

Mecânica Quântica II - FFI 0122

Lista 1

Data de Entrega: 1 de Setembro de 2015, terça-feira

1. Todos os exercícios do capítulo VI (Complemento F_{VI}) do livro do Cohen-Tannoudji. Ver cópia anexa.

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 ; $-j \leq m_z \leq +j$), 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 \mathcal{E}_r . Prove the commutation relations:

$$[L_i, R_j] = i\hbar \varepsilon_{ijk} R_k$$

$$[L_i, P_j] = i\hbar \varepsilon_{ijk} P_k$$

$$[L_i, \mathbf{P}^2] = [L_i, \mathbf{R}^2] = [\mathbf{L}, \mathbf{R} \cdot \mathbf{P}] = 0$$

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5-b)

nd :

36)

37)

38)

9)

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where L_i, R_j, P_j denote arbitrary components of $\mathbf{L}, \mathbf{R}, \mathbf{P}$ 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 $\mathbf{R}_1, \dots, \mathbf{R}_m, \dots, \mathbf{R}_N$, and momenta $\mathbf{P}_1, \dots, \mathbf{P}_m, \dots, \mathbf{P}_N$. 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 \mathbf{J} satisfies the commutation relations which define an angular momentum, and deduce from this that if \mathbf{V} and \mathbf{V}' denote two ordinary vectors of three-dimensional space, then:

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

b. Calculate the commutators of \mathbf{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:

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

and deduce from this the relation:

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

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:

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

Conclusion: what is the difference between the commutation relations of the components of \mathbf{J} along fixed axes and those of the components of \mathbf{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). \mathbf{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:

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

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}_γ of the moving axes $O\alpha, O\beta, O\gamma$ attached to the molecule, and I_\parallel 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 $J_\alpha, J_\beta, J_\gamma$ 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 $K = -J, -J+1, \dots, J-1, J$.

(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_y , 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_y . 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 $I_\parallel = I_\perp$ (spherical rotator)?

5. A system whose state space is \mathcal{E}_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 \mathcal{M} defined by:

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

c. Calculate the commutators:

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

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 , L^2 and L_z form a C.S.C.O. in \mathcal{E}_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 \mathcal{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 \mathcal{E}_l is composed of $2l+1$ eigenvectors $|l, m\rangle$ of L_z ($-l \leq m \leq +l$), 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_x of the component of \mathbf{L} along an axis which is at an angle α with Oz is given by:

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

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:

$$\begin{aligned} (L_x + iL_y)|\psi_0\rangle &= 0 \\ L_z|\psi_0\rangle &= l\hbar|\psi_0\rangle \end{aligned}$$

(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 $\psi_0(X, Y, Z) = c_l \frac{(X + iY)^l}{r^l} f(r)$ [where c_l is defined by equation (D-20) of chapter VI], the one associated with $|l, l\rangle$ being $c_l \frac{(x + iy)^l}{r^l} f(r)$. 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:

$$\Delta J_x \cdot \Delta J_y \geq \frac{\hbar}{2} |\langle J_z \rangle|$$

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:

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

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 $\Delta L_x \cdot \Delta L_y = \frac{\hbar}{2} |\langle L_z \rangle|$ 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:

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

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

b. We now assume that:

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

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 ΔL_x , ΔL_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:

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

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

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

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 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.

CHAPTER VII

Particle in a central potential. The hydrogen atom