Problem 1 (The triangle problem).
In the triangle problem, you are asked to decide whether an n-vertex graph $G$ contains a triangle (a complete subgraph on 3 vertices). The graph is specified by a black box that, for any pair of vertices of $G$, returns a bit indicating whether those vertices are connected by an edge in $G$.

a. What is the classical query complexity of the triangle problem?

b. We say that an edge of $G$ is a triangle edge if it is part of a triangle in $G$. What is the quantum query complexity of deciding whether a particular edge of $G$ is a triangle edge?

c. Now suppose you know the vertices and edges of some $m$-vertex subgraph of $G$. Explain how you can decide whether this subgraph contains a triangle edge using $O(m^2/3\sqrt{n})$ quantum queries.

d. Consider a quantum walk algorithm for the triangle problem (or, equivalently, deciding whether a graph contains a triangle edge). The walk takes place on a graph $G$ whose vertices correspond to subgraphs of $G$ on $m$ vertices, and whose edges correspond to subgraphs that differ by changing one vertex. A vertex of $G$ is marked if it contains a triangle edge. How many queries does this algorithm use to decide whether $G$ contains a triangle? (Hint: Be sure to account for the queries used to initialize the walk, the queries used to move between neighboring vertices of $G$, and the queries used to check whether a given vertex of $G$ is marked. To get a nontrivial result, you should use the search framework mentioned in class that takes many steps according to the walk on $G$ with no marked vertices before performing a phase flip at marked vertices.)

e. Choose a value of $m$ that minimizes the number of queries used by the algorithm. What is the resulting upper bound on the quantum query complexity of the triangle problem?

f. Challenge problem: Generalize this algorithm to decide whether $G$ contains a $k$-clique. How many queries does the algorithm use?

Problem 2 (Grover's algorithm by formula evaluation).
Grover’s algorithm computes the OR of $n$ bits using $O(\sqrt{n})$ quantum queries to those bits. In this problem you will give an alternative algorithm for computing OR by evaluating a NAND formula.

Since $\text{OR}(x_1,\ldots,x_n) = \text{NAND}(\bar{x}_1,\ldots,\bar{x}_n)$, we can represent the OR formula by a NAND tree in which the root has $n$ children, and each of those children has one child, which is a leaf. Given an input $x_1,\ldots,x_n$, we modify the tree by deleting every leaf in the original tree corresponding to an index $i$ for which $x_i = 1$.

We will start our quantum algorithm from the root, so you can restrict your attention to the subspace $S := \text{span}\{H^j|\text{root} : j = 0, 1, 2, \ldots\}$, where $H$ is a weighted adjacency matrix of the tree (with weights to be determined).

a. First consider the input $x_1 = \cdots = x_n = 0$, for which the formula evaluates to 0. Define the weighted adjacency matrix $H$ of the corresponding tree by assigning a weight of $\alpha$ to the edges connected to the root and a weight of 1 to the remaining edges. Compute the spectrum (both eigenvalues and eigenvectors) of $H$ within the subspace $S$.

b. For what values of $\alpha$ does $H$ (as defined in part a) have an eigenstate of eigenvalue 0 with overlap $\Omega(1)$ on the root?
c. Now consider an input with \( x_i = 1 \) for precisely one index \( i \). Compute the spectrum of \( H \) within the subspace \( S \).

d. For what values of \( \alpha \) does \( H \) (as defined in part c) have a minimum eigenvalue of \( \Omega(1/\sqrt{n}) \) (in absolute value)? Choose a value of \( \alpha \) so that this condition and the one from part b are satisfied simultaneously.

e. Compute the spectrum of \( H \) for an arbitrary input, and show that the minimum eigenvalue of \( H \) (again in absolute value) can only be larger than in part c if there is more than one index \( i \) for which \( x_i = 1 \).

f. Explain why your calculations imply a discrete-time quantum walk algorithm for computing the OR of \( n \) bits using \( O(\sqrt{n}) \) queries. (Hint: Refer to problem 5 from assignment 2.)

g. Challenge problem: Describe a simulation of the continuous-time quantum walk generated by \( H \) that computes OR using \( O(\sqrt{n}) \) queries. (Notice that the root of the tree has high degree, so you cannot use results on the simulation of sparse Hamiltonians.)

Problem 3 (Adiabatic evolution of a qubit).

Consider a spin in a magnetic field that is rotated from the \(-x\) direction to the \(-z\) direction in a total time \( T \). Such a spin is described by the Hamiltonian

\[
H(t) = -\cos\left(\frac{\pi t}{2T}\right) \sigma_x - \sin\left(\frac{\pi t}{2T}\right) \sigma_z.
\]

Suppose that at time \( t = 0 \), the spin is in the ground state of \( H(0) \). Plot the behavior of the \( x \), \( y \), and \( z \) components of the spin as a function of time from \( t = 0 \) to \( t = T \), where \( T = 5, 10, \) or 50. Comment on the results in light of the adiabatic theorem.

Problem 4 (Perturbation theory).

Let \( H(s) \) be a Hermitian matrix depending smoothly on a parameter \( s \in \mathbb{R} \). Let \( P(s) \) be the projector onto the eigenstate of \( H(s) \) with the smallest eigenvalue, which is separated by a gap \( \Delta(s) > 0 \) from the rest of the spectrum. (In particular, the eigenstate is non-degenerate for all values of \( s \)).

a. Prove that

\[
\|\dot{P}(s)\| \leq c_1 \frac{\|\dot{H}(s)\|}{\Delta(s)}
\]

for some constant \( c_1 > 0 \), where \( \dot{X}(s) := \frac{d}{ds} X(s) \), and as usual, \( \|X\| \) denotes the spectral norm of \( X \). (Hint: This is a formalization of first-order non-degenerate perturbation theory, as discussed in any introductory textbook on quantum mechanics; you could give a proof along those lines. Alternatively, if you are comfortable with complex analysis, define the resolvent, \( R(z, s) := (H(s) - z)^{-1} \), in terms of which \( P(s) = -\frac{1}{2\pi i} \int_{\Gamma} R(z, s) dz \), where \( \Gamma \) is a contour enclosing only the smallest eigenvalue of \( H(s) \); upper bound \( \|\dot{P}(s)\| \) by integrating around some circular contour.)

b. Prove that

\[
\|\ddot{P}(s)\| \leq c_2 \frac{\|\ddot{H}(s)\|}{\Delta(s)} + c_3 \frac{\|\dot{H}(s)\|^2}{\Delta(s)^2}
\]

for some constants \( c_2, c_3 > 0 \), where \( \dot{X}(s) := \frac{d^2}{ds^2} X \).
Problem 5 (Tunneling in the adiabatic algorithm).

In quantum mechanics, particles can tunnel through a classically impenetrable barrier. In this problem you will see how tunneling allows an adiabatic algorithm to minimize a cost function that could not be minimized by a classical local search algorithm such as simulated annealing.

a. Consider adiabatic optimization of a cost function $h : \{0,1\}^n \to \mathbb{R}$ for which $h(x)$ depends only on $|x| := \sum_i x_i$, the Hamming weight of $x$. In particular, consider the Hamiltonian $H(s) := (1 - s)H_B + sH_P$, where the initial and final Hamiltonians are

$$H_B := -\sum_{j=1}^n \sigma_x^{(j)} \quad H_P := \sum_{x \in \{0,1\}^n} h(x)|x\rangle\langle x|.$$ 

Show that evolution of the initial state $|u\rangle := \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle$ according to the Hamiltonian $H(t/T)$ remains in the subspace span\{[k] : k = 0, 1, \ldots, n\}, where [k] denotes the set of n-bit strings of Hamming weight $k$.

b. Suppose that $h(x) = |x|$, and compute the spectrum of $H(s)$ in the subspace of Hamming weight states as a function of $s \in [0, 1]$. In particular, show that the minimum gap between the ground and excited states of $H(s)$ is at least some constant, independent of $n$.

c. Now suppose that $h(x) = |x| + \Delta(|x|)$, where $\Delta(w)$ is a non-negative function of width $\approx n^\delta$ and height $\approx n^\epsilon$ centered around $w = w_0$. For concreteness, suppose that

$$\Delta(w) = \begin{cases} 
0 & w < w_0 - n^\delta \text{ or } w > w_0 + n^\delta \\
\epsilon & w_0 - n^\delta \leq w \leq w_0 + n^\delta.
\end{cases}$$

Define a local search algorithm as a classical randomized algorithm that works as follows:

- Initialize $x$ to a random bit string.
- For $i = 1$ to $\text{poly}(n)$:
  - Let $y_i$ be some string with $O(1)$ bits equal to 1.
  - If $h(x \oplus y_i) > h(x) + O(1)$, leave $x$ unchanged. Otherwise, leave $x$ unchanged or set $x$ equal to $x \oplus y_i$ according to some specified rule.
- Output $x$.

Argue that if $\delta, \epsilon > 0$ are constants and $w_0 < cn$ for some constant $c < 1/2$, a local search algorithm is unlikely to find the minimum of $h(x)$.

d. Finally, analyze the performance of the adiabatic algorithm for minimizing $h(x) = |x| + \Delta(|x|)$. Since $\Delta(w) \geq 0$, the eigenvalues of $H(s)$ can only be larger than in part b. Thus, to lower bound the gap between the ground and first excited states of $H(s)$, it suffices to upper bound the perturbed ground state energy. Using the original ground state as an ansatz, give an upper bound on the ground state energy of $H(s)$. What are the conditions on $\delta, \epsilon$ such that the minimum gap is at least $1/\text{poly}(n)$?