Lista 1 - Quântica B (2013)

1. Consider a quantum 1D Harmonic Oscillator of mass m and natura frequency ω which is initially prepared $(t=0)$ in the state

$$|\psi_S(0)\rangle = \exp\left(-\frac{i}{\hbar}P_S x_0\right)|0\rangle\,,$$

where $|0\rangle$ is the ground state, P_S is the momentum operator, and x_0 is a scalar.
(a) In the Heisenberg picture, compute $\langle X_H(t)\rangle$ for $t>0$ and relate it with the classical trajectory.
(b) How do you interprete this result with the classical initial conditions?

2. Consider a hidrogen atom in its ground state subject to an electric field $\mathbf{E}=\mathbf{E}_0\cos\omega t$.
(a) What is the minimum frequency of the field in order to have ionization?
(b) What is the transition rate (probability per unit of time) to an ionized state (assuming it can represented by plane waves)?
(c) What is the angular distribution of the ejected electron in this process?
(d) Now consider that the atom is in a certain Eigenstate $|n,l,m\rangle$ and that ω is lower than the corresponding ionization frequency. What can be said about the final Eigenstate $|n',\ell',m'\rangle$?

3. Consider two spin-1/2 particles interacting as

$$V(t) = \frac{E\,(t)}{\hbar^2}\mathbf{S}_1\cdot\mathbf{S}_2,$$

where $E(t)$ vanishes when $t\to\pm\infty$ and approaches to a nonzero value of order $\bar{E}$ on the time interval of length τ. (You may think on a gaussian, for instance.)
(a) At $t\to-\infty$, the system is in the state $|+-\rangle$. Compute exactly the state of the system at time t. With this, show that the probability of finding the system in the state $|-+\rangle$ for $t\to+\infty$ depends only on the integral $I=\int_{-\infty}^{\infty}E(t)\mathrm{d}t$.
(b) Compute the same probability in first-order of time-dependent perturbation theory. By comparing your results with those of item (a), discuss the validity of this calculation.
(c) Make some estimations about the value of the contribution to this probability in second-order of perturbation theory in the limits of $\tau\to0$ and $\tau\to\infty$ and discuss your results with the validity of the approximation conclude in item (b).
(d) Now consider that both spins are subjected to a static magnetic field $\mathbf{B}=B_0\hat{z}$. The corresponding Zeeman Hamiltonian is

$$H_0 = -\frac{\mu_B}{\hbar}B_0\left(g_1 S_1^z + g_2 S_2^z\right),$$

where $g_{1,2}$ are the gyromagnetic ratios (assume them distinct from each other) and μ_B is the Bohr magneton. Consider also that $E(t)=\bar{E}\exp\left(-\left(t/\tau\right)^2\right)$. Compute the same probability of the previous itens in first-order of perturbation theory, and discuss its dependence on B_0 and on τ.
(e) (Optional) Like in item (c), compute the second-order contribution $c^{(2)}_{f\leftarrow i}(\infty)$ in the limits $\tau\to0$ and $\tau\to\infty$.
(*Hint*: Notice that in the limits $\tau\to0$ and $\tau\to\infty$, for estimation purposes, the exchange can be approximated to $E(t)=\bar{E}\tau\delta\,(t)$ and $E(t)=\bar{E}\theta\,(\tau/2-|t|)$, respectively.)

4. Cohen-Tannoudji - complement E-XIII, problem 9.
Transition probability per unit time under the effect of a random perturbation. Simple relaxation model
A physical system, subjected to a perturbation $W(t)$, is at time $t=0$ in the Eigenstate $|\varphi_i\rangle$ of its Hamiltonian H_0. Let $P_{f\leftarrow i}(t)$ be the probability of finding the system at time t in another Eigenstate of H_0, $|\varphi_j\rangle$. The transition probability per unit time $w_{f\leftarrow i}(t)$ is defined by $w_{f\leftarrow i}(t)=\frac{\mathrm{d}}{\mathrm{d}t}P_{f\leftarrow i}(t)$.
(a) Show that , to first order in perturbation theory, we have

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

with $\hbar\omega_{fi} = E_f - E_i$.

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

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

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

This perturbation is said to be "random".

This random perturbation is said to be stationary if the preceding averages are time independent. In this case, we can redifine H_0 in order to make $\overline{W_{fi}} = 0$ and set:

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

which is called the "correlation function" of the perturbation. Usually, $g_{fi}(\tau)$ goes to zero for $|\tau| \gg \tau_c$, a characteristic time scale, called correlation time of the perturbation, i.e., the perturbation has a "memory" which extend into the past (or future) only to an interval of order of τ_c.

($b.\alpha$) The $\mathcal{N}$ (which can be considered infinity for calculations) systems are in the state $|\varphi_i\rangle$ at time $t = 0$ and are subject to a random stationary perturbation, the correlation function of which is $g_{fi}(\tau)$ with correlation time τ_c. Calculate the proportion $\pi_{fi}(t)$ of systems which go to into the state $|\varphi_j\rangle$ per unit time. Show that after a certain value t_1 of t, to be specified, $\pi_{fi}(t)$ no longer depends on t.

($b.\beta$) For fixed τ_c, how does π_{fi} vary with ω_{fi}? Consider the case in which $g_{fi}(\tau) = |v_{fi}|^2 e^{-|\tau|/\tau_c}$, with v_{fi} constant.

($b.\gamma$) The preceding theory is valid only for $t \ll t_2$ [since Eq. (1) results from 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 system. The $\mathcal{N}$ systems under consideration are spin-1/2 particles, with gyromagnetic ratio γ, placed in a static magnetic field $\mathbf{B}_0$ (set $\omega_0 = \gamma B_0$). These particles are enclosed in a spherical shell of radius R. Each of them bounces constantly back and forth between the walls. The mean time between the collisions of the same particle with the wall is called "time of flight" τ_v. During this time, the particle sees only the magnetic field $\mathbf{B}_0$. In a collision with the wall, each particle remains adsorbed on the surface during a mean time τ_a ($\tau_a \ll \tau_v$), during which it seems, in addition to $\mathbf{B}_0$, a constant microscopic field $\mathbf{b}$ due to 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 b_0.

($c.\alpha$) 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 magnetic field $\mathbf{b}$:

$$\overline{b_x(t)b_x(t-\tau)} = \frac{1}{3} b_0^2 \left(\frac{\tau_a}{\tau_b}\right) e^{-|\tau|/\tau_a},$$

and analogous expressions for the y- and z-components, and all the cross terms $\overline{b_x(t)b_y(t-\tau)} = \overline{b_x(t)b_z(t-\tau)} = \cdots = 0$.

($c.\beta$) Let M_z be the z-component of the total magnetization. (Consider $\mathbf{B} = B_0\hat{z}$.) Show that, under the effect of the collisions with the walls, M_z "relaxes", with a time constant T_1:

$$\frac{\mathrm{d}M_z}{\mathrm{d}t} = -\frac{M_z}{T_1}$$

(T_1 is called the longitudinal relaxation time). Calculate T_1 in terms of γ, B_0, τ_v, τ_a, b_0.

($c.\gamma$) Show that studying the variation of T_1 with B_0 permites the experimental determination of the mean adsorption time τ_a.

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

5. Cohen-Tannoudji - complement E-XIII, problem 10.

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

In class, we considered the absorption of radiation by a charged particle attracted by a fixed center (Hydrogen atom with infinitely heavy nucleous). 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. The recoil energy

Consider two particles of masses $m_{1,2}$ of opposite charges $q_{1,2}$ and position and momentum operators $\mathbf{R}_{1,2}$ and $\mathbf{P}_{1,2}$ (a Hydrogen atom). Let $\mathbf{R}$ and $\mathbf{P}$, and $\mathbf{R}_G$ and $\mathbf{P}_G$ be the position and momentum observables of the relative particle and center of mass of the system, respectively. $M = m_1 + m_2$ is the total mass and $m = m_1 m_2/M$ is the reduced mass. The Hamiltonian of the system can be written:

$$H_0 = H_e + H_i,$$

where

$$H_e = \frac{1}{2M} P_G^2$$

describes the translational kinetic energy of the free atom (the "external" degrees of freedom), and H_i describes the internal energy of the atom (the "internal" degrees of freedom). We denote by $|\mathbf{K}\rangle$ the eigenstates of H_e, with Eigenvalues $\hbar^2 K^2/(2M)$. We concern ourselves with only two Eigenstates of H_i, $|\chi_a\rangle$ and $|\chi_b\rangle$ of energies E_a and E_b (with $E_b > E_a$), and set $\hbar\omega_0 = E_b - E_a$.

(a) What energy must be furnished to the atom to move it from state $|\mathbf{K}, \chi_a\rangle$ to state $|\mathbf{K}', \chi_b\rangle$?

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

$$\mathbf{A}(\mathbf{r}, t) = A_0 e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}\hat{e} + \text{c.c.},$$

with A_0 constant. The principal term of the interaction Hamiltonian between this plane wave and the two particle system can be written as

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

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

$$W = W_0 e^{-i\omega t} + W_0^\dagger e^{i\omega t}, \text{ with } W_0 = -\frac{qA_0}{m} \hat{e}\cdot\mathbf{P} e^{i\mathbf{k}\cdot\mathbf{R}_G}. \tag{2}$$

(c) Show that the matrix element $\langle \mathbf{K}', \chi_b | W_0 | \mathbf{K}, \chi_a\rangle$ is different from zero only if there exist a relation between $\mathbf{k}$, $\mathbf{K}$ and $\mathbf{K}'$ (to be specified). Interpret this relation in terms of momentum conservation of the system atom+photon.

(d) Show that if the atom is in the state $|\mathbf{K}, \chi_a\rangle$ is placed in the radiation field, resonance just occurs when the energy $\hbar\omega$ of the photons differs from the atomic transition energy $\hbar\omega_0$ by an amount δE which is to be expressed in terms of $\hbar$, ω_0, $\mathbf{K}$, $\mathbf{k}$, M, and c (since δE is a corrective term, we can replace ω by ω_0 in the final expression for δE). Show that δE is the sum of two terms, one of which, δE_1, depends on $\mathbf{K}$ and on the angle between $\mathbf{K}$ and $\mathbf{k}$ (the Doppler effect), the other term, δE_2, is independs of $\mathbf{K}$. Give a physical interpretation of δE_1 and δE_2 (showing that δE_2 is the recoil kinetic energy of the atom when, having been initially motionless, it absorbs a resonant photon).

Show that δE_2 is negligible compared to δE_1 when $\hbar\omega_0$ is of order of 10 eV (the domain of atomic physics). Choose, for M, a mass of order of the proton ($Mc^2 \approx 10^9$ eV), and, for K, a value corresponding to the thermal velocity at $T = 300$ K. Would this still be true if $\hbar\omega_0$ were of order of 10^5 eV (the domain of nuclear physics)?

II. Recoilles absorption of radiation by a nucleous vibrating about its equilibrium position in a crystal. The Mössbauer effect

The system under consideration is now a nucleous of mass M vibrating at angular frequency Ω about its equilibrium position in a crystalline lattice (the Einstein model). Again, denote by $\mathbf{R}_G$ and $\mathbf{P}_G$ the position and momentum operators of the center of mass of this nucleous, respectively. Its vibrational energy is given by

$$H_e = \frac{1}{2M} P_G^2 + \frac{1}{2} M\Omega \left(X_G^2 + Y_G^2 + Z_G^2\right),$$

which is that of the 3D Harmonic Oscillator. Denote by $|n_x, n_y, n_z\rangle$ the Eigenstate of H_e with Eigenenergy $(n_x + n_y + n_z + 3/2)\,\hbar\Omega$. In addition to these "external" degrees of freedom, the nucleous possesses "internal" degrees of freedom which are associated observables that commute with $\mathbf{R}_G$ and $\mathbf{P}_G$ and are described by H_i. As before, let us concern only with the two lowest levels of H_i: $|\chi_a\rangle$ and $|\chi_b\rangle$. Also, set $\hbar\omega_0 = E_b - E_a > 0$. Typically, $\hbar\omega_0$ is in the γ-ray domain, and thus, $\omega_0 \gg \Omega$.

(e) What energy must be given to the nucleous to allow it go from state $|0, 0, 0, \chi_a\rangle$ to state $|n, 0, 0, \chi_b\rangle$?

(f) This nucleous is placed in the same radiation field as before (and set $\mathbf{k} = k\hat{x}$). It can be shown that, in the electric dipole approximation, the interaction Hamiltonian of the nucleous with the plane wave (responsible for the absorption of γ-rays) can be written as in Eq. (2) with

$$W_0 = A_0 S_i(k) e^{ikX_G},$$

where $S_i(k)$ is an operator which acts on the internal degrees of freedom of the nucleous and, consequently, commutes with $\mathbf{R}_G$ and $\mathbf{P}_G$.

The nucleous is initially in the state $|0, 0, 0, \chi_a\rangle$. Show that under the influence of the incident wave, a resonance appears whenever $\hbar\omega$ coincides with one of the energies calculated in item (e). The intensity of the resonance is $|s(k)|^2 \left|\langle n, 0, 0|\, e^{ikX_G}\, |0, 0, 0\rangle\right|^2$, where the value of k is to be specified and $s(k) = \langle\chi_b\, |S_i(k)|\, \chi_a\rangle$. Show that, because $\omega_0 \gg \Omega$, we can replace k by $k_0 = \omega_0/c$ in the expression for the intensity of the resonance.

(g) Set

$$\pi_n(k_0) = \left|\left\langle \varphi_n \left| e^{ik_0 X_G} \right| \varphi_0 \right\rangle\right|^2,$$

where $|\varphi_n\rangle$ are the Eigenstates of the 1D Hamornic Oscillator of position X_G, mass M, and angular frequency Ω.

($g.\alpha$) Calculate $\pi_n(k_0)$ in terms of $\hbar$, M, Ω, k_0, and n. (*Hint*: stablish a recurrence relation between $\left\langle \varphi_n \left| e^{ik_0 X_G} \right| \varphi_0 \right\rangle$ and $\left\langle \varphi_{n-1} \left| e^{ik_0 X_G} \right| \varphi_0 \right\rangle$, and express all $\pi_n(k_0)$ as a function of $\pi_0(k_0)$, which is to be calculated directly from the wave function of the Harmonic Oscillator. Show that $\pi_n(k_0)$ are given by a Poisson distribution of n with average ξ, where $\xi = \left(\frac{\hbar^2 k_0^2}{2M}\right) / (\hbar\Omega)$.

($g.\beta$) Verify that $\sum_{n=0}^{\infty} \pi_n(k_0) = 1$.

($g.\gamma$) Show that $\sum_{n=0}^{\infty} n\hbar\Omega\pi_n(k_0) = \frac{\hbar^2\omega_0^2}{2Mc^2}$.

(h) Assume that $\hbar\Omega \gg \frac{\hbar^2\omega_0^2}{2Mc^2}$, i.e., the vibrational energy is much greater than the recoil energy (very rigid crystal). Show that the absorption spectrum of the nucleous is essentially composed of a single line at the angular frequency ω_0. This line is called the recoilless absorption line. Justify this name. Why does the Doppler effect disappear?

(i) Now assume that $\hbar\Omega \ll \frac{\hbar^2\omega_0^2}{2Mc^2}$ (very weak crystalline bonds). Show that the absorption spectrum of the nucleous is composed of 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 motionless nucleous. What is the order of magnitude of the width of this spectrum (the dispersion of the line with respect to the barycenter)? Show that one recover the results of the first part in the limit $\Omega \to 0$.

6. (Optional) Consider the 1D dynamics of a particle of charge e e mass m under a periodic potential $V(x) = V(x + a)$. Assume that at $t = 0$ a vector potential is turned on $A(t) = -Et$.

(a) Study the quasi-degenerate perturbation theory between the states e^{ikx} and $e^{i(k-\kappa)x}$ (conveniently normalized) when $k \approx \kappa/2$, where $\kappa = 2\pi/a$. Assume that $A(t)$ varies slowly and that $V(x)$ can be treated perturbatively.

(b) Compute the adiabatic Eigenstates of the system around $k = \kappa/2$.

(c) Compute the transition probability from the lowest- to the highest-energy adiabatic Eigenstate assuming that the transition is more likely to happen around $k = \kappa/2$.

Make any approximation you may find convenient in order to compute the integrals involved.