CHM 428 Assignment 3

April 6, 2024

Due on 13^{th} April, 2024.

1. Compute the following commutators
   (a) $\left[x, \frac{\partial}{\partial x}\right]$
   (b) $\left[\hat{L}_z, x\right]$, where $\hat{L}_z$ is the z-component of the angular momentum.
   (c) $\left[\hat{L}_z, \hat{H}\right]$, where $\hat{H}$ is the hamiltonian of 1-dimensional quantum harmonic oscillator (QHO) moving along x-axis.
   (d) $[\hat{a}_-, \hat{x}\hat{p}_x]$
   (e) $[\hat{n}, \hat{x}]$, where $\hat{n}$ is the number operator from the QHO problem.

2. A quantum harmonic oscillator (QHO) has the Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$.
   (a) Show that its eigenstates have definite parity.
   (b) Show that the expectation value of position and momentum in any eigenstate is 0.
   (c) Given that the uncertainty in position in a particular eigenstate is $\Delta x = a$, determine a lower bound estimate to the energy of the state.
   (d) Using the result of the previous problem estimate the ground state energy of the QHO showing that it is positive.

3. (a) Show that for any two observables $\hat{A}$ and $\hat{B}$ the generalized uncertainty principle holds

$$\Delta A \Delta B \geq \frac{1}{2}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|$$

where $\Delta A = \left\langle \hat{A}^2 \right\rangle - \left\langle \hat{A} \right\rangle^2$. (See Sec.1.16 of Molecular Quantum Mechanics, Atkins and Friedman.)

   (b) Show that the expectation value of position and momentum for a QHO in any eigenstate is 0. (Hint: Write $\hat{x}$ and $\hat{p}$ in terms of the ladder operators).

   (c) For the eigenstates of the QHO compute the uncertainties in position and momentum and verify that they obey the Heisenberg uncertainty principle.

4. If $\hat{a}$ and $\hat{a}^\dagger$ the lowering and raising operators of a harmonic oscillator with fundamental frequency ω then consider the state $|\alpha\rangle = N_\alpha \exp(\alpha \hat{a}^\dagger)|0\rangle$.

   (a) Determine N_α such that $|\alpha\rangle$ is normalized.

   (b) Show that $|\alpha\rangle$ is an eigenstate of $\hat{a}$. (This state is called a coherent state).

   (c) Calculate the uncertainties in position and momentum in the state $|\alpha\rangle$.

   (d) Calculate the average number of quanta in the state, i.e. $\left\langle \hat{N} \right\rangle$.

5. A particle of mass m moves in 1-dimensional quantum harmonic oscillator potential with fundamental frequency ω. At $t = 0$, the particle is prepared in a (unnormalized) state $\Psi(x, 0) = \exp(-\alpha(x + a)^2)$, where $a > 0$ and $\alpha = \frac{m\omega}{2\hbar}$. Determine the wavefunction at any time $t > 0$.

6. Consider a 1-dimensional quantum harmonic oscillator of mass m and fundamental frequency Ω oscillating about the origin. An external force acting on the system modifies its potential energy by $\Delta V(x) = -\lambda x$ ($\lambda > 0$). For this new system

   (a) Determine the eigenstates, eigenvalues and eigenfunctions.

(b) If the system was in a state with $\langle x \rangle = 0$ and $\langle p \rangle = 0$ at time $t = 0$ when the force was applied, then determine the time dependent expectation values of momentum and position for $t > 0$.

7. A 1-dimensional quantum harmonic oscillator of mass m and fundamental frequency Ω oscillating about the origin is in the quantum state $v = 2$. Compute the expectation value of the operators in $\hat{x}^3$ and $\hat{x}^4$ in this state.

8. A model for the hydrogen atom is the isotropic oscillator where the electron is assumed to be bound to the nucleus using an isotropic spring. The potential energy of interaction between the electron and the nucleus in this model is given by $V(r) = \frac{1}{2}kr^2 = \frac{1}{2}k\left(x^2 + y^2 + z^2\right)$ where k is the spring constant. (a) Assuming the equilibrium electron-nuclear distance to be the Bohr radius derive a formula for k in terms of the nuclear and electronic charges and the Bohr radius a_0. (b) Solve the time-independent Schrödinger equation for this isotropic oscillator and obtain the eigenfunctions and eigenvalues. (c) Compare the transition frequencies from the ground to any excited state n to the observed Lyman series for the Hydrogen atom. Is this a good model for the Hydrogen atom?

9. Using the virial theorem show that the potential and kinetic energies of any quantum level of quantum harmonic oscillator are always equal irrespective of the number of dimensions involved.

10. The Hamiltonian for the Hydrogen atom is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{Ke^2}{\hat{r}^2}$$

where $\hat{p}$ and $\hat{r}$ are the momentum and distance coordinates of the proton-electron system; $K = 1/4\pi\epsilon_0$, e is the electronic charge and m the electronic mass. If E is the ground state energy of the atom then show that

$$E = -\left\langle \hat{T} \right\rangle = \frac{1}{2}\left\langle \hat{V} \right\rangle$$