## Complement $E_{XIII}$

## EXERCISES

**1.** Consider a one-dimensional harmonic oscillator of mass $m$, angular frequency $\omega_0$ and charge $q$. Let $| \varphi_n \rangle$ and $E_n = (n + 1/2)\hbar\omega_0$ be the eigenstates and eigenvalues of its Hamiltonian $H_0$.

For $t < 0$, the oscillator is in the ground state $| \varphi_0 \rangle$. At $t = 0$, it is subjected to an electric field "pulse" of duration $\tau$. The corresponding perturbation can be written :

$$W(t) = \begin{cases} - q\mathscr{E}X & \text{for } 0 \leqslant t \leqslant \tau \\ 0 & \text{for } t < 0 \text{ and } t > \tau \end{cases}$$

$\mathscr{E}$ is the field amplitude and $X$ is the position observable. Let $\mathscr{P}_{0n}$ be the probability of finding the oscillator in the state $| \varphi_n \rangle$ after the pulse.

*a.* Calculate $\mathscr{P}_{01}$ by using first-order time-dependent perturbation theory. How does $\mathscr{P}_{01}$ vary with $\tau$, for fixed $\omega_0$?

*b.* Show that, to obtain $\mathscr{P}_{02}$, the time-dependent perturbation theory calculation must be pursued at least to second order. Calculate $\mathscr{P}_{02}$ to this perturbation order.

*c.* Give the exact expressions for $\mathscr{P}_{01}$ and $\mathscr{P}_{02}$ in which the translation operator used in complement $F_V$ appears explicitly. By making a limited power series expansion in $\mathscr{E}$ of these expressions, find the results of the preceding questions.

**2.** Consider two spin 1/2's, $\mathbf{S}_1$ and $\mathbf{S}_2$, coupled by an interaction of the form $a(t)\mathbf{S}_1 \cdot \mathbf{S}_2$; $a(t)$ is a function of time which approaches zero when $|t|$ approaches infinity, and takes on non-negligible values (on the order of $a_0$) only inside an interval, whose width is of the order of $\tau$, about $t = 0$.

*a.* At $t = -\infty$, the system is in the state $| +, - \rangle$ (an eigenstate of $S_{1z}$ and $S_{2z}$ with the eigenvalues $+\hbar/2$ and $-\hbar/2$). Calculate, without approximations, the state of the system at $t = +\infty$. Show that the probability $\mathscr{P}(+ - \longrightarrow - +)$ of finding, at $t = +\infty$, the system in the state $| -, + \rangle$ depends only on the integral

$$\int_{-\infty}^{+\infty} a(t) \, dt.$$

*b.* Calculate $\mathscr{P}(+ - \longrightarrow - +)$ by using first-order time-dependent perturbation theory. Discuss the validity conditions for such an approximation by comparing the results obtained with those of the preceding question.

*c.* Now assume that the two spins are also interacting with a static magnetic field $\mathbf{B}_0$ parallel to $Oz$. The corresponding Zeeman Hamiltonian can be written :

$$H_0 = - B_0(\gamma_1 S_{1z} + \gamma_2 S_{2z})$$

where $\gamma_1$ and $\gamma_2$ are the gyromagnetic ratios of the two spins, assumed to be different.

Assume that $a(t) = a_0 \, e^{-t^2/\tau^2}$. Calculate $\mathscr{P}(+ - \longrightarrow - +)$ by first-order time-dependent perturbation theory. With fixed $a_0$ and $\tau$, discuss the variation of $\mathscr{P}(+ - \longrightarrow - +)$ with respect to $B_0$.

## 3. Two-photon transitions between non-equidistant levels

Consider an atomic level of angular momentum $J = 1$, subject to static electric and magnetic fields, both parallel to $Oz$. It can be shown that three non-equidistant energy levels are then obtained. The eigenstates $| \varphi_M \rangle$ of $J_z$ $(M = -1, 0, +1)$, of energies $E_M$ correspond to them. We set $E_1 - E_0 = \hbar\omega_0$, $E_0 - E_{-1} = \hbar\omega_0'$ $(\omega_0 \neq \omega_0')$.

The atom is also subjected to a radiofrequency field rotating at the angular frequency $\omega$ in the $xOy$ plane. The corresponding perturbation $W(t)$ can be written:

$$W(t) = \frac{\omega_1}{2}\left(J_+ \, e^{-i\omega t} + J_- \, e^{i\omega t}\right)$$

where $\omega_1$ is a constant proportional to the amplitude of the rotating field.

*a.* We set (notation identical to that of chapter XIII):

$$| \psi(t) \rangle = \sum_{M=-1}^{+1} b_M(t) \, e^{-iE_M t/\hbar} \, | \varphi_M \rangle$$

Write the system of differential equations satisfied by the $b_M(t)$.

*b.* Assume that, at time $t = 0$, the system is in the state $| \varphi_{-1} \rangle$. Show that if we want to calculate $b_1(t)$ by time-dependent perturbation theory, the calculation must be pursued to second order. Calculate $b_1(t)$ to this perturbation order.

*c.* For fixed $t$, how does the probability $\mathscr{P}_{-1,+1}(t) = |b_1(t)|^2$ of finding the system in the state $| \varphi_1 \rangle$ at time $t$ vary with respect to $\omega$? Show that a resonance appears, not only for $\omega = \omega_0$ and $\omega = \omega_0'$, but also for $\omega = (\omega_0 + \omega_0')/2$. Give a particle interpretation of this resonance.

**4.** Returning to exercise 5 of complement $H_{XI}$ and using its notation, assume that the field $\mathbf{B}_0$ is oscillating at angular frequency $\omega$, and can be written $\mathbf{B}_0(t) = \mathbf{B}_0 \cos \omega t$. Assume that $b = 2a$ and that $\omega$ is not equal to any Bohr angular frequency of the system (non-resonant excitation).

Introduce the susceptibility tensor $\chi$, of components $\chi_{ij}(\omega)$, defined by:

$$\langle M_i \rangle(t) = \sum_j \mathrm{Re}\left[\chi_{ij}(\omega) \, B_{0j} \, e^{i\omega t}\right]$$

with $i, j = x, y, z$. Using a method analogous to the one in § 2 of complement $A_{XIII}$, calculate $\chi_{ij}(\omega)$. Setting $\omega = 0$, find the results of exercise 5 of complement $H_{XI}$.

## 5. The Autler-Townes effect

Consider a three-level system : $|\varphi_1\rangle$, $|\varphi_2\rangle$, and $|\varphi_3\rangle$, of energies $E_1$, $E_2$ and $E_3$. Assume $E_3 > E_2 > E_1$ and $E_3 - E_2 \ll E_2 - E_1$.

This system interacts with a magnetic field oscillating at the angular frequency $\omega$. The states $|\varphi_2\rangle$ and $|\varphi_3\rangle$ are assumed to have the same parity, which is the opposite of that of $|\varphi_1\rangle$, so that the interaction Hamiltonian $W(t)$ with the oscillating magnetic field can connect $|\varphi_2\rangle$ and $|\varphi_3\rangle$ to $|\varphi_1\rangle$. Assume that, in the basis of the three states $|\varphi_1\rangle$, $|\varphi_2\rangle$, $|\varphi_3\rangle$, arranged in that order, $W(t)$ is represented by the matrix:

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \omega_1 \sin \omega t \\ 0 & \omega_1 \sin \omega t & 0 \end{bmatrix} \hbar$$

where $\omega_1$ is a constant proportional to the amplitude of the oscillating field.

*a.* Set (notation identical to that of chapter XIII):

$$|\psi(t)\rangle = \sum_{i=1}^{3} b_i(t)\, e^{-iE_it/\hbar} |\varphi_i\rangle$$

Write the system of differential equations satisfied by the $b_i(t)$.

*b.* Assume that $\omega$ is very close to $\omega_{32} = (E_3 - E_2)/\hbar$. Making approximations analogous to those used in complement $C_{XIII}$, integrate the preceding system, with the initial conditions:

$$b_1(0) = b_2(0) = \frac{1}{\sqrt{2}} \qquad b_3(0) = 0$$

(neglect, on the right-hand side of the differential equations, the terms whose coefficients, $e^{\pm i(\omega + \omega_{32})t}$, vary very rapidly, and keep only those whose coefficients are constant or vary very slowly, as $e^{\pm i(\omega - \omega_{32})t}$).

*c.* The component $D_z$ along $Oz$ of the electric dipole moment of the system is represented, in the basis of the three states $|\varphi_1\rangle$, $|\varphi_2\rangle$, $|\varphi_3\rangle$, arranged in that order, by the matrix:

$$\begin{bmatrix} 0 & d & 0 \\ d & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

where $d$ is a real constant ($D_z$ is an odd operator and can connect only states of different parities).

Calculate $\langle D_z \rangle(t) = \langle \psi(t) | D_z | \psi(t) \rangle$, using the vector $|\psi(t)\rangle$ calculated in *b*.

Show that the time evolution of $\langle D_z \rangle(t)$ is given by a superposition of sinusoidal terms. Determine the frequencies $\nu_k$ and relative intensities $\pi_k$ of these terms.

These are the frequencies that can be absorbed by the atom when it is placed in an oscillating electric field parallel to $Oz$. Describe the modifications of this absorption spectrum when, for $\omega$ fixed and equal to $\omega_{32}$, $\omega_1$ is increased from zero. Show that the presence of the magnetic field oscillating at the frequency $\omega_{32}/2\pi$ splits the electric dipole absorption line at the frequency $\omega_{21}/2\pi$, and that the separation of the two components of the doublet is proportional to the oscillating magnetic field amplitude (the Autler-Townes doublet).

What happens when, for $\omega_1$ fixed, $\omega - \omega_{32}$ is varied?

## 6. Elastic scattering by a particle in a bound state. Form factor

Consider a particle ($a$) in a bound state $| \varphi_0 \rangle$ described by the wave function $\varphi_0(\mathbf{r}_a)$ localized about a point $O$. Towards this particle ($a$) is directed a beam of particles ($b$), of mass $m$, momentum $\hbar\mathbf{k}_i$, energy $E_i = \hbar^2\mathbf{k}_i^2/2m$ and wave function $\frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}_i \cdot \mathbf{r}_b}$. Each particle ($b$) of the beam interacts with particle ($a$). The corresponding potential energy, $W$, depends only on the relative position $\mathbf{r}_b - \mathbf{r}_a$ of the two particles.

*a.* Calculate the matrix element:

$$\langle a : \varphi_0 ; b : \mathbf{k}_f \,|\, W(\mathbf{R}_b - \mathbf{R}_a) \,|\, a : \varphi_0 ; b : \mathbf{k}_i \rangle$$

of $W(\mathbf{R}_b - \mathbf{R}_a)$ between two states in which particle ($a$) is in the same state $| \varphi_0 \rangle$ and particle ($b$) goes from the state $| \mathbf{k}_i \rangle$ to the state $| \mathbf{k}_f \rangle$. The expression for this matrix element should include the Fourier transform $\overline{W}(\mathbf{k})$ of the potential $W(\mathbf{r}_b - \mathbf{r}_a)$:

$$W(\mathbf{r}_b - \mathbf{r}_a) = \frac{1}{(2\pi)^{3/2}} \int \overline{W}(\mathbf{k}) \, e^{i\mathbf{k} \cdot (\mathbf{r}_b - \mathbf{r}_a)} \, d^3k$$

*b.* Consider the scattering processes in which, under the effect of the interaction $W$, particle ($b$) is scattered in a certain direction, with particle ($a$) remaining in the same quantum state $| \varphi_0 \rangle$ after the scattering process (elastic scattering).

Using a method analogous to the one in chapter XIII [*cf.* comment (*ii*) of § C-3-b], calculate, in the Born approximation, the elastic scattering cross section of particle ($b$) by particle ($a$) in the state $| \varphi_0 \rangle$.

Show that this cross section can be obtained by multiplying the cross section for scattering by the potential $W(\mathbf{r})$ (in the Born approximation) by a factor which characterizes the state $| \varphi_0 \rangle$, called the "form factor".

## 7. A simple model of the photoelectric effect

Consider, in a one-dimensional problem, a particle of mass $m$, placed in a potential of the form $V(x) = -\alpha\delta(x)$, where $\alpha$ is a real positive constant.

Recall (*cf.* exercises 2 and 3 of complement $K_I$) that, in such a potential, there is a single bound state, of negative energy $E_0 = -m\alpha^2/2\hbar^2$, associated with a normalized wave function $\varphi_0(x) = \sqrt{m\alpha/\hbar^2}\, e^{-\frac{m\alpha}{\hbar^2}|x|}$. For each positive value of the energy $E = \hbar^2k^2/2m$, on the other hand, there are two stationary wave functions, corresponding, respectively, to an incident particle coming from the left or from the right. The expression for the first eigenfunction, for example, is:

$$\chi_k(x) = \begin{cases} \dfrac{1}{\sqrt{2\pi}}\left[e^{ikx} - \dfrac{1}{1 + i\hbar^2k/m\alpha}\, e^{-ikx}\right] & \text{for } x < 0 \\[2ex] \dfrac{1}{\sqrt{2\pi}}\, \dfrac{i\hbar^2k/m\alpha}{1 + i\hbar^2k/m\alpha}\, e^{ikx} & \text{for } x > 0 \end{cases}$$

*a.* Show that the $\chi_k(x)$ satisfy the orthonormalization relation (in the extended sense):

$$\langle \chi_k \mid \chi_{k'} \rangle = \delta(k - k')$$

The following relation [*cf.* formula (47) of appendix II] can be used:

$$\int_{-\infty}^{0} e^{iqx}\, dx = \int_{0}^{\infty} e^{-iqx}\, dx = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon + iq}$$
$$= \pi\,\delta(q) - i\,\mathscr{P}\left(\frac{1}{q}\right)$$

Calculate the density of states $\rho(E)$ for a positive energy $E$.

*b.* Calculate the matrix element $\langle \chi_k \mid X \mid \varphi_0 \rangle$ of the position observable $X$ between the bound state $\mid \varphi_0 \rangle$ and the positive energy state $\mid \chi_k \rangle$ whose wave function was given above.

*c.* The particle, assumed to be charged (charge $q$) interacts with an electric field oscillating at the angular frequency $\omega$. The corresponding perturbation is:

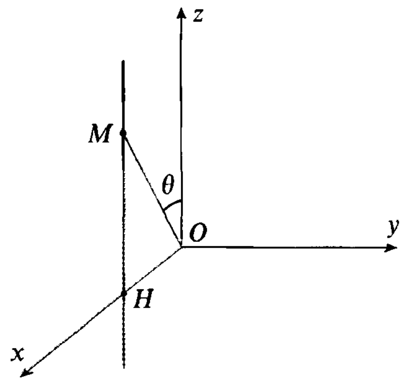
$$W(t) = -q\mathscr{E} X \sin \omega t$$

where $\mathscr{E}$ is a constant.

The particle is initially in the bound state $\mid \varphi_0 \rangle$. Assume that $\hbar\omega > -E_0$. Calculate, using the results of § C of chapter XIII [see, in particular, formula (C-37)], the transition probability $w$ per unit time to an arbitrary positive energy state (the photoelectric or photoionization effect). How does $w$ vary with $\omega$ and $\mathscr{E}$ ?

## 8. Disorientation of an atomic level due to collisions with rare gas atoms

Consider a motionless atom $A$ at the origin of a coordinate frame $Oxyz$ (see figure). This atom $A$ is in a level of angular momentum $J = 1$, to which correspond the three orthonormal kets $| M \rangle$ ($M = -1, 0, +1$), eigenstates of $J_z$ of eigenvalues $M\hbar$.




A second atom $B$, in a level of zero angular momentum, is in uniform rectilinear motion in the $xOz$ plane: it is travelling at the velocity $v$ along a straight line parallel to $Oz$ and situated at a distance $b$ from this axis ($b$ is the "impact parameter"). The time origin is chosen at the time when $B$ arrives at point $H$ of the $Ox$ axis ($OH = b$). At time $t$, atom $B$ is therefore at point $M$, where $HM = vt$. Call $\theta$ the angle between $Oz$ and $OM$.

The preceding model, which treats the external degrees of freedom of the two atoms classically, permits the simple calculation of the effect on the internal degrees of freedom of atom $A$ (which are treated quantum mechanically) of a collision with atom $B$ (which is, for example, a rare gas atom in the ground state). It can be shown that, because of the Van der Waals forces (*cf.* complement $C_{XI}$) between the two atoms, atom $A$ is subject to a perturbation $W$ acting on its internal degrees of freedom, and given by:

$$W = \frac{C}{r^6} J_u^2$$

where $C$ is a constant, $r$ is the distance between the two atoms, and $J_u$ is the component of the angular momentum $\mathbf{J}$ of atom $A$ on the $OM$ axis joining the two atoms.

*a.* Express $W$ in terms of $C$, $b$, $v$, $t$, $J_z$, $J_\pm = J_x \pm iJ_y$. Introduce the dimensionless parameter $\tau = vt/b$.

*b.* Assume that there is no external magnetic field, so that the three states $| +1 \rangle$, $| 0 \rangle$, $| -1 \rangle$ of atom $A$ have the same energy.

Before the collision, that is, at $t = -\infty$, atom $A$ is in the state $| -1 \rangle$. Using first-order time-dependent perturbation theory, calculate the probability $\mathscr{P}_{-1,+1}$ of finding, after the collision (that is, at $t = +\infty$), atom $A$ in the state $| +1 \rangle$. Discuss the variation of $\mathscr{P}_{-1,+1}$ with respect to $b$ and $v$. Similarly, calculate $\mathscr{P}_{-1,0}$.

*c*. Now assume that there is a static field $\mathbf{B}_0$ parallel to $Oz$, so that the three states $| M \rangle$ have an additional energy $M\hbar\omega_0$ (the Zeeman effect), where $\omega_0$ is the Larmor angular frequency in the field $\mathbf{B}_0$.

α. With ordinary magnetic fields ($B_0 \sim 10^2$ gauss), $\omega_0 \simeq 10^9$ rad sec$^{-1}$; $b$ is of the order of 5 Å, and $v$, of the order of $5 \times 10^2$ m . sec$^{-1}$. Show that, under these conditions, the results of question *b* remain valid.

β. Without going into detailed calculations, explain what happens for much higher values of $B_0$. Starting with what value of $\omega_0$ (where $b$ and $v$ have the values indicated in α) will the results of *b* no longer be valid?

*d*. Without going into detailed calculations, explain how to calculate the disorientation probabilities $\mathscr{P}_{-1,+1}$ and $\mathscr{P}_{-1,0}$ for an atom $A$ placed in a gas of atoms $B$ in thermodynamic equilibrium at the temperature $T$, containing a number $n$ of atoms per unit volume sufficiently small that only binary collisions need be considered.

N.B. We give : $\displaystyle\int_{-\infty}^{+\infty} \frac{d\tau}{(1+\tau^2)^4} = \frac{5\pi}{16}$

## 9. Transition probability per unit time under the effect of a random perturbation. Simple relaxation model

A physical system, subject to a perturbation $W(t)$, is at time $t = 0$ in the eigenstate $| \varphi_i \rangle$ of its Hamiltonian $H_0$. Let $\mathscr{P}_{if}(t)$ be the probability of finding the system at time $t$ in another eigenstate of $H_0$, $| \varphi_f \rangle$. The transition probability per unit time $w_{if}(t)$ is defined by $w_{if}(t) = \dfrac{d}{dt}\mathscr{P}_{if}(t)$.

*a*. Show that, to first order in perturbation theory, we have:

$$w_{if}(t) = \frac{1}{\hbar^2}\int_0^t e^{i\omega_{fi}\tau}\, W_{fi}(t) W_{fi}^*(t-\tau)\, d\tau + \text{c.c.} \tag{1}$$

with $\hbar\omega_{fi} = E_f - E_i$ (notation identical to that of chapter XIII).

*b*. Consider a very large number $\mathcal{N}$ of systems $(k)$, which are identical and without mutual interactions ($k = 1, 2, ..., \mathcal{N}$). Each of them has a different microscopic environment and, consequently, "sees" a different perturbation $W^{(k)}(t)$. It is, of course, impossible to know with certainty each of the individual perturbations $W^{(k)}(t)$; we can specify only statistical averages such as:

$$\overline{W_{fi}(t)} = \lim_{\mathcal{N}\to\infty} \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} W_{fi}^{(k)}(t)$$

$$\overline{W_{fi}(t)\, W_{fi}^*(t-\tau)} = \lim_{\mathcal{N}\to\infty} \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} W_{fi}^{(k)}(t)\, W_{fi}^{(k)*}(t-\tau) \tag{2}$$

This perturbation is said to be "random".

This random perturbation is called stationary if the preceding averages do not depend on the time $t$. The unperturbed Hamiltonian $H_0$ is then redefined so as to make all the $\overline{W_{fi}}$ zero, and we set:

$$g_{fi}(\tau) = \overline{W_{fi}(t)\, W^*_{fi}(t - \tau)} \tag{3}$$

$g_{fi}(\tau)$ is called the "correlation function" of the perturbation (for the pair of states $| \varphi_i \rangle$, $| \varphi_f \rangle$). $g_{fi}(\tau)$ generally goes to zero for $\tau \gg \tau_c$, is a characteristic time, called the "correlation time" of the perturbation. The perturbation has a "memory" which extends into the past only over an interval of the order of $\tau_c$.

α. The $\mathcal{N}$ systems are all in the state $| \varphi_i \rangle$ at time $t = 0$ and are subject to a stationary random perturbation, whose correlation function is $g_{fi}(\tau)$ and whose correlation time is $\tau_c$ ($\mathcal{N}$ can be considered to be infinite in the calculations).

Calculate the proportion $\pi_{if}(t)$ of systems which go into the state $| \varphi_f \rangle$ per unit time. Show that after a certain value $t_1$ of $t$, to be specified, $\pi_{if}(t)$ no longer depends on $t$.

β. For fixed $\tau_c$, how does $\pi_{if}$ vary with $\omega_{fi}$? Consider the case for which $g_{fi}(\tau) = |v_{fi}|^2\, \mathrm{e}^{-\tau/\tau_c}$, with $v_{fi}$ constant.

γ. The preceding theory is rigorously valid only for $t \ll t_2$ [since formula (1) results from a perturbation theory]. What is the order of magnitude of $t_2$? Taking $t_2 \gg t_1$, find the condition for introducing a transition probability per unit time which is independent of $t$ [use the form of $g_{fi}(\tau)$ given in the preceding question]. Would it be possible to extend the preceding theory beyond $t = t_2$?

*c*. Application to a simple system.

The $\mathcal{N}$ systems under consideration are $\mathcal{N}$ spin 1/2 particles, with gyromagnetic ratio $\gamma$, placed in a static field $\mathbf{B}_0$ (set $\omega_0 = -\gamma B_0$). These particles are enclosed in a spherical cell of radius $R$. Each of them bounces constantly back and forth between the walls. The mean time between two collisions of the same particle with the wall is called the "flight time" $\tau_v$. During this time, the particle "sees" only the field $\mathbf{B}_0$. In a collision with the wall, each particle remains adsorbed on the surface during a mean time $\tau_a$ ($\tau_a \ll \tau_v$), during which it "sees", in addition to $\mathbf{B}_0$, a constant microscopic magnetic field $\mathbf{b}$, due to the paramagnetic impurities contained in the wall. The direction of $\mathbf{b}$ varies randomly from one collision to another; the mean amplitude of $\mathbf{b}$ is denoted by $b_0$.

α. What is the correlation time of the perturbation seen by the spins? Give the physical justification for the following form, to be chosen for the correlation function of the components of the microscopic field $\mathbf{b}$:

$$\overline{b_x(t)\, b_x(t - \tau)} = \frac{1}{3}\, b_0^2\, \frac{\tau_a}{\tau_v}\, \mathrm{e}^{-\tau/\tau_a} \tag{4}$$

and analogous expressions for the components along $Oy$ and $Oz$, all the cross terms $\overline{b_x(t) b_y(t - \tau)}$... being zero.

$\beta$. Let $\mathcal{M}_z$ be the component along the $Oz$ axis defined by the field $\mathbf{B}_0$ of the macroscopic magnetization of the $\mathcal{N}$ particles. Show that, under the effect of the collisions with the wall, $\mathcal{M}_z$ "relaxes", with a time constant $T_1$:

$$\frac{\mathrm{d}\mathcal{M}_z}{\mathrm{d}t} = -\frac{\mathcal{M}_z}{T_1}$$

($T_1$ is called the longitudinal relaxation time). Calculate $T_1$ in terms of $\gamma$, $B_0$, $\tau_a$, $\tau_v$, $b_0$.

$\gamma$. Show that studying the variation of $T_1$ with $B_0$ permits the experimental determination of the mean adsorption time $\tau_a$.

$\delta$. We have at our disposition several cells, of different radii $R$, constructed from the same material. By measuring $T_1$, how can we determine experimentally the mean amplitude $b_0$ of the microscopic field at the wall?

## 10. Absorption of radiation by a many-particle system forming a bound state. The Doppler effect. Recoil energy. The Mössbauer effect

In complement $A_{XIII}$, we consider the absorption of radiation by a charged particle attracted by a fixed center $O$ (the hydrogen atom model for which the nucleus is infinitely heavy). In this exercise, we treat a more realistic situation, in which the incident radiation is absorbed by a system of many particles of finite masses interacting with each other and forming a bound state. Thus, we are studying the effect on the absorption phenomenon of the degrees of freedom of the center of mass of the system.

### I. ABSORPTION OF RADIATION BY A FREE HYDROGEN ATOM. THE DOPPLER EFFECT. RECOIL ENERGY

Let $\mathbf{R}_1$ and $\mathbf{P}_1$, $\mathbf{R}_2$ and $\mathbf{P}_2$ be the position and momentum observables of two particles, (1) and (2), of masses $m_1$ and $m_2$ and opposite charges $q_1$ and $q_2$ (a hydrogen atom). Let $\mathbf{R}$ and $\mathbf{P}$, $\mathbf{R}_G$ and $\mathbf{P}_G$ be the position and momentum observables of the relative particle and the center of mass (*cf.* chap. VII, § B). $M = m_1 + m_2$ is the total mass, and $m = m_1 m_2/(m_1 + m_2)$ is the reduced mass. The Hamiltonian $H_0$ of the system can be written:

$$H_0 = H_e + H_i \tag{1}$$

where:

$$H_e = \frac{1}{2M}\mathbf{P}_G^2 \tag{2}$$

is the translational kinetic energy of the atom, assumed to be free ("external" degrees of freedom), and where $H_i$ (which depends only on $\mathbf{R}$ and $\mathbf{P}$) describes the internal energy of the atom ("internal" degrees of freedom). We denote by $|\mathbf{K}\rangle$ the eigenstates of $H_e$, with eigenvalues $\hbar^2\mathbf{K}^2/2M$. We concern ourselves with only two eigenstates of $H_i$, $|\chi_a\rangle$ and $|\chi_b\rangle$, of energies $E_a$ and $E_b$ ($E_b > E_a$). We set:

$$E_b - E_a = \hbar\omega_0 \tag{3}$$

*a*. What energy must be furnished to the atom to move it from the state $|\mathbf{K};\chi_a\rangle$ (the atom in the state $|\chi_a\rangle$ with a total momentum $\hbar\mathbf{K}$) to the state $|\mathbf{K}';\chi_b\rangle$?

*b*. This atom interacts with a plane electromagnetic wave of wave vector **k** and angular frequency $\omega = ck$, polarized along the unit vector **e** perpendicular to **k**. The corresponding vector potential $\mathbf{A}(\mathbf{r}, t)$ is:

$$\mathbf{A}(\mathbf{r}, t) = \mathscr{A}_0\, \mathbf{e}\, \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} + c.c. \tag{4}$$

where $\mathscr{A}_0$ is a constant. The principal term of the interaction Hamiltonian between this plane wave and the two-particle system can be written (*cf.* complement $A_{XIII}$, §1-b):

$$W(t) = -\sum_{i=1}^{2} \frac{q_i}{m_i}\, \mathbf{P}_i \cdot \mathbf{A}(\mathbf{R}_i, t) \tag{5}$$

Express $W(t)$ in terms of $\mathbf{R}$, $\mathbf{P}$, $\mathbf{R}_G$, $\mathbf{P}_G$, $m$, $M$ and $q$ (setting $q_1 = -q_2 = q$), and show that, in the electric dipole approximation which consists of neglecting $\mathbf{k}\cdot\mathbf{R}$ (but not $\mathbf{k}\cdot\mathbf{R}_G$) compared to 1, we have:

$$W(t) = W\mathrm{e}^{-i\omega t} + W^\dagger \mathrm{e}^{i\omega t} \tag{6}$$

where:

$$W = -\frac{q\mathscr{A}_0}{m}\, \mathbf{e}\cdot\mathbf{P}\, \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}_G} \tag{7}$$

*c*. Show that the matrix element of $W$ between the state $|\mathbf{K};\chi_a\rangle$ and the state $|\mathbf{K}';\chi_b\rangle$ is different from zero only if there exists a certain relation between **K**, **k**, **K**′ (to be specified). Interpret this relation in terms of the total momentum conservation during the absorption of an incident photon by the atom.

*d*. Show from this that if the atom in the state $|\mathbf{K};\chi_a\rangle$ is placed in the plane wave (4), resonance occurs when the energy $\hbar\omega$ of the photons associated with the incident wave differs from the energy $\hbar\omega_0$ of the atomic transition $|\chi_a\rangle \longrightarrow |\chi_b\rangle$ by a quantity $\delta$ which is to be expressed in terms of $\hbar$, $\omega_0$, **K**, **k**, $M$, $c$ (since $\delta$ is a corrective term, we can replace $\omega$ by $\omega_0$ in the expression for $\delta$). Show that $\delta$ is the sum of two terms, one of which, $\delta_1$, depends on **K** and on the angle between **K** and **k** (the Doppler effect), and the other, $\delta_2$, is independent of **K**. Give a physical interpretation of $\delta_1$ and $\delta_2$ (showing that $\delta_2$ is the recoil kinetic energy of the atom when, having been initially motionless, it absorbs a resonant photon).

Show that $\delta_2$ is negligible compared to $\delta_1$ when $\hbar\omega_0$ is of the order of 10 eV (the domain of atomic physics). Choose, for $M$, a mass of the order of that of the proton ($Mc^2 \simeq 10^9$ eV), and, for $|\mathbf{K}|$, a value corresponding to a thermal velocity at $T = 300$ °K. Would this still be true if $\hbar\omega_0$ were of the order of $10^5$ eV (the domain of nuclear physics)?

## 11. RECOILLESS ABSORPTION OF RADIATION BY A NUCLEUS VIBRATING ABOUT ITS EQUILIBRIUM POSITION IN A CRYSTAL. THE MÖSSBAUER EFFECT

The system under consideration is now a nucleus of mass $M$ vibrating at the angular frequency $\Omega$ about its equilibrium position in a crystalline lattice (the Einstein model; *cf.* complement $A_V$, § 2). We again denote by $\mathbf{R}_G$ and $\mathbf{P}_G$ the position and momentum of the center of mass of this nucleus. The vibrational energy of the nucleus is described by the Hamiltonian:

$$H_e = \frac{1}{2M}\mathbf{P}_G^2 + \frac{1}{2}M\Omega^2(X_G^2 + Y_G^2 + Z_G^2) \tag{8}$$

which is that of a three-dimensional isotropic harmonic oscillator. Denote by $| \psi_{n_x,n_y,n_z} \rangle$ the eigenstate of $H_e$ of eigenvalue $(n_x + n_y + n_z + 3/2)\hbar\Omega$. In addition to these external degrees of freedom, the nucleus possesses internal degrees of freedom with which are associated observables which all commute with $\mathbf{R}_G$ and $\mathbf{P}_G$. Let $H_i$ be the Hamiltonian which describes the internal energy of the nucleus. As above, we concern ourselves with two eigenstates of $H_i$, $| \chi_a \rangle$ and $| \chi_b \rangle$, of energies $E_a$ and $E_b$, and we set $\hbar\omega_0 = E_b - E_a$. Since $\hbar\omega_0$ falls into the $\gamma$-ray domain, we have, of course:

$$\omega_0 \gg \Omega \tag{9}$$

*e*. What energy must be furnished to the nucleus to allow it to go from the state $| \psi_{0,0,0}; \chi_a \rangle$ (the nucleus in the vibrational state defined by the quantum numbers $n_x = 0$, $n_y = 0$, $n_z = 0$ and the internal state $| \chi_a \rangle$) to the state $| \psi_{n,0,0}; \chi_b \rangle$?

*f*. This nucleus is placed in an electromagnetic wave of the type defined by (4), whose wave vector $\mathbf{k}$ is parallel to $Ox$. It can be shown that, in the electric dipole approximation, the interaction Hamiltonian of the nucleus with this plane wave (responsible for the absorption of the $\gamma$-rays) can be written as in (6), with:

$$W = \mathscr{A}_0 S_i(k)\, e^{ikX_G} \tag{10}$$

where $S_i(k)$ is an operator which acts on the internal degrees of freedom and consequently commutes with $\mathbf{R}_G$ and $\mathbf{P}_G$. Set $s(k) = \langle \chi_b | S_i(k) | \chi_a \rangle$.

The nucleus is initially in the state $| \psi_{0,0,0}; \chi_a \rangle$. Show that, under the influence of the incident plane wave, a resonance appears whenever $\hbar\omega$ coincides with one of the energies calculated in *e*, with the intensity of the corresponding resonance proportional to $|s(k)|^2 \, |\langle \psi_{n,0,0} | e^{ikX_G} | \psi_{0,0,0} \rangle|^2$, where the value of $k$ is to be specified. Show, furthermore, that condition (9) allows us to replace $k$ by $k_0 = \omega_0/c$ in the expression for the intensity of the resonance.

*g*. We set:

$$\pi_n(k_0) = |\langle \varphi_n | e^{ik_0X_G} | \varphi_0 \rangle|^2 \tag{11}$$

where the states $| \varphi_n \rangle$ are the eigenstates of a one-dimensional harmonic oscillator of position $X_G$, mass $M$ and angular frequency $\Omega$.

α. Calculate $\pi_n(k_0)$ in terms of $\hbar$, $M$, $\Omega$, $k_0$, $n$ (see also exercise 7 of complement $M_V$). Set $\xi = \dfrac{\hbar^2 k_0^2}{2M}\Big/\hbar\Omega$. Hint: establish a recurrence relation between $\langle \varphi_n | e^{ik_0 X_G} | \varphi_0 \rangle$ and $\langle \varphi_{n-1} | e^{ik_0 X_G} | \varphi_0 \rangle$, and express all the $\pi_n(k_0)$ in terms of $\pi_0(k_0)$, which is to be calculated directly from the wave function of the harmonic oscillator ground state. Show that the $\pi_n(k_0)$ are given by a Poisson distribution.

β. Verify that $\sum\limits_{n=0}^{\infty} \pi_n(k_0) = 1$.

γ. Show that $\sum\limits_{n=0}^{\infty} n\hbar\Omega\, \pi_n(k_0) = \hbar^2\omega_0^2/2Mc^2$.

*h*. Assume that $\hbar\Omega \gg \hbar^2\omega_0^2/2Mc^2$, that is, that the vibrational energy of the nucleus is much greater than the recoil energy (very rigid crystalline bonds). Show that the absorption spectrum of the nucleus is essentially composed of a single line of angular frequency $\omega_0$. This line is called the recoilless absorption line. Justify this name. Why does the Doppler effect disappear?

*i*. Now assume that $\hbar\Omega \ll \hbar^2\omega_0^2/2Mc^2$ (very weak crystalline bonds). Show that the absorption spectrum of the nucleus is composed of a very large number of equidistant lines whose barycenter (obtained by weighting the abscissa of each line by its relative intensity) coincides with the position of the absorption line of the free and initially motionless nucleus. What is the order of magnitude of the width of this spectrum (the dispersion of the lines about their barycenter)? Show that one obtains the results of the first part in the limit $\Omega \longrightarrow 0$.

**Exercise 3 :**

References : see Brossel's lectures in (15.2).

**Exercise 5 :**

References : see Townes and Schawlow (12.10), chap. 10, § 9.

**Exercise 6 :**

References : see Wilson (16.34).

**Exercise 9 :**

References : see Abragam (14.1), chap. VIII; Slichter (14.2), chap. 5.

**Exercise 10 :**

References : see De Benedetti (16.23); Valentin (16.1), annexe XV.