FI 002 – Mecânica Quântica II – Lista 1

P.01. P.8.9, Merzbacher:
Solve the energy eigenvalue problem for a particle that is confined in a two-dimensional square box whose sides have length L and are oriented along the x- and y -coordinate axes with one corner at the origin. Find the eigenvalues and eigenfunctions, and calculate the number of eigenstates per unit energy interval for high energies.
A small perturbation $V = Cxy$ is now introduced. Find the approximate energy change of the ground state and the splitting of the first excited energy level. For the given perturbation, construct the optimal superpositions of the unperturbed wave functions in the case of the first excited state.

P.02. P.18.1, Merzbacher:
The Hamiltonian of a rigid rotator in a magnetic field perpendicular to the x axis is of the form $AL^2 + BL_z + CL_y$, if the term that is quadratic in the field is neglected. Obtain the exact energy eigenvalues and eigenfunctions of the Hamiltonian. Then, assuming $B \gg C$, use second-order perturbation theory to get approximate eigenvalues and compare these with the exact answers.
Hint: Exercise 16.4, Merzbacher.

03. P.18.2, Merzbacher:
A charged particle is constrained to move on a spherical shell in a weak uniform electric field. Obtain the energy spectrum to second order in the field strength.
Hint: Eq. (12.196), Arfken and P.5.12, Sakurai.

P.04. P.18.5, Merzbacher:
A slightly anisotropic three-dimensional harmonic oscillator has $\omega_z = \omega + \Delta\omega$ and $\omega_x = \omega_y = \omega$, with $\Delta\omega \ll \omega$. A charged particle moves in a field of this oscillator and it is at the same time exposed to a uniform magnetic filed in the x direction. Assuming that the Zeeman splitting is comparable to the splitting produced by the anisotropy, but small compared to $\hbar\omega$, calculate to first order the energies of the components of the first excited state. Discuss various limiting cases.
Obs.: Consider the symmetric gauge.

05. P.18.9, Merzbacher:
Obtain the relativistic correction to $\propto p^4$ to the nonrelativistic kinetic energy of an electron, and, using first-order perturbation theory, evaluate the energy shift that it produces in the ground state of hydrogen.

06. P.18.10, Merzbacher:
Using the Hamiltonian for an atomic electron in a magnetic field, determine, for a state of zero angular momentum, the energy change to order B^2, if the system is in a uniform magnetic field represented by the vector potential $\mathbf{A} = \mathbf{B} \times \mathbf{r}/2$. Defining the atomic diamagnetic susceptibility χ by $E = -\chi B^2/2$, calculate χ for the ground state of the hydrogen atom.

P.07. P.18.14, Merzbacher:
A rotator whose orientation is specified by the angular coordinates θ and ϕ performs a hindered rotation described by the Hamiltonian

$$H = AL^2 + B\hbar^2 \cos 2\varphi$$

with $A \gg B$. Calculate the S, P, and D energy levels of this system in first-order perturbation theory, and work out the corresponding unperturbed energy eigenfunctions.

08. Exercise 18.16, Merzbacher:
Calculate the linear Stark effect for the $n = 3$ levels of the hydrogen atom.

09. P.11.6, Baym:
Using Brillouin-Wigner perturbation theory show that $\partial E_n/\partial \epsilon_n = Z$ is exact to all orders in the perturbation, where Z is the wave function renormalization constant, E_n the exact energy, ϵ_n the unperturbed energy, and the derivative is at constant matrix elements ϵ_m and $n \neq m$.
Hint: See Chapter 11, Baym.

P.10. P.16.1, Messiah:
The interaction $V(q)$ is added to the Hamiltonian $H = (p^2 + m^2\omega^2 q^2)/2m$. Calculate with the perturbation theory the first- and second-order energy-level shifts for the following two cases:

a) $V = bq.$

b) $V = \frac{1}{2} m\alpha^2 q^2.$

In cases (a) and (b), the shifts can be exactly calculated. Compare the exact result with that of the perturbation theory.

11. P.5.32 (a), Sakurai:
Consider the positronium problem you solved in Chapter 3, Problem 3.4. In the presence of a uniform and static magnetic field B along the z-axis, the Hamiltonian is given by

$$H = A\mathbf{S}_1 \cdot \mathbf{S}_2 + \left(\frac{eB}{mc}\right)(S_{1z} - S_{2z})\,.$$

Solve this problem to obtain the energy levels of all four states using degenerate time-independent perturbation theory (instead of diagonalizing the Hamiltonian matrix). Regard the first and second terms in the expression for H as H_0 and V, respectively. Compare your results with the exact expressions.

P.12. P.11.5, Cohen-Tannoudji:
Consider a system of angular momentum $\mathbf{J}$. We confine ourselves in this exercise to a three-dimensional subspace, spanned by the three kets $|+1\rangle$, $|0\rangle$, and $|-1\rangle$, common eigenstates of J^2 and J_z. The Hamiltonian H_0 of the system is:

$$H_0 = aJ_z + \frac{b}{\hbar} J_z^2,$$

where a and b are two positive constants, which have the dimensions of an angular frequency.

a) What are the energy levels of the system? For what value of the ratio b/a is there degeneracy?

b) A static field $\mathbf{B}_0$ is applied in a direction $\hat{u}$ with polar angles θ and ϕ. The interaction with $\mathbf{B}_0$ of the magnetic moment of the system:

$$\mu = \gamma \mathbf{J}$$

(γ: the gyromagnetic ratio, assumed to be negative) is described by the Hamiltonian:

$$W = \omega_0 J_u$$

where $\omega_0 = -\gamma B_0$ is the Larmor angular frequency in the field $\mathbf{B}_0$ and J_u is the component of $\mathbf{J}$ in the $\hat{u}$ direction:

$$J_u = J_z \cos\theta + J_x \sin\theta \cos\phi + J_y \sin\theta \sin\phi.$$

Write the matrix which represents W in the basis of the three eigenstates of H_0.

c) Assume that $b = a$ and that the $\hat{u}$ direction is parallel to Ox. We also have $\omega_0 \ll a$. Calculate the energies and eigenstates of the system, to first order in ω_0 for the energies and to zeroeth order for the eigenstates.

d) Assume that $b = 2a$ and that we again have $\omega_0 \ll a$, the direction of $\hat{u}$ now being arbitrary. In the $|+1\rangle$, $|0\rangle$, $|-1\rangle$ basis, what is the expansion of the ground state $|\psi_0\rangle$ of $H_0 + W$, to first order in ω_0? Calculate the mean value $\langle\mu\rangle$ of the magnetic moment μ of the system in the state $|\psi_0\rangle$. Are $\langle\mu\rangle$ and $\mathbf{B}_0$ parallel? Show that one can write:

$$\langle\mu_i\rangle = \sum_j \chi_{ij} B_j$$

with $i, j = x, y, z$. Calculate the coefficients χ_{ij} (the components of the susceptibility tensor).

13. P.11.7, Cohen-Tannoudji: Consider a nucleus of spin $I = 3/2$, whose state space is spanned by the four vectors $|m\rangle$ ($m = -3/2, -1/2, +1/2, +3/2$) common eigenvectors of I^2 and I_z. This nucleus is placed at the coordinate origin in a non-uniform electric field derived from a potential $U(x, y, z)$. The directions of the axes are chosen such that, at the origin:

$$\frac{\partial^2 U}{\partial x \partial y} = \frac{\partial^2 U}{\partial y \partial z} = \frac{\partial^2 U}{\partial z \partial x} = 0.$$

Recall that U satisfies Laplace equation $\nabla^2 U = 0$. We shall assume that the interaction Hamiltonian between the electric field gradient at the origin and the electric quadrupole moment of the nucleus can be written

$$H_0 = \frac{qQ}{2I(2I-1)\hbar^2}\left(a_x I_x^2 + a_y I_y^2 + a_z I_z^2\right)$$

where q is the electron charge, Q is a constant with the dimensions of a surface and proportional to the quadrupole moment of the nucleus, and

$$a_x = \left(\frac{\partial^2 U}{\partial x^2}\right)_0, \qquad a_y = \left(\frac{\partial^2 U}{\partial y^2}\right)_0, \qquad a_z = \left(\frac{\partial^2 U}{\partial z^2}\right)_0$$

(the index 0 indicates that the derivatives are evaluated at the origin).

a) Show that, if U is symmetrical with respect to revolution about Oz, H_0 has the form:

$$H_0 = A\left[3I_z^2 - I(I+1)\hbar^2\right]$$

where A is a constant to be specified. What are the eigenvalues of H_0, their degrees of degeneracy and the corresponding eigenstates?

b) Show that, in the general case, H_0 can be written:

$$H_0 = A\left[3I_z^2 - I(I+1)\hbar^2\right] + B\left(I_+^2 + I_-^2\right)$$

where A and B are constants, to be expressed in terms of a_x and a_y. What is the matrix which represents H_0 in the $|m\rangle$ basis? Show that it can be broken down into two 2×2 submatrices. Determine the eigenvalues of H_0 and their degrees of degeneracy, as well as the corresponding eigenstates.

c) In addition to its quadrupole moment, the nucleus has a magnetic moment $\mu = \gamma \mathbf{I}$ (γ: the gyromagnetic ratio). Onto the electrostatic field is superposed a magnetic field $\mathbf{B}_0$, of arbitrary direction $\hat{u}$. We set $\omega_0 = -\gamma B_0$. What term W must be added to H_0 in order to take into account the coupling between μ and $\mathbf{B}_0$? Calculate the energies of the system to first order in B_0.

d) Assume $\mathbf{B}_0$ to be parallel to Oz and weak enough for the eigenstates found in (b) and the energies to first order in ω_0 found in (c) to be good approximations. What are the Bohr frequencies which can appear in the evolution of $\langle I_x \rangle$? Deduce from them the shape of the nuclear magnetic resonance spectrum which can be observed with a radiofrequency field oscillating along Ox.