L3-Magistère de Physique Fondamentale
L3 ENS Paris-Saclay

QUANTUM MECHANICS II
Partial examination — March 6, 2023.

Duration: 2 hours

Books and mobile phones are forbidden.
Lecture notes given by the teachers, personal notes and calculators are allowed.

The examination is composed of three independent exercises.

Exercise A – Singlet and triplet states

Two spin-1/2 particles are in a singlet state $|\psi_{0,0}\rangle$, with total spin $S = 0$ and quantum number $M = 0$.

1. We consider the basis $\{|+\rangle, |-\rangle\}$ of the Hilbert space of a spin-1/2. Introduce the so-called tensor-product basis of the total Hilbert space of two spins and write the singlet state in this basis. You can answer this question without explaining your reasoning.

2. Consider the operators:

$$S_x^{(1)} \otimes S_x^{(2)} \qquad S_y^{(1)} \otimes S_y^{(2)} \qquad S_z^{(1)} \otimes S_z^{(2)}. \tag{1}$$

   Write the expectation value of each of the three operators on $|\psi_{0,0}\rangle$.

Consider now the triplet state $|\psi_{1,0}\rangle$ of two spin-1/2, with total spin $S = 1$ and quantum number $M = 0$.

3. Write the state $|\psi_{1,0}\rangle$ in the tensor-product basis. You can answer this question without explaining your reasoning.

4. Compute the expectation value of each of the three operators in Eq. (1) on $|\psi_{1,0}\rangle$.

5. Compare the results obtained at points 2. and 4. Could you have anticipated this result? Justify your answer in one line.

Exercise B – A highly-excited state of the hydrogen atom

A hydrogen atom is prepared in the energy level $|1, 0, 0\rangle$, with usual quantum-number notation $|n, l, m\rangle$. A theorist and an experimentalist are interested in preparing it in the energy level $|60, 2, 0\rangle$. To this goal they have prepared an apparatus that can send electromagnetic waves with wavevector $\vec{k}$ parallel to the x axis $\hat{u}_x$ and which are linearly polarized, with the electric field $\vec{E}(\vec{r}, t)$ parallel to the z axis $\hat{u}_z$. In principle, their experimental apparatus based on lasers allows for a wide tunability of the frequency of the radiation ω, and they can even send bichromatic radiation composed of two frequencies ω_1 and ω_2.

The atom is placed at the origin of the Cartesian axes and in the following we will neglect the motion of the proton and the spins of the electron and of the proton. In the framework of the electric-dipole approximation, the light-matter coupling Hamiltonian reads:

$$H_{lm} = +q\, \hat{\vec{r}} \cdot \vec{E}(0, t). \tag{2}$$

where $\hat{\vec{r}}$ is the position of the electron and $q > 0$ is the elementary charge.

A direct transition.

The first strategy that they devise is that of inducing a direct transition with monochromatic radiation.

1. Using the notion of selection rules, show that an electromagnetic transition from the energy level $|1,0,0\rangle$ to $|60,2,0\rangle$ is not possible in the framework of first-order time-dependent perturbation theory.

A two-step transition with an intermediate state.

As a second strategy, they think at preparing the state $|60,2,0\rangle$ with a two-step process and using radiation with two frequencies ω_1 and ω_2. The idea is that the first frequency can be used to drive the transition to an intermediate state $|n,l,m\rangle$ and that the second frequency can subsequently drive the transition to the desired final state $|60,2,0\rangle$.

2. Using first-order time-dependent perturbation theory and the notion of selection rules, identify all states $|n,l,m\rangle$ to which a transition from $|1,0,0\rangle$ is possible. Show that the state $|30,1,0\rangle$ belongs to this set.

3. Consider now a transition from the state $|30,1,0\rangle$ to the final state $|60,2,0\rangle$. Is this transition possible (always according to first-order time-dependent perturbation theory)? To solve this question, it can be useful to look at the explicit formulas for the spherical harmonics listed here below and in particular to express $\cos^2\theta$ as a linear combination of two spherical harmonics.

4. Consider now a three-level model with the basis vectors $|1,0,0\rangle$, $|30,1,0\rangle$ and $|60,2,0\rangle$. The dynamics of the experimental apparatus proposed above can be described by the Hamiltonian:

$$H(t) = \begin{pmatrix} -E_I & W_1 e^{i\omega_1 t} & 0 \\ W_1^* e^{-i\omega_1 t} & -\frac{E_I}{30^2} & W_2 e^{i\omega_2 t} \\ 0 & W_2^* e^{-i\omega_2 t} & -\frac{E_I}{60^2} \end{pmatrix}. \tag{3}$$

   Explain briefly the physical significance of all the matrix elements.

5. The state vector can be represented as a three-component vector, for which we propose the following ansatz:

$$|\Psi(t)\rangle = \begin{pmatrix} c_1(t) \\ c_2(t)e^{-i\omega_1 t} \\ c_3(t)e^{-i(\omega_1+\omega_2)t} \end{pmatrix}. \tag{4}$$

   Show that the differential equations obeyed by the $c_i(t)$ do not depend on time.

6. The initial state is $|1,0,0\rangle$: what are the initial conditions for the $c_i(t)$?

7. A simple analytical solution of the problem can be derived when:

$$\hbar\omega_1 = E_I\left(-\frac{1}{30^2}+1\right), \qquad \hbar\omega_2 = E_I\left(-\frac{1}{60^2}+\frac{1}{30^2}\right), \qquad W_1 = W_2 \in \mathbb{R}. \tag{5}$$

   Show that the problem can be recast as an effective Schrödinger equation with the effective state vector and Hamiltonian:

$$|\Psi_{\text{eff}}(t)\rangle = \begin{pmatrix} c_1(t) \\ c_2(t) \\ c_3(t) \end{pmatrix}; \qquad H_{\text{eff}} = \begin{pmatrix} 0 & W & 0 \\ W & 0 & W \\ 0 & W & 0 \end{pmatrix}; \qquad W \in \mathbb{R}. \tag{6}$$

8. The eigenvalues of H_{eff} are

$$\lambda_1 = \sqrt{2}W, \qquad \lambda_2 = 0, \qquad \lambda_3 = -\sqrt{2}W, \tag{7}$$

and the respective eigenvectors are:

$$|v_1\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} \sqrt{2} \\ 1 \\ \sqrt{2} \end{pmatrix}; \qquad |v_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}; \qquad |v_3\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} \sqrt{2} \\ -1 \\ \sqrt{2} \end{pmatrix}. \tag{8}$$

Solve the dynamics of the system: what is the state vector $|\Psi(t)\rangle$ at time t?

9. Compute the probability of finding the system in the level $|60, 2, 0\rangle$ at time t. What its maximal value as a function of time? Would you say that the two physicists achieved their goal?

Exercise C – A perturbed square potential well

We consider an electron (mass m) moving in a two-dimensional plane and trapped in an infinite potential well:

$$V(x, y) = \begin{cases} 0 & \text{if } x \in [0, a] \text{ AND } y \in [0, b]; \\ +\infty & \text{otherwise.} \end{cases} \tag{9}$$

The two lengths a and b are very similar but different, we will thus parametrise $b = a + \epsilon$ with $\epsilon \ll a$. The eigenvalues and eigenvectors of the associated Hamiltonian are:

$$e_{n,n'} = \frac{\hbar^2 \pi^2 n^2}{2ma^2} + \frac{\hbar^2 \pi^2 n'^2}{2mb^2}; \qquad \psi_{n,n'}(x, y) = \sqrt{\frac{4}{ab}} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{n'\pi y}{b}\right); \qquad n, n' \in \{1, 2, 3 \ldots\}. \tag{10}$$

In this exercise we neglect the spin of the electron.

At time $t = 0$ the system is in the ground state $|\Psi_g\rangle$ (characterised by quantum numbers $n = n' = 0$) and a time-dependent potential of the form

$$W(x, y, t) = \epsilon_0 \, \frac{x}{a} \, \sin(\omega t) \qquad \text{for } t \geq 0 \tag{11}$$

is switched on, where ϵ_0 is a typical energy scale. We are interested in characterising the time evolution of the system; in particular, at a time $\tau \geq 0$ we measure the energy of the system and we want to investigate whether the system will be in an excited energy level. To this goal, we will use the time-dependent perturbation theory.

1. Using first-order time-dependent perturbation theory, write the probability $P_{g\to f}(\tau)$ of measuring the system in an excited energy level $|\Psi_f\rangle$ at time τ. One or more integrals are expected to appear, you do not need to solve them.

The effect of the frequency ω.

We now consider the transition from the ground state $|\Psi_g\rangle$ to the excited state $|\Psi_e\rangle$ with quantum numbers $n = 2$ and $n' = 1$.

2. Consider the transition probability $P_{g\to e}(\tau)$: solve *only* the integral over time that you wrote at point 1 and show that it is the sum of two terms. Give a physical interpretation of both terms. Explain why when one is interested in describing a transition to $|\Psi_e\rangle$, one of the two terms can be neglected.

3. Plot $P_{g\to e}(\tau)$ as a function of τ and characterize the values of its maxima and minima, as well as the values of τ at which they are attained. The following integral can be useful: $\int_0^\pi x \sin(2x) \sin(x) dx = -8/9$.

4. The frequency ω can be tuned but we want to remain in a regime where $\max_\tau P_{g\to e}(\tau)$ is much smaller than 1 in order to be able to use time-dependent perturbation theory. Give a condition on ω so that this is obtained.

5. The blind application of time-dependent perturbation theory identifies a frequency ω_0 such that $\max_\tau P_{0\to 1}(\tau)$ diverges to the infinity. What is this frequency? Is this result physical?

6. What happens to the system when the oscillation takes place exactly at the frequency ω_0? You can answer this question with qualitative arguments since the rigorous calculation is rather long.

Numerical application

7. Consider an electron in a semiconductor, whose mass is renormalised by the ionic lattice, and takes the typical value $m = 10^{-30}$ kg. The potential well, realised with microfabrication techniques, has an edge whose length is of the order $0.01\,\mu$m. Estimate the order of magnitude of the frequency $\omega/2\pi$ at which the perturbation should oscillate in order to induce a transition to $|\Psi_e\rangle$ with a significant probability.

END OF THE EXAMINATION

Some spherical harmonics.

$$l = 0 \qquad Y_{0,0}(\theta,\phi) = \sqrt{\frac{1}{4\pi}};$$

$$l = 1 \qquad Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta; \qquad Y_{1,\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}e^{\pm i\phi}\sin\theta;$$

$$l = 2 \qquad Y_{2,0}(\theta,\phi) = \sqrt{\frac{5}{16\pi^2}}(3\cos^2\theta - 1); \qquad Y_{2,\pm1}(\theta,\phi) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\phi};$$

$$Y_{2,\pm2}(\theta,\phi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm i2\phi};$$