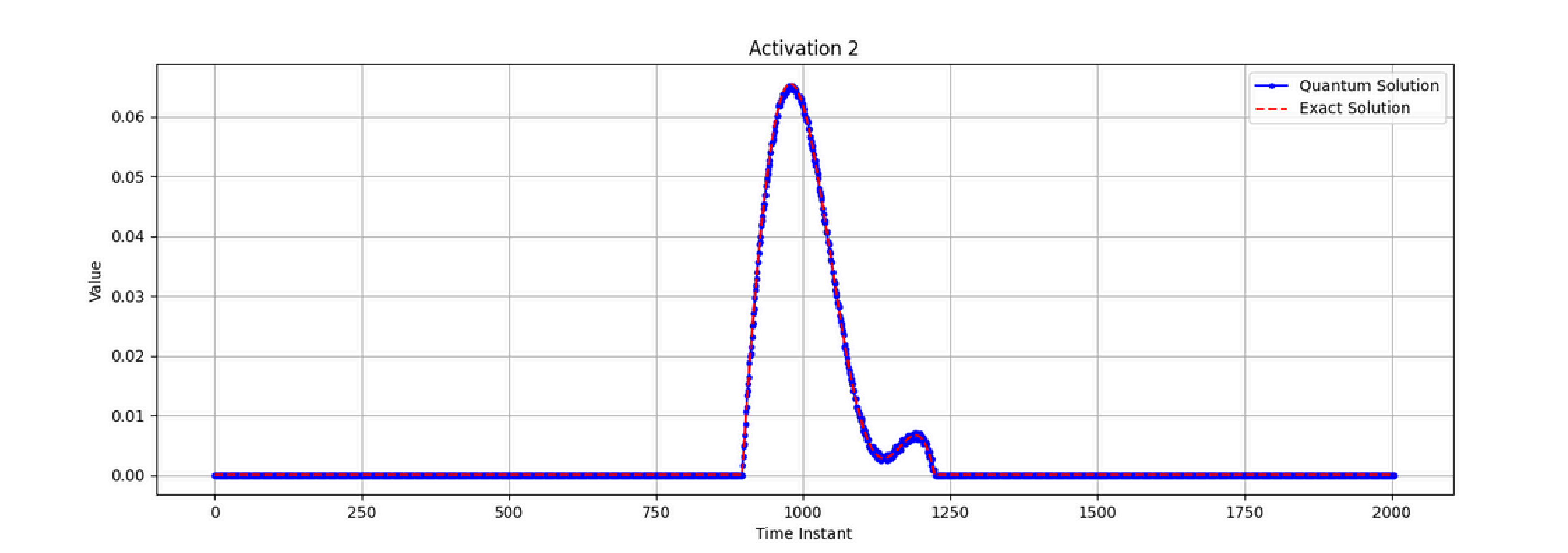


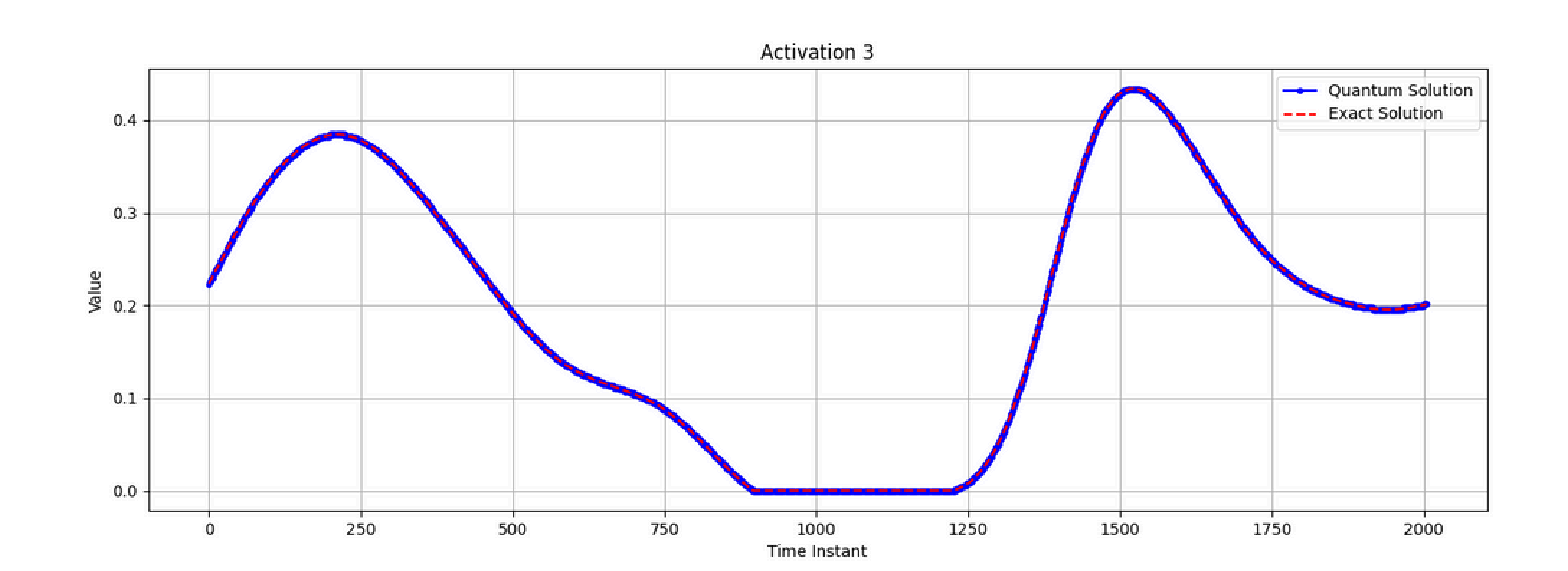


Results

Number of qubits per activation: 8, antagonists muscles decoupled







Conclusions

and future works

We have shown that using quantum annealing it is possible to find an **optimal solution** for this type of problem.

These are the activations observed in a person under **standard conditions**. The main interest is to predict the activation pattern of a person with **muscle alteration** caused by diseases or malformations. These solutions are actually computed using a stochastic approach that takes a **long time**. The quantum approach can **simplify** it. As shown, during annealing we find not only the ground state but also some higher energy levels that are associated with **sub-optimal** solutions.

We are conducting further studies to verify the compatibility of the results obtained with the stochastic and quantum annealing approaches.

Thanks for your attention