Homework #5
Due by 12/17/2025 before class

1. [10 pt] Use the energy $E_+(R)$ computed in the class for the hydrogen molecule ion to estimate what is its vibration frequency.

2. (a) [10 pt] Consider a 1D simple harmonic oscillator

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{1}$$

subjected to a perturbation $V = \lambda x$ where λ is a small constant. Calculate the energy shift of the ground state to the lowest non-vanishing order. Compare your result with the exact solution by shifting the origin of the harmonic oscillator

(b) [10 pt] Consider a 2D isotropic harmonic oscillator

$$H_0 = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2), \tag{2}$$

subjected to a perturbation $V = \alpha m\omega^2 xy$ where α is a small parameter. Solve the zeroth-order energy eigenstates and the corresponding energy up to the first order for the three lowest-lying states. Again, compare your result with the exact solution.

3. Two identical spin-1/2 fermions with mass m move in a 1D infinite square well potential

$$V = \begin{cases} 0 & 0 \le x \le L \\ \infty & x < 0,\, x > L \end{cases} \tag{3}$$

(a) [5 pt] First we neglect the interaction between the two particles. What is the lowest energy of the system and the corresponding wave function when the spins of the two particles are in a symmetric state $\frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle)$? What about the anti-symmetric spin state $\frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$?

(b) [10 pt] Now suppose the two particles interact through a short-range attractive potential which is approximated by a delta function

$$V = -\lambda\delta(x_1 - x_2) \qquad (\lambda > 0). \tag{4}$$

Estimate how the energies computed in (a) change under the first-order perturbation theory.

4. [15 pt] Write a code to compute the Bravyi-Kitaev transformation for n fermionic modes. Define the weight of a multi-qubit operator as the number of qubits on which it acts nontrivially. What is the maximal weight for the transformation for $n = 5$ modes? Plot the maximal weight vs. n up to $n = 1000$, and compare it with $\log_2 n + 1$ and $\log_2(n + 1)$.

5. In the class, we map a 1D nearest-neighbor transverse-field Ising model with open boundary conditions to a quadratic fermionic Hamiltonian. If we start from an Ising model with periodic boundary conditions, the mapping will be more complicated. Instead, here we simply generalize the mapped quadratic fermionic Hamiltonian into periodic boundary conditions:

$$H = -J \sum_{i=1}^{N} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i - c_i c_{i+1} - c_{i+1}^\dagger c_i^\dagger) + 2B \sum_{i=1}^{N} c_i^\dagger c_i, \tag{5}$$

where we identify $c_1 = c_{N+1}$.

(a) [5 pt] We can construct operators in momentum space $a_k \equiv \frac{1}{\sqrt{N}} \sum_{j=1}^{N} c_j e^{2\pi ijk/N}$ ($k = 0, 1, \cdots, N-1$) and the reverse transformation $c_j \equiv \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} a_k e^{-2\pi ijk/N}$ ($j = 1, 2, \cdots, N$). Verify that the a_k operators defined in this way satisfy the fermionic anti-commutation relations.

(b) [10 pt] Express the Hamiltonian in the momentum space. You should get several pairs of coupled modes with no interaction between different pairs.

(c) [10 pt] For two fermionic modes a and b, we can define two new modes $c = ua - ivb^\dagger$ and $d = ub + iva^\dagger$, where u and v are two real parameters satisfying $u^2 + v^2 = 1$. This is called the Bogoliubov transformation. Verify that c and d also satisfy the fermionic anti-commutation relations. What parameters u_k and v_k should we choose to turn the mode a_k and its coupled mode into two uncoupled fermionic modes?

(d) [5 pt] Each creation or annihilation of a fermion corresponds to a flip in the parity of the original spin system. Recall that in the class we are interested in the energy gap inside the symmetry branch with even parity. This corresponds to two fermions in the system. Compute the energy gap as a function of J and B. For simplicity, you can consider the limit $N \to \infty$ so that the momentum $2\pi k/N$ is almost continuous.

6. [10 pt] In the class, we consider 6 Fock basis states for two electrons in the four molecular orbitals in the hydrogen molecule. What are the total spin and the parity under spatial reflection for these 6 states? Given that the total spin and the parity are two conserved quantities for the Hamiltonian, show that these quantities allow us to predict the nonzero matrix elements of the Hamiltonian without performing detailed calculation.