HW5 (25 points)

For this homework consider the set $A = \{6, 2, 12, 7, 3, 18, 11\}$.

Problem 1. *(Points :3)* Design a QUBO for the Partition optimization problem. For that, first read Section-II of

https://arxiv.org/pdf/2211.02653.pdf.

Then, write down a QUBO based on the similarity of the Partition problem and the SubsetSum problem – these are described below.

SubsetSum Given a set $A = \{x_1, \ldots, x_n\}$ of integers (say positive), and a target (positive) integer T, is there a subset $A' \subseteq A$ whose sum is T (i.e., $\sum_{x \in A'} x = T$).

Partition (Decision) Given a set $A = \{x_1, \ldots, x_n\}$ of integers (say positive), is there a way to divide A into two non-overlapping subsets A' and A'' (so, $A' \cup A'' = A$ and $A' \cap A'' = \emptyset$), such that $\sum_{x \in A'} x = \sum_{x \in A''} x$.

Partition (Optimization) Given a set $A = \{x_1, \ldots, x_n\}$ of integers (say positive), partition A into two non-overlapping subsets A' and A'' (so, $A' \cup A'' = A$ and $A' \cap A'' = \emptyset$), such that $|\sum_{x \in A'} x - \sum_{x \in A''} x|$ is minimized.

You should write the QUBO for the optimization version of **Partition** for the above A.

Problem 2. *(Points :2)* Write down a Hamiltonian H whose ground state energy equals the optimal value of the Partition problem on A. The standard approach is to replace the variable x_i by the operator $\frac{I - Z_i}{2}$.

Problem 3. *(Points :6)* Let $|\psi\rangle = |+\rangle^{\otimes 7}$. Use IBM's Qiskit simulator or a QPU to estimate $\langle\psi| H |\psi\rangle$. Submit the details of the experiments, all intermediate calculations/Jupyter notebook, and final result. Does your experiment produce the optimal value?

Problem 4. *(Points :6)* Use VQE (refer to Qiskit API for qiskit.algorithms.minimum_eigensolvers.VQE) to estimate the ground state energy of H. State choices made for estimator, number of parameters, ansatz, optimizer, and the other attributes of the VQE class. Submit a table or a plot that shows, for each evaluation, the values of the parameters, the estimated mean value.

Problem 5. *(Points :2+2+4=8)* Consider the setting of Grover's search with a unique solution. Let x denote the unique solution of $f()$, and let U_f be the oracle to identify the solution.

$$U_f |y\rangle |b\rangle = |y\rangle |b\rangle \text{ for } y \neq x \text{ }, U_f |x\rangle |b\rangle = |x\rangle |b \oplus 1\rangle$$

Consider the states $|x\rangle$ and $|x^\perp\rangle$ where the latter is a normalized state that is orthogonal to $|x\rangle$; observe that they form a 2-dimensional basis. Let t be any small positive real number.

1. Show that $e^{-i|x\rangle\langle x|t} = I + (e^{-it} - 1)|x\rangle\langle x|$ (Hint:use Taylor expansion if everything fails).
2. Show the action of the operator $I + (e^{-it} - 1)|x\rangle\langle x|$ on the states $|x\rangle$ and $|x^\perp\rangle$.
3. Based on the above observations, explain how to implement the operator $e^{-i|x\rangle\langle x|t}$. You will need to call U_f and may need an additional ancillæ as well (in that case, you must return the ancillæ to its initial $|0\rangle$ state). Explain the action of your circuit on any state $|\phi\rangle = \alpha|x\rangle + \beta|x^\perp\rangle$.