CHEM 544 Fall 2017 - Homework 4

Due on Friday, December 1.

Answer all questions. To gain full credit you should explain your reasoning and show all working. Please write neatly and remember to include your name on the front page of your answers.

Solve the following problems in “Molecular Quantum Mechanics, 5th edition, by P. Atkins and R. Friedman”.

Chapter 4

1. Exercises 4.2, 4.3 and 4.5
2. Problems 4.2, 4.11, 4.12, 4.26 and 4.29

Additional problems

1. **Problem 4.9-modified.** Evaluate the effect of (a) \( \exp(-i\pi \sigma_x/2) \), (b) \( \exp(-i\pi \sigma_y/4) \) and (c) \( \exp(-i\pi \sigma_z/2) \) on an \( |\alpha\rangle \) spin state where \( \sigma_q \) are the Pauli operators. Hint. Expand the exponential operators as in Problem 1.18.
2. **Hydrogen atom.** Consider a hydrogen atom under magnetic fields (S=1/2 electron and I=1/2 nuclear spins) described by the following Hamiltonian,

\[
H = (\mu_B / \hbar) g_e S \cdot B + (A_0 / \hbar^2) S \cdot I
\]

where \( S \) and \( I \) are spin operators for electron and nuclear spins, \((\mu_B / \hbar) g_e = 28 \) (GHz/Tesla), the hyperfine coupling constant \((A/\hbar^2) = 1.4 \) (GHz) and \( B = (0, 0, B_0) \).

Simulate and plot the energy diagram (the energy levels as a function of magnetic fields) for \( B_0 = 0–1 \) (Tesla) and show the eigenstates of all the energy levels at \( B_0 = 0 \) and 1 (Tesla).

(Submit a printout of your program with the homework too).