Quantum Mechanics and Spectroscopy
CHEM 3PA3
Assignment 18 **Name:** _____

1. What is the electronic and nuclear Schrödinger equations for the hydrogen atom, showing the dependence on physical constants like the charge and mass of the electron.

2. Is the product of two Hermitian operators always Hermitian? If not, under what conditions is this true?

3. Consider a particle with unit mass and unit charge confined in a 3-dimensional box, with potential,

$$V_{3D-box}(x,y,z) = V_{1D-box}(x) + V_{1D-box}(y) + V_{1D-box}(z)$$

$$V_{1D-box}(i) = \begin{cases} +\infty, & i \leq 0 \\ 0 & 0 < i < a \\ -\infty, & i \geq a \end{cases}$$

We place this box in linearly polarized light, which induces a time-dependent potential with the form

$$V_{light}(x,y,z,t) = -2Vx\sin(\omega t - kz).$$

What is the time-dependent Schrödinger equation for this system, using atomic units (so $\hbar = 1$)?

4. Consider a Nitrogen atom in its ground state, with $M_s = S = 3/2$, where M_s is the spin angular momentum around the z axis. The Robertson-Schrödinger relation then allows us to state that for this state of the Nitrogen atom, in atomic units,

$$\left\langle \Psi \middle| \hat{S}_x^2 \middle| \Psi \right\rangle \left\langle \Psi \middle| \hat{S}_y^2 \middle| \Psi \right\rangle \geq \frac{9}{16}.$$

Show, mathematically, why this result is true, that is, derive this result.

5. Consider a Holmium atom with electron configuration$[Xe]4f^{11}6s^2$, what are the values for the following quantum numbers for the ground state described by ${}^4I$ term symbol? When the term symbol is not sufficient to fully specify the quantum number, please list all the possible values.

   (a) L (total orbital angular momentum)

   (b) M_L (orbital angular momentum around the z-axis)

   (c) S (total spin angular momentum)

   (d) M_S (spin angular momentum around the z-axis)

   What are the possible values of J for the ground state term of the Holmium atom? Which value of J does Hund's rule predict to be most stable?