Physics 521, Quantum Mechanics I

Problem Set #10: Angular Momentum in Quantum Mechanics

Cohen-Tannoudji et al., Chapter VI,

Sakurai 3.1, 3.5, 3.6, Merzbacher Chapter 11

Due: Tues. Nov. 25, 2014

Problem 1: Cohen-Tannoudji et al. Vol. I, Prob. 5, p. 767 (10 Points).

Using Spherical Harmonics

Problem 2: Cohen-Tannoudji et al. Vol. I, Prob. 6, p. 768 (20 Points).

The Electric Quadrapole Moment

Problem 3: The Isotropic Harmonic Oscillator in Two Dimensions (25 Points)

Consider a particle moving in a 2D isotropic harmonic potential $\hat{V}(x,y) = \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2)$.

(a) Show that the Hamiltonian commutes with $\hat{L}_z$. Please interpret.

(b) Defining the usual polar coordinates (ρ,ϕ) via $x = \rho\cos\phi$, $y = \rho\sin\phi$, show that the Hamiltonian can be written as

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_\rho^2 + \frac{\hat{L}_z^2}{\rho^2}\right) + \frac{1}{2}m\omega^2\hat{\rho}^2,$$

where $\hat{p}_\rho^2 = -\hbar^2\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)$ is the radial momentum squared and $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$.

(c) Separating coordinates , writing the energy eigenstates $\psi_{n,m}(\rho,\phi) = R_{n,m}(\rho)\Phi_m(\phi)$, with $\Phi_m(\phi)$ the usual eigenstates of $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$, find the "radial equation, for $R_{n,m}(\rho)$.

(d) In class we solved this problem, separating in Cartesian coordinates $\Psi_{n_x,n_y}(x,y) = u_{n_x}(x)u_{n_y}(y)$ where $u_{n_x}(x)$ and $u_{n_y}(y)$ are the usual energy eigenfunctions in 1D. The energy eigenvalues are $E_n = \hbar\omega(n+1)$ with degeneracy $n+1$. It must be possible to expand these eigenfunction in terms of the eigenfunction in polar coordinates. Express the five eigenfunctions $\Psi_{0,0}(x,y)$, $\Psi_{1,0}(x,y)$, $\Psi_{0,1}(x,y)$, $\Psi_{1,1}(x,y)$, $\Psi_{2,0}(x,y)$, $\Psi_{0,2}(x,y)$ in this basis. That is write

$$\Psi_{n_x,n_y}(x,y) = \sum_{m=?}^{?} c_{n,m}\psi_{n,m}(\rho,\phi), \quad n = n_x + n_y,$$

and thus find the eigenstates $\psi_{n,m}(\rho,\phi)$ for n=0,1, and 2.

(e) Show that $R_{n,m}(\rho)$ satisfy the radial equation you found in (c)

(f) Finally, given the state $\Psi_{1,1}(x,y)$, what are the probabilities of finding the system with angular momentum eigenvalues $m = 2,1,0,-1,-2$ respectively?

where L_i, R_j, P_j denote arbitrary components of **L**, **R**, **P** in an orthonormal system, and ε_{ijk} is defined by:

$$\varepsilon_{ijk}\begin{cases} = 0 & \text{if two (or three) of the indices } i, j, k \text{ are equal} \\ = 1 & \text{if these indices are an even permutation of } x, y, z \\ = -1 & \text{if the permutation is odd.}\end{cases}$$

4. Rotation of a polyatomic molecule

Consider a system composed of N different particles, of positions $\mathbf{R}_1, ..., \mathbf{R}_m, ..., \mathbf{R}_N$, and momenta $\mathbf{P}_1, ..., \mathbf{P}_m, ..., \mathbf{P}_N$. We set:

$$\mathbf{J} = \sum_m \mathbf{L}_m$$

with:

$$\mathbf{L}_m = \mathbf{R}_m \times \mathbf{P}_m$$

a. Show that the operator **J** satisfies the commutation relations which define an angular momentum, and deduce from this that if **V** and **V′** denote two ordinary vectors of three-dimensional space, then:

$$[\mathbf{J}\,.\,\mathbf{V}, \mathbf{J}\,.\,\mathbf{V}'] = i\hbar(\mathbf{V} \times \mathbf{V}')\,.\,\mathbf{J}$$

b. Calculate the commutators of **J** with the three components of $\mathbf{R}_m$ and with those of $\mathbf{P}_m$. Show that:

$$[\mathbf{J}, \mathbf{R}_m\,.\,\mathbf{R}_p] = 0$$

c. Prove that:

$$[\mathbf{J}, \mathbf{J}\,.\,\mathbf{R}_m] = 0$$

and deduce from this the relation:

$$[\mathbf{J}\,.\,\mathbf{R}_m, \mathbf{J}\,.\,\mathbf{R}_{m'}] = i\hbar(\mathbf{R}_{m'} \times \mathbf{R}_m)\,.\,\mathbf{J} = i\hbar\ \mathbf{J}\,.\,(\mathbf{R}_{m'} \times \mathbf{R}_m)$$

We set:

$$\mathbf{W} = \sum_m a_m \mathbf{R}_m$$

$$\mathbf{W}' = \sum_m a'_m \mathbf{R}_m$$

where the coefficients a_m and a'_m are given. Show that:

$$[\mathbf{J}\,.\,\mathbf{W}, \mathbf{J}\,.\,\mathbf{W}'] = -\,i\hbar(\mathbf{W} \times \mathbf{W}')\,.\,\mathbf{J}$$

Conclusion: what is the difference between the commutation relations of the components of **J** along fixed axes and those of the components of **J** along the moving axes of the system being studied?

d. Consider a molecule which is formed by N unaligned atoms whose relative distances are assumed to be invariant (a rigid rotator). **J** is the sum of the angular momenta of the atoms with respect to the center of mass of the molecule, situated at a fixed point O; the $Oxyz$ axes constitute a fixed orthonormal frame. The three principal inertial axes of the system are denoted by $O\alpha$, $O\beta$ and $O\gamma$, with the ellipsoid of inertia assumed to be an ellipsoid of revolution about $O\gamma$ (a symmetrical rotator). The rotational energy of the molecule is then:

$$H = \frac{1}{2}\left[\frac{J_\gamma^2}{I_{//}} + \frac{J_\alpha^2 + J_\beta^2}{I_\perp}\right]$$

where J_α, J_β and J_γ are the components of **J** along the unit vectors $\mathbf{w}_\alpha$, $\mathbf{w}_\beta$ and $\mathbf{w}_\gamma$ of the moving axes $O\alpha$, $O\beta$, $O\gamma$ attached to the molecule, and $I_{//}$ and $I_\perp$ are the corresponding moments of inertia. We grant that:

$$J_\alpha^2 + J_\beta^2 + J_\gamma^2 = J_x^2 + J_y^2 + J_z^2 = \mathbf{J}^2$$

(*i*) Derive the commutation relations of J_α, J_β, J_γ from the results of *c*.

(*ii*) We introduce the operators $N_\pm = J_\alpha \pm iJ_\beta$. Using the general arguments of chapter VI, show that one can find eigenvectors common to $\mathbf{J}^2$ and J_γ, of eigenvalues $J(J+1)\hbar^2$ and $K\hbar$, with $K = -J, -J+1, ..., J-1, J$.

(*iii*) Express the Hamiltonian H of the rotator in terms of $\mathbf{J}^2$ and J_γ^2. Find its eigenvalues.

(*iv*) Show that one can find eigenstates common to $\mathbf{J}^2$, J_z and J_γ, to be denoted by $|J, M, K\rangle$ [the respective eigenvalues are $J(J+1)\hbar^2$, $M\hbar$, $K\hbar$]. Show that these states are also eigenstates of H.

(*v*) Calculate the commutators of $J_\pm$ and $N_\pm$ with $\mathbf{J}^2$, J_z, J_γ. Derive from them the action of $J_\pm$ and $N_\pm$ on $|J, M, K\rangle$. Show that the eigenvalues of H are at least $2(2J+1)$-fold degenerate if $K \neq 0$, and $(2J+1)$-fold degenerate if $K = 0$.

(*vi*) Draw the energy diagram of the rigid rotator (J is an integer since **J** is a sum of orbital angular momenta; *cf.* chapter X). What happens to this diagram when $I_{//} = I_\perp$ (spherical rotator)?

5. A system whose state space is $\mathscr{E}_\mathbf{r}$ has for its wave function:

$$\psi(x, y, z) = N(x + y + z)\,e^{-r^2/\alpha^2}$$

where α, which is real, is given and N is a normalization constant.

a. The observables L_z and $\mathbf{L}^2$ are measured; what are the probabilities of finding 0 and $2\hbar^2$? Recall that:

$$Y_1^0(\theta, \varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

b. If one also uses the fact that:

$$Y_1^{\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi}$$

is it possible to predict directly the probabilities of all possible results of measurements of $\mathbf{L}^2$ and L_z in the system of wave function $\psi(x, y, z)$?

6. Consider a system of angular momentum $l = 1$. A basis of its state space is formed by the three eigenvectors of L_z : $|+1\rangle$, $|0\rangle$, $|-1\rangle$, whose eigenvalues are, respectively, $+\hbar$, 0, and $-\hbar$, and which satisfy:

$$L_\pm \,|\, m \rangle = \hbar\sqrt{2}\,|\, m \pm 1 \rangle$$
$$L_+ \,|\, 1 \rangle = L_- \,|\, -1 \rangle = 0$$

This system, which possesses an electric quadrupole moment, is placed in an electric field gradient, so that its Hamiltonian can be written:

$$H = \frac{\omega_0}{\hbar}(L_u^2 - L_v^2)$$

where L_u and L_v are the components of **L** along the two directions Ou and Ov of the xOz plane which form angles of 45° with Ox and Oz; ω_0 is a real constant.

a. Write the matrix which represents H in the $\{ |+1\rangle, |0\rangle, |-1\rangle \}$ basis. What are the stationary states of the system, and what are their energies? (These states are to be written $|E_1\rangle$, $|E_2\rangle$, $|E_3\rangle$, in order of decreasing energies.)

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

$$|\,\psi(0)\,\rangle = \frac{1}{\sqrt{2}}[\,|+1\rangle - |-1\rangle]$$

What is the state vector $|\psi(t)\rangle$ at time t? At t, L_z is measured; what are the probabilities of the various possible results?

c. Calculate the mean values $\langle L_x \rangle(t)$, $\langle L_y \rangle(t)$ and $\langle L_z \rangle(t)$ at t. What is the motion performed by the vector $\langle \mathbf{L} \rangle$?

d. At t, a measurement of L_z^2 is performed.

(*i*) Do times exist when only one result is possible?

(*ii*) Assume that this measurement has yielded the result $\hbar^2$. What is the state of the system immediately after the measurement? Indicate, without calculation, its subsequent evolution.

7. Consider rotations in ordinary three-dimensional space, to be denoted by $\mathscr{R}_{\mathbf{u}}(\alpha)$, where **u** is the unit vector which defines the axis of rotation and α is the angle of rotation.

a. Show that, if M' is the transform of M under an infinitesimal rotation of angle ε, then:

$$\mathbf{OM'} = \mathbf{OM} + \varepsilon\mathbf{u} \times \mathbf{OM}$$

b. If **OM** is represented by the column vector $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$, what is the matrix associated with $\mathscr{R}_{\mathbf{u}}(\varepsilon)$? Derive from it the matrices which represent the components of the operator $\mathscr{M}$ defined by:

$$\mathscr{R}_{\mathbf{u}}(\varepsilon) = 1 + \varepsilon\, \mathscr{M}.\,\mathbf{u}$$