Complement L_{III}

EXERCISES

1. In a one-dimensional problem, consider a particle whose wave function is :

$$\psi(x) = N \frac{e^{ip_0 x/\hbar}}{\sqrt{x^2 + a^2}}$$

where a and p_0 are real constants and N is a normalization coefficient.

a. Determine N so that $\psi(x)$ is normalized.

b. The position of the particle is measured. What is the probability of finding a result between $-\frac{a}{\sqrt{3}}$ and $+\frac{a}{\sqrt{3}}$?

c. Calculate the mean value of the momentum of a particle which has $\psi(x)$ for its wave function.

2. Consider, in a one-dimensional problem, a particle of mass m whose wave function at time t is $\psi(x, t)$.

a. At time t, the distance d of this particle from the origin is measured. Write, as a function of $\psi(x, t)$, the probability $\mathscr{P}(d_0)$ of finding a result greater than a given length d_0. What are the limits of $\mathscr{P}(d_0)$ when $d_0 \longrightarrow 0$ and $d_0 \longrightarrow \infty$?

b. Instead of performing the measurement of question *a*, one measures the velocity v of the particle at time t. Express, as a function of $\psi(x, t)$, the probability of finding a result greater than a given value v_0.

3. The wave function of a free particle, in a one-dimensional problem, is given at time $t = 0$ by :

$$\psi(x, 0) = N \int_{-\infty}^{+\infty} dk \, e^{-|k|/k_0} \, e^{ikx}$$

where k_0 and N are constants.

a. What is the probability $\mathscr{P}(p_1, 0)$ that a measurement of the momentum, performed at time $t = 0$, will yield a result included between $-p_1$ and $+p_1$? Sketch the function $\mathscr{P}(p_1, 0)$.

b. What happens to this probability $\mathscr{P}(p_1, t)$ if the measurement is performed at time t ? Interpret.

c. What is the form of the wave packet at time $t = 0$? Calculate for this time the product $\Delta X \, . \, \Delta P$; what is your conclusion? Describe qualitatively the subsequent evolution of the wave packet.

4. Spreading of a free wave packet

Consider a free particle.

a. Show, applying Ehrenfest's theorem, that $\langle X \rangle$ is a linear function of time, the mean value $\langle P \rangle$ remaining constant.

b. Write the equations of motion for the mean values $\langle X^2 \rangle$ and $\langle XP + PX \rangle$. Integrate these equations.

c. Show that, with a suitable choice of the time origin, the root-mean-square deviation ΔX is given by :

$$(\Delta X)^2 = \frac{1}{m^2}(\Delta P)_0^2\, t^2 + (\Delta X)_0^2$$

where $(\Delta X)_0$ and $(\Delta P)_0$ are the root-mean-square deviations at the initial time.

How does the width of the wave packet vary as a function of time (see § 3-c of complement G_I)? Give a physical interpretation.

5. Particle subject to a constant force

In a one-dimensional problem, consider a particle of potential energy $V(X) = -fX$, where f is a positive constant [$V(X)$ arises, for example, from a gravity field or a uniform electric field].

a. Write Ehrenfest's theorem for the mean values of the position X and the momentum P of the particle. Integrate these equations; compare with the classical motion.

b. Show that the root-mean-square deviation ΔP does not vary over time.

c. Write the Schrödinger equation in the $\{ | p \rangle \}$ representation. Deduce from it a relation between $\frac{\partial}{\partial t} | \langle p | \psi(t) \rangle |^2$ and $\frac{\partial}{\partial p} | \langle p | \psi(t) \rangle |^2$. Integrate the equation thus obtained; give a physical interpretation.

6. Consider the three-dimensional wave function

$$\psi(x, y, z) = N\, e^{-\left[\frac{|x|}{2a} + \frac{|y|}{2b} + \frac{|z|}{2c}\right]}$$

where a, b and c are three positive lengths.

a. Calculate the constant N which normalizes ψ.

b. Calculate the probability that a measurement of X will yield a result included between 0 and a.

c. Calculate the probability that simultaneous measurements of Y and Z will yield results included respectively between $-b$ and $+b$, and $-c$ and $+c$.

d. Calculate the probability that a measurement of the momentum will yield a result included in the element $dp_x dp_y dp_z$ centered at the point $p_x = p_y = 0$; $p_z = \hbar/c$.

7. Let $\psi(x, y, z) = \psi(\mathbf{r})$ be the normalized wave function of a particle. Express in terms of $\psi(\mathbf{r})$ the probability for:

a. a measurement of the abscissa X, to yield a result included between x_1 and x_2;

b. a measurement of the component P_x of the momentum, to yield a result included between p_1 and p_2;

c. simultaneous measurements of X and P_z, to yield:

$$x_1 \leqslant x \leqslant x_2$$
$$p_z \geqslant 0$$

d. simultaneous measurements of P_x, P_y, P_z, to yield:

$$p_1 \leqslant p_x \leqslant p_2$$
$$p_3 \leqslant p_y \leqslant p_4$$
$$p_5 \leqslant p_z \leqslant p_6$$

Show that this probability is equal to the result of b when $p_3, p_5 \longrightarrow -\infty$; $p_1, p_6 \longrightarrow +\infty$;

e. a measurement of the component $U = \frac{1}{\sqrt{3}}(X + Y + Z)$ of the position, to yield a result included between u_1 and u_2.

8. Let $\mathbf{J}(\mathbf{r})$ be the probability current associated with a wave function $\psi(\mathbf{r})$ describing the state of a particle of mass m [chap. III, relations (D-17) and (D-19)].

a. Show that:

$$m \int d^3r \; \mathbf{J}(\mathbf{r}) = \langle \mathbf{P} \rangle$$

where $\langle \mathbf{P} \rangle$ is the mean value of the momentum.

b. Consider the operator $\mathbf{L}$ (orbital angular momentum) defined by $\mathbf{L} = \mathbf{R} \times \mathbf{P}$. Are the three components of $\mathbf{L}$ Hermitian operators? Establish the relation:

$$m \int d^3r \; [\mathbf{r} \times \mathbf{J}(\mathbf{r})] = \langle \mathbf{L} \rangle.$$

9. One wants to show that the physical state of a (spinless) particle is completely defined by specifying the probability density $\rho(\mathbf{r}) = |\psi(\mathbf{r})|^2$ and the probability current $\mathbf{J}(\mathbf{r})$.

a. Assume the function $\psi(\mathbf{r})$ known and let $\xi(\mathbf{r})$ be its argument:

$$\psi(\mathbf{r}) = \sqrt{\rho(\mathbf{r})}\, e^{i\xi(\mathbf{r})}$$

Show that:

$$\mathbf{J}(\mathbf{r}) = \frac{\hbar}{m}\, \rho(\mathbf{r})\, \nabla\xi(\mathbf{r})$$

Deduce that two wave functions leading to the same density $\rho(\mathbf{r})$ and current $\mathbf{J}(\mathbf{r})$ can differ only by a global phase factor.

b. Given arbitrary functions $\rho(\mathbf{r})$ and $\mathbf{J}(\mathbf{r})$, show that a quantum state $\psi(\mathbf{r})$ can be associated with them only if $\nabla \times \mathbf{v}(\mathbf{r}) = 0$, where $\mathbf{v}(\mathbf{r}) = \mathbf{J}(\mathbf{r})/\rho(\mathbf{r})$ is the velocity associated with the probability fluid.

c. Now assume that the particle is submitted to a magnetic field $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ [see chap. III, definition (D-20) of the probability current in this case]. Show that:

$$\mathbf{J} = \frac{\rho(\mathbf{r})}{m}\left[\hbar \nabla \xi(\mathbf{r}) - q\mathbf{A}(\mathbf{r})\right]$$

and:

$$\nabla \times \mathbf{v}(\mathbf{r}) = -\frac{q}{m}\mathbf{B}(\mathbf{r})$$

10. Virial theorem

a. In a one-dimensional problem, consider a particle with the Hamiltonian:

$$H = \frac{P^2}{2m} + V(X)$$

where:

$$V(X) = \lambda X^n$$

Calculate the commutator $[H, XP]$. If there exists one or several stationary states $|\varphi\rangle$ in the potential V, show that the mean values $\langle T \rangle$ and $\langle V \rangle$ of the kinetic and potential energies in these states satisfy the relation: $2\langle T \rangle = n\langle V \rangle$.

b. In a three-dimensional problem, H is written:

$$H = \frac{\mathbf{P}^2}{2m} + V(\mathbf{R})$$

Calculate the commutator $[H, \mathbf{R} \cdot \mathbf{P}]$. Assume that $V(\mathbf{R})$ is a homogeneous function of nth order in the variables X, Y, Z. What relation necessarily exists between the mean kinetic energy and the mean potential energy of the particle in a stationary state?

Apply this to a particle moving in the potential $V(r) = -e^2/r$ (hydrogen atom).

Recall that a homogeneous function V of nth degree in the variables x, y and z by definition satisfies the relation:

$$V(\alpha x, \alpha y, \alpha z) = \alpha^n V(x, y, z)$$

and satisfies Euler's identity:

$$x\frac{\partial V}{\partial x} + y\frac{\partial V}{\partial y} + z\frac{\partial V}{\partial z} = nV(x, y, z).$$

c. Consider a system of N particles of positions $\mathbf{R}_i$ and momenta $\mathbf{P}_i$ ($i = 1, 2, \ldots N$). When their potential energy is a homogeneous (nth degree) function of the set of components X_i, Y_i, Z_i, can the results obtained above be generalized? An application of this can be made to the study of an arbitrary molecule formed of nuclei of charges $-Z_i q$ and electrons of charge q. All these particles interact by pairs through Coulomb forces. In a stationary state of the molecule, what relation exists between the kinetic energy of the system of particles and their energy of mutual interaction?

11. Two-particle wave function

In a one-dimensional problem, consider a system of two particles (1) and (2) with which is associated the wave function $\psi(x_1, x_2)$.

a. What is the probability of finding, in a measurement of the positions X_1 and X_2 of the two particles, a result such that:

$$x \leqslant x_1 \leqslant x + \mathrm{d}x$$
$$\alpha \leqslant x_2 \leqslant \beta$$

b. What is the probability of finding particle (1) between x and $x + \mathrm{d}x$ [when no observations are made on particle (2)]?

c. Give the probability of finding at least one of the particles between α and β.

d. Give the probability of finding one and only one particle between α and β.

e. What is the probability of finding the momentum of particle (1) included between p' and p'' and the position of particle (2) between α and β?

f. The momenta P_1 and P_2 of the two particles are measured; what is the probability of finding $p' \leqslant p_1 \leqslant p''$; $p''' \leqslant p_2 \leqslant p''''$?

g. The only quantity measured is the momentum P_1 of the first particle. Calculate, first from the results of *e* and then from those of *f*, the probability of finding this momentum included between p' and p''. Compare the two results obtained.

h. The algebraic distance $X_1 - X_2$ between the two particles is measured; what is the probability of finding a result included between $-d$ and $+d$? What is the mean value of this distance?

12. Infinite one-dimensional well

Consider a particle of mass m submitted to the potential:

$$V(x) = 0 \quad \text{if} \quad 0 \leqslant x \leqslant a.$$
$$V(x) = +\infty \quad \text{if} \quad x < 0 \quad \text{or} \quad x > a.$$

$|\varphi_n\rangle$ are the eigenstates of the Hamiltonian H of the system, and their eigenvalues are $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$ (*cf.* complement $\mathrm{H_I}$). The state of the particle at the instant $t = 0$ is:

$$|\psi(0)\rangle = a_1\,|\varphi_1\rangle + a_2\,|\varphi_2\rangle + a_3\,|\varphi_3\rangle + a_4\,|\varphi_4\rangle$$

a. What is the probability, when the energy of the particle in the state $|\psi(0)\rangle$ is measured, of finding a value smaller than $\frac{3\pi^2\hbar^2}{ma^2}$?

b. What is the mean value and what is the root-mean-square deviation of the energy of the particle in the state $|\psi(0)\rangle$?

c. Calculate the state vector $|\psi(t)\rangle$ at the instant t. Do the results found in *a* and *b* at the instant $t = 0$ remain valid at an arbitrary time t?

d. When the energy is measured, the result $\frac{8\pi^2\hbar^2}{ma^2}$ is found. After the measurement, what is the state of the system? What is the result if the energy is measured again?

13. Infinite two-dimensional well (*cf.* complement G_{II})

In a two-dimensional problem, consider a particle of mass m; its Hamiltonian H is written:

$$H = H_x + H_y$$

with:

$$H_x = \frac{P_x^2}{2m} + V(X) \qquad H_y = \frac{P_y^2}{2m} + V(Y)$$

The potential energy $V(x)$ [or $V(y)$] is zero when x (or y) is included in the interval $[0, a]$ and is infinite everywhere else.

a. Of the following sets of operators, which form a C.S.C.O.?

$$\{ H \}, \{ H_x \}, \{ H_x, H_y \}, \{ H, H_x \}$$

b. Consider a particle whose wave function is:

$$\psi(x, y) = N \cos\frac{\pi x}{a} \cos\frac{\pi y}{a} \sin\frac{2\pi x}{a} \sin\frac{2\pi y}{a}$$

when $0 \leqslant x \leqslant a$ and $0 \leqslant y \leqslant a$, and is zero everywhere else (where N is a constant).

α. What is the mean value $\langle H \rangle$ of the energy of the particle? If the energy H is measured, what results can be found, and with what probabilities?

β. The observable H_x is measured; what results can be found, and with what probabilities? If this measurement yields the result $\frac{\pi^2\hbar^2}{2ma^2}$, what will be the results of a subsequent measurement of H_y, and with what probabilities?

γ. Instead of performing the preceding measurements, one now performs a simultaneous measurement of H_x and P_y. What are the probabilities of finding :

$$E_x = \frac{9\pi^2\hbar^2}{2ma^2}$$

and :

$$p_0 \leqslant p_y \leqslant p_0 + \mathrm{d}p \text{ ?}$$

14. Consider a physical system whose state space, which is three-dimensional, is spanned by the orthonormal basis formed by the three kets $|u_1\rangle$, $|u_2\rangle$, $|u_3\rangle$. In this basis, the Hamiltonian operator H of the system and the two observables A and B are written:

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

where ω_0, a and b are positive real constants.

The physical system at time $t = 0$ is in the state:

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

a. At time $t = 0$, the energy of the system is measured. What values can be found, and with what probabilities? Calculate, for the system in the state $|\psi(0)\rangle$, the mean value $\langle H \rangle$ and the root-mean-square deviation ΔH.

b. Instead of measuring H at time $t = 0$, one measures A; what results can be found, and with what probabilities? What is the state vector immediately after the measurement?

c. Calculate the state vector $|\psi(t)\rangle$ of the system at time t.

d. Calculate the mean values $\langle A \rangle(t)$ and $\langle B \rangle(t)$ of A and B at time t. What comments can be made?

e. What results are obtained if the observable A is measured at time t? Same question for the observable B. Interpret.

15. Interaction picture

(It is recommended that complement F_{III} and perhaps complement G_{III} be read before this exercise is undertaken.)

Consider an arbitrary physical system. Denote its Hamiltonian by $H_0(t)$ and the corresponding evolution operator by $U_0(t, t')$:

$$\begin{cases} i\hbar \dfrac{\partial}{\partial t} U_0(t, t_0) = H_0(t)\, U_0(t, t_0) \\ U_0(t_0, t_0) = \mathbb{1} \end{cases}$$

Now assume that the system is perturbed in such a way that its Hamiltonian becomes:

$$H(t) = H_0(t) + W(t)$$

The state vector of the system in the "interaction picture", $|\psi_I(t)\rangle$, is defined from the state vector $|\psi_S(t)\rangle$ in the Schrödinger picture by:

$$|\psi_I(t)\rangle = U_0^\dagger(t, t_0)\,|\psi_S(t)\rangle$$

a. Show that the evolution of $|\psi_I(t)\rangle$ is given by:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_I(t)\rangle = W_I(t)\,|\psi_I(t)\rangle$$

where $W_I(t)$ is the transform operator of $W(t)$ under the unitary transformation associated with $U_0^\dagger(t, t_0)$:

$$W_I(t) = U_0^\dagger(t, t_0)\,W(t)\,U_0(t, t_0)$$

Explain qualitatively why, when the perturbation $W(t)$ is much smaller than $H_0(t)$, the motion of the vector $|\psi_I(t)\rangle$ is much slower than that of $|\psi_S(t)\rangle$.

b. Show that the preceding differential equation is equivalent to the integral equation:

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle + \frac{1}{i\hbar}\int_{t_0}^{t}\mathrm{d}t'\,W_I(t')\,|\psi_I(t')\rangle$$

where : $|\psi_I(t_0)\rangle = |\psi_S(t_0)\rangle$.

c. Solving this integral equation by iteration, show that the ket $|\psi_I(t)\rangle$ can be expanded in a power series in W of the form:

$$|\psi_I(t)\rangle = \left\{\mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t}\mathrm{d}t'\,W_I(t') + \frac{1}{(i\hbar)^2}\int_{t_0}^{t}\mathrm{d}t'\,W_I(t')\int_{t_0}^{t'}\mathrm{d}t''\,W_I(t'') + \ldots\right\}|\psi_I(t_0)\rangle$$

16. Correlations between two particles

(It is recommended that the complement E_{III} be read in order to answer question *e* of this exercise.)

Consider a physical system formed by two particles (1) and (2), of the same mass m, which do not interact with each other and which are both placed in an infinite potential well of width a (*cf.* complement H_I, § 2-c). Denote by $H(1)$ and $H(2)$ the Hamiltonians of each of the two particles and by $|\varphi_n(1)\rangle$ and $|\varphi_q(2)\rangle$ the corresponding eigenstates of the first and second particle, of energies $\dfrac{n^2\pi^2\hbar^2}{2ma^2}$ and $\dfrac{q^2\pi^2\hbar^2}{2ma^2}$. In the state space of the global system, the basis chosen is composed of the states $|\varphi_n\varphi_q\rangle$ defined by:

$$|\varphi_n\varphi_q\rangle = |\varphi_n(1)\rangle \otimes |\varphi_q(2)\rangle$$

a. What are the eigenstates and the eigenvalues of the operator $H = H(1) + H(2)$, the total Hamiltonian of the system? Give the degree of degeneracy of the two lowest energy levels.

b. Assume that the system, at time $t = 0$ is in the state :

$$| \psi(0) \rangle = \frac{1}{\sqrt{6}} | \varphi_1\varphi_1 \rangle + \frac{1}{\sqrt{3}} | \varphi_1\varphi_2 \rangle + \frac{1}{\sqrt{6}} | \varphi_2\varphi_1 \rangle + \frac{1}{\sqrt{3}} | \varphi_2\varphi_2 \rangle$$

α. What is the state of the system at time t?

β. The total energy H is measured. What results can be found, and with what probabilities?

γ. Same questions if, instead of measuring H, one measures $H(1)$.

c. α. Show that $| \psi(0) \rangle$ is a tensor product state. When the system is in this state, calculate the following mean values : $\langle H(1) \rangle$, $\langle H(2) \rangle$ and $\langle H(1)H(2) \rangle$. Compare $\langle H(1) \rangle \langle H(2) \rangle$ with $\langle H(1)H(2) \rangle$; how can this result be explained?

β. Show that the preceding results remain valid when the state of the system is the state $| \psi(t) \rangle$ calculated in *b*.

d. Now assume that the state $| \psi(0) \rangle$ is given by :

$$| \psi(0) \rangle = \frac{1}{\sqrt{5}} | \varphi_1\varphi_1 \rangle + \sqrt{\frac{3}{5}} | \varphi_1\varphi_2 \rangle + \frac{1}{\sqrt{5}} | \varphi_2\varphi_1 \rangle$$

Show that $| \psi(0) \rangle$ cannot be put in the form of a tensor product. Answer for this case all the questions asked in *c*.

e. α. Write the matrix, in the basis of the vectors $| \varphi_n\varphi_p \rangle$, which represents the density operator $\rho(0)$ corresponding to the ket $| \psi(0) \rangle$ given in *b*. What is the density matrix $\rho(t)$ at time t? Calculate, at the instant $t = 0$, the partial traces:

$$\rho(1) = \text{Tr}_2 \rho \quad \text{and} \quad \rho(2) = \text{Tr}_1 \rho$$

Do the density operators ρ, $\rho(1)$ and $\rho(2)$ describe pure states? Compare ρ with $\rho(1) \otimes \rho(2)$; what is your interpretation?

β. Answer the same questions as in α, but choosing for $| \psi(0) \rangle$ the ket given in *d*.

The subject of the following exercises is the density operator: they therefore assume the concepts and results of complement E_{III} *to be known.*

17. Let ρ be the density operator of an arbitrary system, where $| \chi_l \rangle$ and π_l are the eigenvectors and eigenvalues of ρ. Write ρ and ρ^2 in terms of the $| \chi_l \rangle$ and π_l. What do the matrices representing these two operators in the $\{ | \chi_l \rangle \}$ basis look like – first, in the case where ρ describes a pure state and then, in the case of a statistical mixture of states? (Begin by showing that, in a pure case, ρ has only one non-zero diagonal element, equal to 1, while for a statistical mixture, ρ has several diagonal elements included between 0 and 1.) Show that ρ corresponds to a pure case if and only if the trace of ρ^2 is equal to 1.

18. Consider a system whose density operator is $\rho(t)$, evolving under the influence of a Hamiltonian $H(t)$. Show that the trace of ρ^2 does not vary over time. Conclusion : can the system evolve so as to be successively in a pure state and a statistical mixture of states?

19. Let (1) + (2) be a global system, composed of two subsystems (1) and (2). A and B denote two operators acting in the state space $\mathscr{E}(1) \otimes \mathscr{E}(2)$. Show that the two partial traces $\text{Tr}_1 \{ AB \}$ and $\text{Tr}_1 \{ BA \}$ are equal when A (or B) actually acts only in the space $\mathscr{E}(1)$, that is, when A (or B) can be written:

$$A = A(1) \otimes \mathbb{1}(2) \qquad [\text{or } B = B(1) \otimes \mathbb{1}(2)].$$

Application: if the operator H, the Hamiltonian of the global system, is the sum of two operators which act, respectively, only in $\mathscr{E}(1)$ and only in $\mathscr{E}(2)$:

$$H = H(1) + H(2),$$

calculate the variation $\frac{\text{d}}{\text{d}t}\rho(1)$ of the reduced density operator $\rho(1)$. Give the physical interpretation of the result obtained.

Exercise 5

References: Flügge (1.24), §§40 and 41; Landau and Lifshitz (1.19), §22.

Exercise 10

References: Levine (12.3), chap. 14; Eyring et al (12.5), § 18 b

Exercise 15

References: see references of complement G_{III}.