**Quantum Electrodynamics and Quantum Optics**

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE (EPFL)

*Exercise No.7*

## 7.1 Semiclassical Atom-Field interaction

In this exercise we study the interaction of a two level system (i.e. an atom) with a classical electromagnetic field. First we review how to describe the dynamics of a charged particle moving in an electromagnetic field in the Hamilton formalism[1], and then we quantize the motion of a particle bound in an atom.

1. Consider a charged particle with mass $m$ and charge $e$, where its position and velocity are expressed by $\mathbf{r}$ and $\dot{\mathbf{r}} = \mathbf{v}$. The particle is moving in an electromagnetic field with electric and magnetic fields of $\mathbf{E}(t, \mathbf{r})$ and $\mathbf{B}(t, \mathbf{r})$. Show that the Lagrangian

$$L = \frac{1}{2}m\mathbf{v}^2 - eU + e\mathbf{A} \cdot \mathbf{v}, \tag{1}$$

describes the dynamics of this particle, meaning it recovers the Lorentz force $\mathbf{F} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. Here we have introduced the electromagnetuc potentials $U$ and $\mathbf{A}$, where $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\nabla U - \frac{\partial}{\partial t}\mathbf{A}$.

2. Find the corresponding generalized momentum for this system ($p_j = \partial L / \partial v_j$), and then show that the Hamiltonian of this system is given by:

$$H = \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + eU \tag{2}$$

3. Now we would like to treat the problem of an electron, bound in an atom, in the presence of an external *classical* electromagnetic field. In a radiation gauge where $\nabla \cdot \mathbf{A} = 0$ and $U = 0$, and adapting Eq. 2 we can write the Hamilton **operator** for this system:

$$\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} - e\mathbf{A}(\hat{\mathbf{r}}, t))^2 + \hat{V}(\hat{\mathbf{r}}), \tag{3}$$

where $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ are position and momentum operators of the electron and $\hat{V}(\hat{\mathbf{r}})$ is the static nucleus potential in the atom. Note that the vector potential is kept as a classical field. Here we make an important approximation, known as the **Dipole approximation**. Typically the wavelength of the external field is much bigger that the dimensions of the atom and we can neglect the spatial variation of the external field and aproximate it with its value at the center of mass position of the atom ($\mathbf{r}_0$) meaning $\mathbf{A}(\hat{\mathbf{r}}, t) \approx \mathbf{A}(\mathbf{r}_0, t) = \mathbf{A}_0(t)$. Now we can write the Schrödinger equation (SE) for this bound electron in the coordinate space (i.e. $\hat{\mathbf{r}} \to \mathbf{r}$ and $\hat{\mathbf{p}} \to -i\hbar\nabla$):

$$[-\frac{\hbar^2}{2m}(\nabla - \frac{ie}{\hbar}\mathbf{A}_0(t))^2 + V(\mathbf{r})]\psi(\mathbf{r}, t) = i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t}. \tag{4}$$

Now define a new gauge transformed wave function $\phi(\mathbf{r}, t) = \exp\left[-\frac{ie}{\hbar}\mathbf{A}_0(t) \cdot \mathbf{r}\right]\psi(\mathbf{r}, t)$. (Note that the Schrödinger equation leads to wave functions which is defined only up to an arbitrary constant global phase factor.). Rewrite the Schrödinger equation with the new wave function ($\phi$) and deduce a new form for the electromagnetic Hamiltonian.

[1] You can refer to the book 'Classical Mechanics' by Goldstein, chapter 1 and 2

$$H = H_0 + H_I \tag{5}$$
$$H_0 = \frac{(-i\hbar\nabla)^2}{2m} + V(\mathbf{r}) \tag{6}$$
$$H_I = -e\mathbf{r}\cdot\mathbf{E}(\mathbf{r}_o, t) \tag{7}$$

The interaction term is typically called the **Dipole Interaction Hamiltonian**.

4. [2] The external electric field has the form $\mathbf{E}_0(t) = \mathbf{E}_0\cos(\omega t)$. As we will see later in the exercise the field interacts strongly with the two levels of the atom for which the transition frequency is close to the oscillation frequency of the field. In the situation we can model the atom as a two level system.

   Now consider two eigenstates of the atom (i.e. $H_0$): $|1\rangle$ and $|2\rangle$ with the corresponding wave functions $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$ and energy eigenvalues of $\omega_1$ and $\omega_2$. Furthermore assume that the transition occurs between states with different parity (e.g. $\phi_2(-\mathbf{r}) = -\phi_2(\mathbf{r})$ and $\phi_1(-\mathbf{r}) = \phi_1(\mathbf{r})$).

   (a) In this two dimensional space the state of the atom can be expressed as $|\Psi(t)\rangle = \alpha(t)e^{-i\omega_1 t}|1\rangle + \beta(t)e^{-i\omega_2 t}|2\rangle$. Show that the probability amplitudes for the ground and excited states obey:

$$\frac{d\alpha}{dt} = i\frac{\Omega}{2}e^{i(\omega-\omega_{21})t}\beta \tag{8}$$
$$\frac{d\beta}{dt} = i\frac{\Omega}{2}e^{-i(\omega-\omega_{21})t}\alpha \tag{9}$$

   Here, the Rabi Frequency is given by $\Omega \equiv \frac{\mathbf{d}_{12}\cdot\mathbf{E}_0}{\hbar}$, where the dipole matrix element is $\mathbf{d}_{12} \equiv \langle 1|e\mathbf{r}|2\rangle$. $\omega_{21} = \omega_2 - \omega_1$ is the transition frequency. Derive the general solutions of these equations for arbitrary detuning (and for the initial condition $|\Psi(t=0)\rangle = |1\rangle$).

   (b) Show that the probability of being in the excited states has the form

$$P_2(t) = |\langle\Psi(t)|2\rangle|^2 = \frac{1}{1+(\Delta\omega/\Omega)^2}\sin^2(\frac{\tilde{\Omega}t}{2}) \tag{10}$$

   with $\Delta\omega = \omega - \omega_{12}$ and $\tilde{\Omega} = \sqrt{\Omega^2 + \Delta\omega^2}$.

   (c) Calculate for the resonant case (i.e. $\Delta\omega = 0$) the expectation value of the Dipole moment, i.e. $\langle\Psi(t)|e\mathbf{r}|\Psi(t)\rangle$. Show that the dipole moment exhibits a fast modulation at the optical frequency ($\omega$) as well as a slow *amplitude* modulation at Rabi frequency.

   (d) Finally, use *Poynting theorem*[3] from classical electrodynamics (e.g. see Amon Yariv, Quantum electronics, Chapter 5) along with the calculated (point-like) dipole $\langle\mathbf{P}(\mathbf{r}_o,t)\rangle = \langle\Psi(t)|e\mathbf{r}|\Psi(t)\rangle\cdot\delta(\mathbf{r}_o-\mathbf{r})$ from above to evaluate in which direction the energy flows (i.e. to or from the electromagnetic field). Specifically, show that on resonance ($\Delta\omega = 0$) the total amount of energy that flows from time $t = 0...\pi/\Omega$ (i.e. the Rabi-up cycle) is exactly equal to $\hbar\omega$, while for from $t = \pi/\Omega...2\pi/\Omega$ ( Rabi down cycle) the amount of energy is given back to the field, i.e. it equals $-\hbar\omega$.[4]

[2] For assistance see "Quantum Optics", M.O Scully, Chapter 5

[3] *Hint*: The Poynting theorem states that amount of work that is done in the time interval T on the field $\mathbf{E}(\mathbf{r}_o,t)$ by the dipole $\langle\mathbf{P}(\mathbf{r}_o,t)\rangle$ is given by:

$$U = \int_T\int_V \mathbf{E}(\mathbf{r}_o,t)\frac{d}{dt}\langle\mathbf{P}(\mathbf{r}_o,t)\rangle dV dt$$

[4] This shows that even within the framework of the semiclassical theory, the energy is taken or given to the optical field in a quantized fashion. Howeverm this quantization clearly arises in this context due to the fact that the atom exhibits quantized levels.

### 7.2 Polarization selection rules in the Hydrogen atom (*)

Previously (in the "Semi-classical atom-field interaction" exercise) we considered two orbitals with opposite parity interaction with linearly polarized light. The dipole interaction term in this case is given for polarization along z-direction by:

$$H_I = -e\mathbf{r}\cdot\mathbf{E}(\mathbf{r}_o,t) = -ez|\mathbf{E}(\mathbf{r}_o,t)| \tag{11}$$

The dipole interaction between the ground state $(n,l,m) = (1,0,0)$ and the excited state $(2,1,0)$ is in this case non-zero. However, light can also be right or left circularly polarized. In this case the field at the location of the atom is given by:

$$\mathbf{E}^L(\mathbf{r}_o,t) = \frac{\mathbf{E}(\mathbf{r}_o)}{2}(\hat{\mathbf{x}}\cos(\omega t) - \hat{\mathbf{y}}\sin(\omega t)) \tag{12}$$

$$\mathbf{E}^R(\mathbf{r}_o,t) = \frac{\mathbf{E}(\mathbf{r}_o)}{2}(\hat{\mathbf{x}}\cos(\omega t) + \hat{\mathbf{y}}\sin(\omega t)) \tag{13}$$

Here the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors. Next consider the three orbitals of the Hydrogen atom:

$$\phi_{100}(\mathbf{r}) = \sqrt{\frac{1}{\pi a_0^3}}e^{-r/a_0} \tag{14}$$

$$\phi_{210}(\mathbf{r}) = \sqrt{\frac{1}{\pi a_0^3}}e^{-r/2a_0}\frac{1}{a_0}z \tag{15}$$

$$\phi_{211}(\mathbf{r}) = \sqrt{\frac{1}{\pi a_0^3}}e^{-r/2a_0}\frac{1}{a_0}(x+iy) \tag{16}$$

$$\phi_{21-1}(\mathbf{r}) = \sqrt{\frac{1}{\pi a_0^3}}e^{-r/2a_0}\frac{1}{a_0}(x-iy) \tag{17}$$

1. First, show that transition from the ground state to $(n,l,m) = (2,1,\pm1)$ cannot be excited via linear polarized light. Start your analysis from the minimal coupling Hamiltonian $H_I = -e\mathbf{r}\cdot\mathbf{E}(\mathbf{r}_o,t)$, and make use explicitly of the rotating wave approximation.

2. Second, show that the transition from $m = 0$ to $m = -1$ can only proceed via left circular polarized (LCP) light (which is also called $\sigma^-$ light). Furthermore show that in this case, you do not have to neglect counter rotating terms as in the case of linear polarization. In fact, these terms never appear.[5]

3. Finally, show that the transition from $m = 0$ to $m = +1$ can only proceed via right circular polarized light (which is also called $\sigma^+$ light). Again, no counter rotating terms appear in the analysis.

   *Note:* The cummulative results are known as conservation of the angular momentum of the photon. It can have the value $\pm1$ or 0. Transitions thus need to conserve the angular momentum and consequently transitions from $m = 0$ to $m = 1$ require $\sigma^+$ (RCP) and from $m = 0$ to $m = 1$ require $\sigma^-$ (LCP) light. However the above analysis makes clear that the conservation of spin is simply a symmetry argument (in essence again a manifestation of Noether's Theorem)

[5] cf. Quantum Optics, Scully, Chapter 5

### 7.3 Coherent population trapping

In this exercise we will discuss a $\Lambda$-type two level system, in which two ground states $|b\rangle$ and $|c\rangle$ are coupled to a common upper state $|a\rangle$. This scenario can for instance be the case when having a ground state which exhibits Hyperfine splitting. The Hamiltonian is thus given by:

$$\hat{H}_0 = \hbar(\omega_a |a\rangle \langle a| + \omega_b |b\rangle \langle b| + \omega_c |c\rangle \langle c|) \tag{18}$$

Assume that you have two coupling lasers $E(t) = E_1 \cos(\omega_1 t)$ and $E(t) = E_2 \cos(\omega_2 t)$ where $E_1$ and $E_2$ are real numbers. The interaction Hamiltonian (with the Rotating Wave Approximation - RWA) is given by:

$$\hat{H}_D = -\frac{\hbar}{2}(\Omega_{R1} \exp(-i(\omega_1 - \omega_{ab})t) |a\rangle \langle b| + \Omega_{R2} \exp(-i(\omega_2 - \omega_{ac})t) |a\rangle \langle c| + \text{h.c.}) \tag{19}$$

Here the quantities $\Omega_{R1}$, $\Omega_{R2}$ denote the Rabi frequencies associated with the transition $|a\rangle \rightarrow |b\rangle$ and $|a\rangle \rightarrow |c\rangle$.

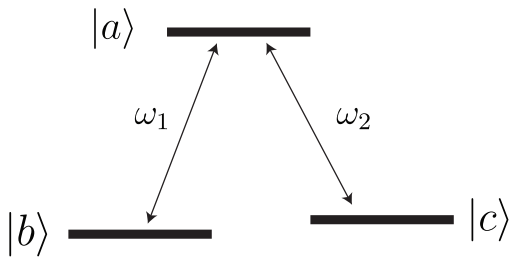


Figure 1: $\Lambda$-type system containing two ground state levels coupled to a joint excited state

1. Derive the equations of motion for the probability amplitudes of the state vector $|\Psi\rangle = a(t)|a\rangle + b(t)|b\rangle + c(t)|c\rangle$ for the case that both fields are resonant. Show that the eigenstates in the presence of the laser fields are given by:

$$|\Psi_+\rangle = \frac{1}{\sqrt{2}}\left(|a\rangle + \frac{\Omega_{R1}^*}{\Omega}|b\rangle + \frac{\Omega_{R2}^*}{\Omega}|c\rangle\right) \tag{20}$$

$$|\Psi_0\rangle = \frac{\Omega_{R2}}{\Omega}|b\rangle - \frac{\Omega_{R1}}{\Omega}|c\rangle \tag{21}$$

$$|\Psi_-\rangle = \frac{1}{\sqrt{2}}\left(|a\rangle - \frac{\Omega_{R1}^*}{\Omega}|b\rangle - \frac{\Omega_{R2}^*}{\Omega}|c\rangle\right) \tag{22}$$

   where $\Omega \equiv \sqrt{|\Omega_{R1}|^2 + |\Omega_{R2}|^2}$. Derive the corresponding eigenvalues and show that one of the above states, $|\Psi_0\rangle$, has a zero eigenvalue. This implies that this state undergoes no time evolution. Furthermore, note that this state is also not coupled to the excited state. Hence, the system is not excited into the state $|a\rangle$, despite the two resonant laser fields.

2. To understand the physical principle of this effect, consider the two following eigenstates:

$$|NC\rangle = \frac{\Omega_{R2}}{\Omega}|b\rangle - \frac{\Omega_{R1}}{\Omega}|c\rangle \tag{23}$$

$$|C\rangle = \frac{\Omega_{R1}}{\Omega}|b\rangle + \frac{\Omega_{R2}}{\Omega}|c\rangle \tag{24}$$

   Show, by evaluating the transition matrix element $\langle a|\hat{H}_D|NC\rangle$ and $\langle a|\hat{H}_D|C\rangle$ and showing that the $|NC\rangle$ is not coupled to the excited state (it has a vanishing dipole transition matrix element), whereas $|C\rangle$ is coupled to the excited state. In the calculations, you should take notice of the fact that the superposition of the two ground states leads to a destructive interference of population in the excited state; this is what gives rise to the lack of coupling to the excited state. Therefore, the dark state is in essence an electronic interference phenomena.[6]

[6]Consequently, if the system is prepared in the state $|NC\rangle$ (i.e. the state $|\Psi_0\rangle$ from the exercise) the population

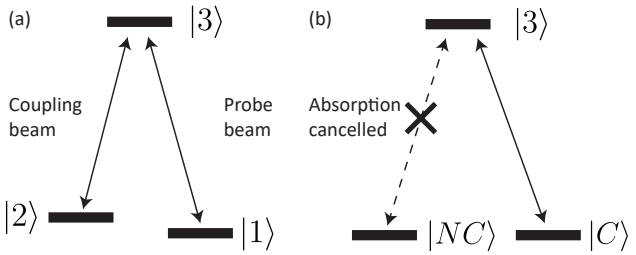


Figure 2: Physical picture of the new eigenstate of the system in terms of (a) coupled and (b) uncoupled (dark) state

remains in this state for all times. Hence, the "population" stays in the eigenstate and is "trapped". Since no quanta of light is absorbed from the two interacting modes, our physical picture suggests that, the three level system is transparent to radiation, even though we tune it to a resonance. Since the state we have prepared doesn't interact with the fields, it is called a *dark state*