Complement F_{VI}

EXERCISES

1. Consider a system of angular momentum $j = 1$, whose state space is spanned by the basis $\{ | +1 \rangle, | 0 \rangle, | -1 \rangle \}$ of three eigenvectors common to $\mathbf{J}^2$ (eigenvalue $2\hbar^2$) and J_z (respective eigenvalues $+\hbar$, 0 and $-\hbar$). The state of the system is:

$$| \psi \rangle = \alpha | +1 \rangle + \beta | 0 \rangle + \gamma | -1 \rangle$$

where α, β, γ are three given complex parameters.

a. Calculate the mean value $\langle \mathbf{J} \rangle$ of the angular momentum in terms of α, β and γ.

b. Give the expression for the three mean values $\langle J_x^2 \rangle$, $\langle J_y^2 \rangle$ and $\langle J_z^2 \rangle$ in terms of the same quantities.

2. Consider an arbitrary physical system whose four-dimensional state space is spanned by a basis of four eigenvectors $| j, m_z \rangle$ common to $\mathbf{J}^2$ and J_z ($j = 0$ or 1; $-j \leqslant m_z \leqslant +j$), of eigenvalues $j(j+1)\hbar^2$ and $m_z\hbar$, such that:

$$J_{\pm} | j, m_z \rangle = \hbar \sqrt{j(j+1) - m_z(m_z \pm 1)} \, | j, m_z \pm 1 \rangle$$
$$J_+ | j, j \rangle = J_- | j, -j \rangle = 0$$

a. Express in terms of the kets $| j, m_z \rangle$, the eigenstates common to $\mathbf{J}^2$ and J_x, to be denoted by $| j, m_x \rangle$.

b. Consider a system in the normalized state:

$$| \psi \rangle = \alpha | j = 1, m_z = 1 \rangle + \beta | j = 1, m_z = 0 \rangle + \gamma | j = 1, m_z = -1 \rangle + \delta | j = 0, m_z = 0 \rangle$$

(*i*) What is the probability of finding $2\hbar^2$ and $\hbar$ if $\mathbf{J}^2$ and J_x are measured simultaneously?

(*ii*) Calculate the mean value of J_z when the system is in the state $| \psi \rangle$, and the probabilities of the various possible results of a measurement bearing only on this observable.

(*iii*) Same questions for the observable $\mathbf{J}^2$ and for J_x.

(*iv*) J_z^2 is now measured; what are the possible results, their probabilities, and their mean value?

3. Let $\mathbf{L} = \mathbf{R} \times \mathbf{P}$ be the angular momentum of a system whose state is $\mathscr{E}_{\mathbf{r}}$. Prove the commutation relations :

$$[L_i, R_j] = i\hbar \, \varepsilon_{ijk} \, R_k$$
$$[L_i, P_j] = i\hbar \, \varepsilon_{ijk} \, P_k$$
$$[L_i, \mathbf{P}^2] = [L_i, \mathbf{R}^2] = [L_i, \mathbf{R} \cdot \mathbf{P}] = 0$$

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:

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

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 $\mathbf{J}$ 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 $\mathbf{J}$ 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 $\mathbf{L}$ 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 $\mathcal{R}_{\mathbf{u}}(\alpha)$, where $\mathbf{u}$ 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 $\mathbf{OM}$ is represented by the column vector $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$, what is the matrix associated with $\mathcal{R}_{\mathbf{u}}(\varepsilon)$? Derive from it the matrices which represent the components of the operator $\boldsymbol{\mathcal{M}}$ defined by:

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

c. Calculate the commutators :

$$[\mathcal{M}_x, \mathcal{M}_y]; \quad [\mathcal{M}_y, \mathcal{M}_z]; \quad [\mathcal{M}_z, \mathcal{M}_x]$$

What are the quantum mechanical analogues of the purely geometrical relations obtained ?

d. Starting with the matrix which represents $\mathcal{M}_z$, calculate the one which represents $e^{\alpha \mathcal{M}_z}$; show that $\mathcal{R}_z(\alpha) = e^{\alpha \mathcal{M}_z}$; what is the analogue of this relation in quantum mechanics?

8. Consider a particle in three-dimensional space, whose state vector is $|\psi\rangle$, and whose wave function is $\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle$. Let A be an observable which commutes with $\mathbf{L} = \mathbf{R} \times \mathbf{P}$, the orbital angular momentum of the particle. Assuming that A, $\mathbf{L}^2$ and L_z form a C.S.C.O. in $\mathscr{E}_\mathbf{r}$, call $|n, l, m\rangle$ their common eigenkets, whose eigenvalues are, respectively, a_n (the index n is assumed to be discrete), $l(l+1)\hbar^2$ and $m\hbar$.

Let $U(\varphi)$ be the unitary operator defined by:

$$U(\varphi) = e^{-i\varphi L_z/\hbar}$$

where φ is a real dimensionless parameter. For an arbitrary operator K, we call $\tilde{K}$ the transform of K by the unitary operator $U(\varphi)$:

$$\tilde{K} = U(\varphi) K U^\dagger(\varphi)$$

a. We set $L_+ = L_x + iL_y$, $L_- = L_x - iL_y$. Calculate $\tilde{L}_+ |n, l, m\rangle$ and show that L_+ and $\tilde{L}_+$ are proportional; calculate the proportionality constant. Same question for L_- and $\tilde{L}_-$.

b. Express $\tilde{L}_x$, $\tilde{L}_y$ and $\tilde{L}_z$ in terms of L_x, L_y and L_z. What geometrical transformation can be associated with the transformation of $\mathbf{L}$ into $\tilde{\mathbf{L}}$?

c. Calculate the commutators $[X \pm iY, L_z]$ and $[Z, L_z]$. Show that the kets $(X \pm iY)|n, l, m\rangle$ and $Z|n, l, m\rangle$ are eigenvectors of L_z and calculate their eigenvalues. What relation must exist between m and m' for the matrix element $\langle n', l', m' | X \pm iY | n, l, m\rangle$ to be non-zero? Same question for:

$$\langle n', l', m' | Z | n, l, m\rangle.$$

d. By comparing the matrix elements of $\widetilde{X \pm iY}$ and $\tilde{Z}$ with those of $X \pm iY$ and Z, calculate $\tilde{X}$, $\tilde{Y}$, $\tilde{Z}$ in terms of X, Y, Z. Give a geometrical interpretation.

9. Consider a physical system of fixed angular momentum l, whose state space is $\mathscr{E}_l$, and whose state vector is $|\psi\rangle$; its orbital angular momentum operator is denoted by $\mathbf{L}$. We assume that a basis of $\mathscr{E}_l$ is composed of $2l+1$ eigenvectors $|l, m\rangle$ of L_z $(-l \leqslant m \leqslant +l)$, associated with the wave functions $f(r)Y_l^m(\theta, \varphi)$. We call $\langle \mathbf{L} \rangle = \langle \psi | \mathbf{L} | \psi \rangle$ the mean value of $\mathbf{L}$.

a. We begin by assuming that:

$$\langle L_x \rangle = \langle L_y \rangle = 0$$

Out of all the possible states of the system, what are those for which the sum $(\Delta L_x)^2 + (\Delta L_y)^2 + (\Delta L_z)^2$ is minimal? Show that, for these states, the root-mean-square deviation ΔL_α of the component of $\mathbf{L}$ along an axis which is at an angle α with Oz is given by:

$$\Delta L_\alpha = \hbar \sqrt{\frac{l}{2}} \sin \alpha$$

b. We now assume that $\langle \mathbf{L} \rangle$ has an arbitrary direction with respect to the $Oxyz$ axes. We denote by $OXYZ$ a frame whose OZ axis is directed along $\langle \mathbf{L} \rangle$, with the OY axis in the xOy plane.

(*i*) Show that the state $| \psi_0 \rangle$ of the system for which:

$$(\Delta L_x)^2 + (\Delta L_y)^2 + (\Delta L_z)^2$$

is minimal is such that:

$$(L_x + iL_y) | \psi_0 \rangle = 0$$
$$L_z | \psi_0 \rangle = l\hbar | \psi_0 \rangle$$

(*ii*) Let θ_0 be the angle between Oz and OZ, and φ_0, the angle between Oy and OY; prove the relations:

$$L_X + iL_Y = \cos^2 \frac{\theta_0}{2} e^{-i\varphi_0} L_+ - \sin^2 \frac{\theta_0}{2} e^{i\varphi_0} L_- - \sin \theta_0 L_z$$

$$L_Z = \sin \frac{\theta_0}{2} \cos \frac{\theta_0}{2} e^{-i\varphi_0} L_+ + \sin \frac{\theta_0}{2} \cos \frac{\theta_0}{2} e^{i\varphi_0} L_- + \cos \theta_0 L_z$$

If we set:

$$| \psi_0 \rangle = \sum_m d_m | l, m \rangle$$

show that:

$$d_m = \tan \frac{\theta_0}{2} e^{i\varphi_0} \sqrt{\frac{l + m + 1}{l - m}} d_{m+1}$$

Express d_m in terms of d_l, θ_0, φ_0 and l.

(*iii*) To calculate d_l, show that the wave function associated with $| \psi_0 \rangle$ is $\psi_0(X, Y, Z) = c_l \dfrac{(X + iY)^l}{r^l} f(r)$ [where c_l is defined by equation (D-20) of chapter VI], the one associated with $| l, l \rangle$ being $c_l \dfrac{(x + iy)^l}{r^l} f(r)$. By replacing X, Y and Z in this expression for $\psi_0(X, Y, Z)$ by their values in terms of x, y, z, find the value of d_l and the relation:

$$d_m = \left(\sin \frac{\theta_0}{2} \right)^{l-m} \left(\cos \frac{\theta_0}{2} \right)^{l+m} e^{-im\varphi_0} \sqrt{\frac{(2l)!}{(l + m)! \, (l - m)!}}$$

(*iv*) With the system in the state $|\psi_0\rangle$, L_z is measured. What are the probabilities of the various possible results? What is the most probable result? Show that, if l is much greater than 1, the results correspond to the classical limit.

10. Let $\mathbf{J}$ be the angular momentum operator of an arbitrary physical system whose state vector is $|\psi\rangle$.

a. Can states of the system be found for which the root-mean-square deviations ΔJ_x, ΔJ_y and ΔJ_z are simultaneously zero?

b. Prove the relation:

$$\Delta J_x \,.\, \Delta J_y \geqslant \frac{\hbar}{2}|\langle J_z \rangle|$$

and those obtained by cyclic permutation of x, y, z.

Let $\langle \mathbf{J} \rangle$ be the mean value of the angular momentum of the system. The $Oxyz$ axes are assumed to be chosen in such a way that $\langle J_x \rangle = \langle J_y \rangle = 0$. Show that:

$$(\Delta J_x)^2 + (\Delta J_y)^2 \geqslant \hbar\,|\langle J_z \rangle|$$

c. Show that the two inequalities proven in question *b.* both become equalities if and only if $J_+|\psi\rangle = 0$ or $J_-|\psi\rangle = 0$.

d. The system under consideration is a spinless particle for which $\mathbf{J} = \mathbf{L} = \mathbf{R} \times \mathbf{P}$. Show that it is not possible to have both $\Delta L_x \,.\, \Delta L_y = \frac{\hbar}{2}|\langle L_z \rangle|$ and $(\Delta L_x)^2 + (\Delta L_y)^2 = \hbar\,|\langle L_z \rangle|$ unless the wave function of the system is of the form:

$$\psi(r, \theta, \varphi) = F(r, \sin\theta\, e^{\pm i\varphi})$$

11. Consider a three-dimensional harmonic oscillator, whose state vector $|\psi\rangle$ is:

$$|\psi\rangle = |\alpha_x\rangle \otimes |\alpha_y\rangle \otimes |\alpha_z\rangle$$

where $|\alpha_x\rangle$, $|\alpha_y\rangle$ and $|\alpha_z\rangle$ are quasi-classical states (*cf.* complement G_V) for one-dimensional harmonic oscillators moving along Ox, Oy and Oz, respectively. Let $\mathbf{L} = \mathbf{R} \times \mathbf{P}$ be the orbital angular momentum of the three-dimensional oscillator.

a. Prove:

$$\langle L_z \rangle = i\hbar\,(\alpha_x \alpha_y^* - \alpha_x^* \alpha_y)$$
$$\Delta L_z = \hbar\sqrt{|\alpha_x|^2 + |\alpha_y|^2}$$

and the analogous expressions for the components of $\mathbf{L}$ along Ox and Oy.

b. We now assume that:

$$\langle L_x \rangle = \langle L_y \rangle = 0 \quad , \quad \langle L_z \rangle = \lambda\hbar > 0$$

Show that α_z must be zero. We then fix the value of λ. Show that, in order to minimize $\Delta L_x + \Delta L_y$, we must choose:

$$\alpha_x = - i\alpha_y = \sqrt{\frac{\lambda}{2}}\, e^{i\varphi_0}$$

(where φ_0 is an arbitrary real number). Do the expressions $\Delta L_x \,.\, \Delta L_y$ and $(\Delta L_x)^2 + (\Delta L_y)^2$ in this case have minimum values which are compatible with the inequalities obtained in question *b.* of the preceding exercise?

c. Show that the state of a system for which the preceding conditions are satisfied is necessarily of the form:

$$| \psi \rangle = \sum_k c_k(\alpha_d) \,| \chi_{n_d = k, n_g = 0, n_z = 0} \rangle$$

with:

$$| \chi_{n_d = k, n_g = 0, n_z = 0} \rangle = \frac{(a_x^\dagger + i a_y^\dagger)^k}{\sqrt{2^k k!}} \,| \varphi_{n_x = 0, n_y = 0, n_z = 0} \rangle$$

$$c_k(\alpha) = \frac{\alpha^k}{\sqrt{k!}}\, e^{-|\alpha|^2/2} \quad ; \quad \alpha_d = e^{i\varphi_0} \sqrt{\lambda}$$

(the results of complement G_V and of § 4 of complement D_{VI} can be used). Show that the angular dependence of $| \chi_{n_d = k, n_g = 0, n_z = 0} \rangle$ is $(\sin\theta\, e^{i\varphi})^k$.

$\mathbf{L}^2$ is measured on a system in the state $| \psi \rangle$. Show that the probabilities of the various possible results are given by a Poisson distribution. What results can be obtained in a measurement of L_z which follows a measurement of $\mathbf{L}^2$ whose result was $l(l + 1)\hbar^2$?

Reference:

Exercise 4: Landau and Lifshitz (1.19), § 101; Ter Haar (1.23), §§8.13 and 8.14.