Homework #4
Due by 11/26/2025 before class

1. [10 pt] Consider a particle with a mass of m in a potential $V(x) = \alpha x^4$ ($\alpha > 0$). Use the variational ansatz $\psi(x) = Ae^{-\lambda x^2}$ to approximate the ground state energy and the ground state wavefunction, where A is a normalization factor.

2. Again, consider a particle with a mass of m in a potential $V(x) = \alpha x^4$ ($\alpha > 0$). This time we solve this problem numerically. Let us set $m = 1$, $\alpha = 1$ and $\hbar = 1$.

(a) [10 pt] Express the position and the momentum operators as $x = (a + a^\dagger)/\sqrt{2}$ and $p = i(a^\dagger - a)/\sqrt{2}$, where a and $a^\dagger$ are the annihilation and the creation operators. Further express the Hamiltonian in terms of a and $a^\dagger$. Choose a suitable cutoff for the excitation number n_{cut}, and express H as a matrix in the Fock basis $\{|0\rangle, |1\rangle, \cdots, |n_{\text{cut}}\rangle\}$. Compute the energies for the ground state and the first excited state. Keep three digits in your results. Note that you should increase n_{cut} to verify that your solution has converged.

(b) [10 pt] To use the shooting method, we want to work with a finite domain of the wavefunction. In this case, we can construct a length unit as $(\hbar^2/\alpha m)^{1/6} = 1$. When sufficiently far away from $x = 0$, we can expect that the wavefunction vanishes. Therefore, as an approximation, we can restrict our wavefunction to the domain of $[-5, 5]$ with the boundary conditions $\psi(-5) = 0$ and $\psi(5) = 0$. Furthermore, owing to the reflection symmetry of the Hamiltonian about $x = 0$, it is guaranteed that all the nondegenerate energy eigenstates have specific parity, namely, $\psi_n(x) = \psi_n(-x)$ for even parity, or $\psi_n(x) = -\psi_n(-x)$ for odd parity. Now use the shooting method to find the energies for the ground state (initial value $\psi(0) = 1$, $\psi'(0) = 0$ for even parity) and the first excited state (initial value $\psi(0) = 0$, $\psi'(0) = 1$ for odd parity). Plot the wavefunctions you find. Again, keep three digits in your results. [Hint: You may use *scipy.integrate.solve_ivp* of Python, *ode45* of MATLAB, or similar numerical tools to solve an initial value problem for a system of ordinary differential equations.]

3. Consider the numerical optimization of a complicated objective function $f(x, y)$. Suppose we start from the origin $(0, 0)$, around which the objective function can be approximated by a model function $m(x, y) = 8x + 12y + x^2 - 2y^2$.

(a) [5 pt] Compute the stationary point of $m(x, y)$. Show that it is neither a maximum nor a minimum, but a saddle point.

(b) [10 pt] Now suppose the model function is valid in a trust region with a radius of $\Delta = 5$ around the origin. What is our best choice for the next step? Compare your result

with the direction of the gradient descent method. [Hint: You can use any numerical tools to find the root of a single-variable polynomial, but DO NOT solve two-variable problems directly numerically. Keep three digits in your result.]

4. [15 pt] Consider an objective function $f(x) = |x|^{3/2}$ which is continuously differentiable. Suppose we use the gradient descent method to find its local minimum iteratively, with a constant step size $\alpha > 0$. That is, we update

$$x_{n+1} = x_n - \alpha f'(x_n). \tag{1}$$

Prove that, for any constant $\alpha > 0$, this algorithm will not converge to the minimizer $x^* = 0$. In other words, prove that for any $\alpha > 0$ and $\delta > 0$, there exists an initial point $|x_0| < \delta$ within the δ-neighborhood of x^*, s.t. the sequence $\{x_n\}$ generated by Eq. (1) does not converge to x^* in the limit $n \to \infty$. To ensure convergence, we need to update the step size along the iteration using, e.g., the Backtracking algorithm.

5. [20 pt] For the example we see in the class using the quantum variational algorithm to prepare the logical state of the Steane code, consider $p = 1$ ($p + 1$ layers of single-qubit rotations and p layers of CNOT gates). Write Qiskit codes to simulate the gradient with respect to the rotation angle of the first qubit in the first layer, using the finite difference method and the parameter shift method, respectively. Plot the error of your sampled gradient versus the trial number $M = 10, 10^2, 10^3, 10^4, 10^5$ for these two methods. (You should choose a suitable scaling for δ versus M in the finite difference method.) To determine the error of the gradient, you can write one further Qiskit code to compute the exact gradient g from the simulated wave vector. Then you can repeat the above sampling process for $K = 10$ times, each with M trials, to obtain K sampled gradients $\{g_i\}$. The average absolute error can be computed as

$$e \equiv \frac{1}{K} \sum_{i=1}^{K} |g_i - g| \tag{2}$$

To be specific, the gradients can be evaluated at the parameters $\alpha_{ik} = 1$ for all the variational parameters.

6. (a) [10 pt] Similar to what we have done in the class, write a Qiskit code to solve the max cut problem with $n = 5$ vertices using the QAOA variational ansatz. Use the finite difference method to evaluate the gradient, and consider $p = 3$ layers and $M = 1000$ trials for each evaluation. For convenience, you can use the quantum-annealing-inspired initial values of $\alpha = 0.1 \times [1, 2/3, 1/3]$ and $\beta = 0.1 \times [1/3, 2/3, 1]$, which corresponds to a step size $\Delta t = 0.1$ in the quantum annealing algorithm. Solve the numerical optimization problem for 100 times, and plot the histogram of the final cut number (the expectation value over the final quantum state). As you can see, there will be randomness due to the sampling of the gradient.

(b) [10 pt] For the best set of variational parameters you find, compute the standard deviation of the cut number $\Delta W = \sqrt{\langle W^2 \rangle - \langle W \rangle^2}$ from $M = 10000$ measurement samples. For an ideal eigenstate, the standard deviation should be zero. Therefore we can use it to characterize the quality of our solution even if the true ground state may not be known.