Quantum Mechanics

Problem Sheet 5

Basics

1. More commutation relations involving the angular momentum. Remember that both $\hat{\underline{R}}$ and $\hat{\underline{L}}$ are vectors, i.e. each of them is a triplet of operators.

2. More about the Hamiltonian in spherical coordinates. Useful for practice.

3. There are two aspects to this problem: i) you are looking for bound states, i.e. states with $E < 0$; (ii) you are dealing with a 3D problem, with a spherical potential.

4. More practice with matrix elements. Make sure you remember the definition of the matrix element of an operator between two states. Check that you can apply successfully this definition to this simple example.

5. Review the computation of the quantum rotator discussed in the lectures. This problem finishes off the discussion of the energy levels. You are then asked to compute some matrix elements again. Read carefully the question, the solution does not require *long* computations!!

Further problems

1. 3-state system. You **must** try this exercise to make sure you understood the 2-state system that we discussed at length.

2. Parity operator in spherical coordinates.

3. Coupled harmonic oscillators. This exercise is an excellent practice to learn how to use annihilation and creation operators.

Basics

1. Compute the commutation relations of the position operator $\hat{\underline{R}}$ and the angular momentum $\hat{\underline{L}}$. Deduce the commutation relations of $\hat{R}^2$ with the angular momentum $\hat{\underline{L}}$.

2. Let us introduce the operator:

$$\hat{P}_r \psi = -i\hbar \frac{1}{r} \frac{\partial}{\partial r}(r\psi) \, ;$$

   show that the Hamiltonian can be written as:

$$\hat{H} = \frac{1}{2m} \left(\hat{P}_r^2 + \frac{\hat{L}^2}{r^2} \right) \, .$$

3. Find the bound states for a particle with $\ell = 0$ in a three-dimensional spherical potential well:

$$V(r) = \begin{cases} -V_0 \, , & \text{for } r < a \, , \\ 0 \, , & \text{for } r > a \, . \end{cases}$$

4. The space of functions with $\ell = 1$ is a three-dimensional subspace of the space of possible functions $f(\theta\phi)$. A basis for this subspace is given by the three spherical harmonics $Y_1^m(\theta, \phi)$ for $m = -1, 0, 1$. Explicitly construct the three 3×3 matrices that represent L_x, L_y and L_z:

$$(L_i)_{m,m'} = \langle \ell = 1, m | \hat{L}_i | \ell = 1, m' \rangle = \int \sin\theta d\theta d\phi \, Y_1^m(\theta, \phi)^* \hat{L}_i Y_1^{m'}(\theta, \phi) \, .$$

   Compute explicitly using the matrix representation the commutator of $\hat{L}_1$ with $\hat{L}_2$.

   Compute the expectation value of $\hat{L}_x$ in the state

$$\psi(\underline{r}) = F(r) \left[\frac{\sqrt{2}}{\sqrt{5}} Y_1^1(\theta, \phi) - \frac{\sqrt{3}}{\sqrt{5}} Y_1^0(\theta, \phi) \right] \, ,$$

   where $F(r)$ denotes the radial dependence of the wave function.

   What are the possible outcomes if we measure L_z in this state?

5. Compute the energy levels of the quantum rotator discussed in the lectures. Discuss their degeneracy, and compute the distance between successive levels.

   Let $\hat{Z} = r_e \cos\theta$ be the operator associated to the projection of the molecule axis along the z direction. Using the fact that:

$$\cos\theta \, Y_\ell^m(\theta, \phi) = \sqrt{\frac{\ell^2 - m^2}{4\ell^2 - 1}} Y_{\ell-1}^m(\theta, \phi) + \sqrt{\frac{(\ell+1)^2 - m^2}{4(\ell+1)^2 - 1}} Y_{\ell+1}^m(\theta, \phi) \, ,$$

   Show that:

$$\langle \ell', m' | Z | \ell, m \rangle = r_e \delta_{m',m} \left[\delta_{\ell',\ell-1} \sqrt{\frac{\ell^2 - m^2}{4\ell^2 - 1}} + \delta_{\ell',\ell+1} \sqrt{\frac{(\ell+1)^2 - m^2}{4(\ell+1)^2 - 1}} \right] \, .$$

   Deduce the time evolution of $\langle Z(t) \rangle = \langle \Psi(t) | \hat{Z} | \Psi(t) \rangle$, where $\Psi(\theta, \phi, t)$ describes the state of the system at time t.

Further problems

1. Consider a system whose state space is spanned by the orthonormal basis $\mathcal{B} = \{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$. In this basis the Hamiltonian $\hat{H}$ and the two observables $\hat{A}$ and $\hat{B}$ are written as:

$$H = \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad A = a \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad B = b \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

where ω_0, a, and b are positive real constants.

At time $t = 0$ the system is in the state:

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}}|u_1\rangle + \frac{1}{2}|u_2\rangle + \frac{1}{2}|u_3\rangle.$$

What are the possible values of the energy at time $t = 0$? What are the probabilities of finding each of them? Calculate the mean value of the energy for the state $|\Psi(0)\rangle$. A is measured at time $t = 0$. What results can be found, and with what probabilities? What is the state vector immediately after the measurement? Calculate the state vector at time t. What are the possible values of H at time t? Calculate the mean values of H, A, and B at time t. Comments? What results are obtained if A is measured at time t? Same question for B. Interpret your result.

2. The parity operator changes the sign of the position vector of a particle: $\underline{r} \to -\underline{r}$. Express this geometrical transformation in spherical coordinates. Check the properties of the first few spherical harmonics under parity.

3. Consider two harmonic oscillators, 1 and 2, and assume their potential energy to be:

$$V_0(\hat{X}_1, \hat{X}_2) = \frac{1}{2}m\omega^2(\hat{X}_1 - a)^2 + \frac{1}{2}m\omega^2(\hat{X}_2 + a)^2.$$

Factorize the Hamiltonian, and define the creation and annihilation operators. Using the latter find the eigenstates and eigenvalues of the Hamiltonian.

Consider now the case where the two oscillators are coupled by an extra term in the potential:

$$\Delta V = \lambda m\omega^2(\hat{X}_1 - \hat{X}_2)^2.$$

Introduce the observables:

$$\hat{X}_G = \frac{1}{2}(\hat{X}_1 + \hat{X}_2), \quad \hat{P}_G = \hat{P}_1 + \hat{P}_2, \quad \hat{X}_R = (\hat{X}_1 - \hat{X}_2), \quad \hat{P}_R = \frac{1}{2}(\hat{P}_1 - \hat{P}_2).$$

Compute the commutation relations between these new operators. Keeping in mind the commutation relations computed above, rewrite the Hamiltonian in terms of the new operators. (Two new frequencies $\omega_G = \omega$, and $\omega_R = \omega\sqrt{1 + 4\lambda}$ should appear.) Define new creation and annihilation operators, and find the eigenvalues and eigenvectors of the coupled oscillators.