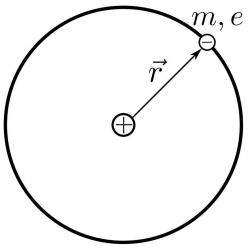
1 Introduction and review of basic concepts in Quantum optics

1.1 Atom-field interactions

Our starting point will be to consider an atom in the absence of external field. We can view this atom as just an electron (with charge e) bound to the nucleus via the Coulomb interaction $V(r)$. The dynamics of this system is described by a Schrödinger equation:



$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H_0\psi(\vec{r},t), \tag{1.1}$$

where $\psi(\vec{r},t)$ is the wave function the contains all information about the system. The Hamiltonian on the right hand side of the equation here reads simply

$$H_0 = \frac{\vec{P}^2}{2m} + V(r)\ , \tag{1.2}$$

where m is the mass of the electron, $\vec{P} = -i\hbar\vec{\nabla}$ the momentum operator, and $V\left(|\vec{r}| = r\right)$ the Coulomb potential.

In the presence of external fields, the Hamiltonian that describes this problem is the so-called *minimal-coupling Hamiltonian*

$$H\left(\vec{r},t\right) = \frac{1}{2m}\left[\vec{P} - e\vec{A}\left(\vec{r},t\right)\right]^2 + e\Phi\left(\vec{r},t\right) + V(r), \tag{1.3}$$

which accounts for the action of the vector and scalar potentials $\vec{A}$ and Φ, respectively, which describe the external fields. In the following, we will use the concept of gauge invariance and the dipole approximation to obtain a simplified version of this Hamiltonian, which will be the starting point of many of the calculations throughout the course.

Gauge invariance:

We know from Classical Field Theory that the electric and magnetic fields can be written in terms of the scalar and vector potentials as

- $\vec{E}\left(\vec{r},t\right) = -\vec{\nabla}\Phi\left(\vec{r},t\right) - \frac{\partial\vec{A}(\vec{r},t)}{\partial t}$
- $\vec{B}\left(\vec{r},t\right) = \vec{\nabla}\times\vec{A}\left(\vec{r},t\right)$.

We also know that these fields (and in general the physics of the problem) must remain the same under a **gauge transformation**:

- $\Phi'(\vec{r},t) = \Phi(\vec{r},t) - \frac{\hbar}{e}\frac{\partial\chi(\vec{r},t)}{\partial t}$
- $\vec{A}'(\vec{r},t) = \vec{A}(\vec{r},t) + \frac{\hbar}{e}\vec{\nabla}\chi(\vec{r},t)$,

this is the so-called gauge invariance. In quantum mechanics, this gauge invariance is established instead by saying that the Schrödinger equation remains invariant under a transformation of the wave function of the form

$$\psi'(\vec{r},t) = U\psi(\vec{r},t) = e^{i\chi(\vec{r},t)}\psi(\vec{r},t) \ . \tag{1.4}$$

Let us see what this means for the Hamiltonian in the original Schrödinger equation:

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = H(\vec{r},t)\,\psi(\vec{r},t)\,. \tag{1.5}$$

Our aim is to write a Schrödinger equation for ψ'. We do this as

$$\begin{aligned} i\hbar\frac{\partial\overbrace{U\psi}^{\psi'}}{\partial t} &= i\hbar\left[\frac{\partial U}{\partial t}\psi + U\frac{\partial\psi}{\partial t}\right] = i\hbar\underbrace{\frac{\partial U}{\partial t}}_{(1.4)}\psi + U\underbrace{i\hbar\frac{\partial\psi}{\partial t}}_{(1.5)} \\ &= -\hbar\frac{\partial\chi}{\partial t}\underbrace{U\psi}_{\psi'} + UH\underbrace{\psi}_{U^\dagger\psi'} \quad \left(UU^\dagger = U^\dagger U = \mathbb{1}\right) \\ &= \underbrace{\left[UHU^\dagger - \hbar\frac{\partial\chi}{\partial t}\right]}_{H'(\vec{r},t)}\psi' \end{aligned}$$

Hence, the Hamiltonian after the transformation reads

$$\begin{aligned} H' &= UHU^\dagger - \hbar\frac{\partial\chi}{\partial t} = e^{i\chi}\frac{1}{2m}\left[i\hbar\vec{\nabla} + e\vec{A}\right]^2 e^{-i\chi} + e\Phi + V(r) - \hbar\frac{\partial\chi}{\partial t} \\ &= e\Phi' + V(r) + \frac{e^{i\chi}}{2m}\left[-\hbar^2\vec{\nabla}^2 + e^2\vec{A}^2 + i\hbar e\vec{\nabla}\cdot\vec{A} + i\hbar e\vec{A}\cdot\vec{\nabla}\right]e^{-i\chi} \\ &= e\Phi' + V(r) + \frac{1}{2m}\left[-\hbar^2\vec{\nabla}^2 + \hbar^2\left(\vec{\nabla}\chi\right)^2 + i\hbar^2\vec{\nabla}^2\chi + 2i\hbar^2\vec{\nabla}\chi\cdot\vec{\nabla}\right. \\ &\left. + e^2\vec{A}^2 + i\hbar e\vec{\nabla}\cdot\vec{A} + \hbar e\vec{\nabla}\chi\cdot\vec{A} + i\hbar e\vec{A}\cdot\vec{\nabla} + \hbar e\vec{A}\cdot\vec{\nabla}\chi + i\hbar e\vec{A}\cdot\vec{\nabla}\right] \\ &\overset{(*)}{=} \frac{1}{2m}\left[i\hbar\vec{\nabla} + e\vec{A}'(\vec{r},t)\right]^2 + e\Phi' + V(r) \end{aligned}$$

Our aim is now to choose a gauge and a gauge function $\chi(\vec{r},t)$ that simplifies (1.3). We now make a choice of gauge, the *Coulomb or radiation gauge*, such that

$$\Phi = 0 \text{ and } \vec{\nabla}\cdot\vec{A} = 0.$$

This simplifies the Hamiltonian to

$$H'(\vec{r},t) = \frac{1}{2m}\left[\vec{P} - e\left(\vec{A} + \frac{\hbar}{e}\vec{\nabla}\chi\right)\right]^2 - \hbar\frac{\partial\chi}{\partial t} + V(r) \tag{1.6}$$

where the vector potential satisfies the *wave equation*

$$\vec{\nabla}^2\vec{A} - \frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} = 0.$$

A general solution for this equation is given by

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

where $\vec{A_0}$ is the amplitude of the vector potential, and $\vec{k}$ is the wave vector of the radiation with $|\vec{k}| = \frac{2\pi}{\lambda} = \frac{\omega}{c}$.

Dipole approximation:

In the expression of $\vec{A}$, we will be interested in the variation of the vector potential in the position of the electron $\vec{r}$ around the position of the atom $\vec{r_0}$ (which here I can assume to be, without loss of generality, the origin). Hence, here the position $\vec{r}$ in which I am interested is approximately the position of the electron with respect to the nucleus. The typical distance between nucleus and electron is a few Ångströms. On the other hand, for typical optical transitions $\lambda \approx$ a few hundred nanometers. Under these circumstances we find that $\vec{k}\cdot\vec{r} \ll 1$, which allows us to take a Taylor expansion such that

$$\begin{aligned}\vec{A}(\vec{r},t) &= \vec{A_0}e^{-i\omega t}\left(1 + i\vec{k}\cdot\vec{r} + \cdots\right) + \text{h.c.} \\ &\approx \vec{A_0}e^{-i\omega t} + \vec{A_0}^{\dagger}e^{i\omega t} \equiv \vec{A}_0(t)\end{aligned} \tag{1.7}$$

where we have kept only the first term of the expansion. This is the *dipole approximation*, and it is equivalent to consider that the external field is constant over the extension of the atom.

Taking now (1.7) into the Hamiltonian (1.6) we have:

$$H'(\vec{r},t) = \frac{1}{2m}\left[\vec{P} - e\left(\vec{A_0} + \frac{\hbar}{e}\vec{\nabla}\chi\right)\right]^2 - \hbar\frac{\partial\chi}{\partial t} + V(r) \ ,$$

where now $\vec{A_0}$ is only a function of time. We now proceed to choose a gauge function χ. By choosing

$$\chi(\vec{r},t) = -\frac{e}{\hbar}\vec{r}\cdot\vec{A_0}(t)$$

the Hamiltonian can be notably simplified, as here

- $\vec{\nabla}\chi = -\frac{e}{\hbar}\vec{A_0}(t)$,
- $\frac{\partial\chi}{\partial t} = -\frac{e}{\hbar}\vec{r}\cdot\frac{\partial\vec{A_0}(t)}{\partial t} \equiv \frac{e}{\hbar}\vec{r}\cdot\vec{E_0}(t)$,

such that

$$H'(\vec{r},t) = \frac{\vec{P}^2}{2m} - e\vec{r}\cdot\vec{E_0}(t) + V(r),$$

and, finally,

$$\boxed{H' = H_0 - \vec{d}\cdot\vec{E_0}(t)} \tag{1.8}$$

where we have used the dipole moment operator:

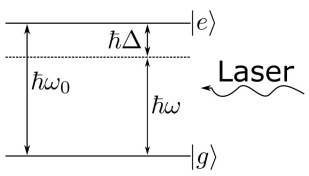
$$\vec{d} = e\vec{r} \tag{1.9}$$

In summary, here we have chosen a gauge and a gauge transformation to obtain (within the dipole approximation) the simplest possible expression for the Hamiltonian that describes the interaction between a bound electron in an atom and an external field.

1.2 Interaction of a two-level atom with a single-mode classical field

In this section, we will start from the Hamiltonian (1.8) and describe the dynamics of a single atom with a laser field.

The atom is modelled as a two-level system, i.e., the electron can be either in the ground $|g\rangle$ or the excited $|e\rangle$ state. Within this *two-level approximation* the two levels are separated energetically by:



$$\hbar\omega_0 = E_e - E_g, \tag{1.10}$$

where E_e and E_g are the energies of the excited and ground state, respectively.

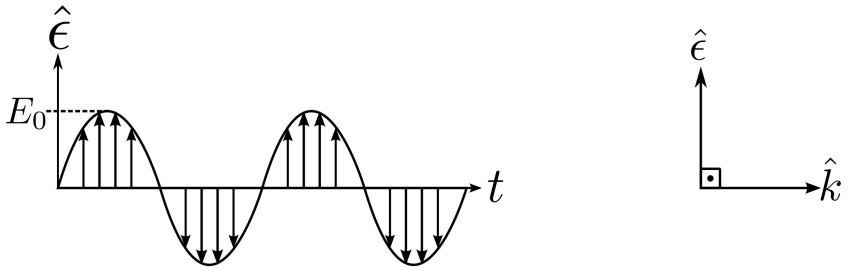
The external field is here considered to be a monochromatic laser field with frequency ω very close to ω_0. The difference between the two frequencies is called *detuning*:

$$\boxed{\Delta = \omega_0 - \omega} \tag{1.11}$$

This field can be expressed as

$$\vec{E_0}(t) = E_0 \cos\Big(\vec{k}\cdot\vec{r_0} - \omega t\Big)\hat{\epsilon} \tag{1.12}$$

where E_0 is the amplitude of the field, $\vec{r_0}$ is the position of the atom, and $\hat{\epsilon}$ is the unit polarization vector, which is perpendicular to the wave vector $\vec{k}$.



Let us now come back to the Hamiltonian we obtained before and see how it looks in this particular case. Let us start with H_0. The eigenstates of H_0 are precisely $|g\rangle$ and $|e\rangle$, i.e.,

$$\begin{aligned} H_0\,|g\rangle &= E_g\,|g\rangle \\ H_0\,|e\rangle &= E_e\,|e\rangle\,. \end{aligned}$$

Since there are no other levels considered in the atom, $\{|g\rangle, |e\rangle\}$ form an *orthonormal basis*, which then satisfies

- $|g\rangle\langle g| + |e\rangle\langle e| = \mathbb{1}$

- $\langle g|g\rangle = \langle e|e\rangle = 1$
- $\langle g|e\rangle = \langle e|g\rangle = 0$

Using these properties, we can write H_0 as

$$\begin{aligned} H_0 &= \left(|g\rangle\langle g| + |e\rangle\langle e|\right) H_0 \left(|g\rangle\langle g| + |e\rangle\langle e|\right) \\ &= E_g \, |g\rangle\langle g| + E_e \, |e\rangle\langle e| \, . \end{aligned} \tag{1.13}$$

The part of the Hamiltonian that describes the interaction between the atoms and the field can be written as

$$\begin{aligned} -\vec{d}\cdot\vec{E_0} &\overset{(1.12)}{=} -E_0 \cos\Big(\vec{k}\cdot\vec{r_0} - \omega t\Big)\hat{\epsilon}\cdot\vec{d} \\ &= -E_0 \cos\Big(\vec{k}\cdot\vec{r_0} - \omega t\Big)\hat{\epsilon}\cdot\Big[\left(|g\rangle\langle g| + |e\rangle\langle e|\right)\vec{d}\left(|g\rangle\langle g| + |e\rangle\langle e|\right)\Big] \\ &= -E_0 \cos\Big(\vec{k}\cdot\vec{r_0} - \omega t\Big)\hat{\epsilon}\cdot\Big[\ \langle g|\vec{d}|e\rangle\,|g\rangle\langle e| + \ \langle e|\vec{d}|g\rangle\,|e\rangle\langle g| \\ &\qquad + \underbrace{\cancel{\langle g|\vec{d}|g\rangle\,|g\rangle\langle g|} + \cancel{\langle e|\vec{d}|e\rangle\,|e\rangle\langle e|}}_{\text{selection rules, parity *}}\Big] \end{aligned}$$

such that

$$-\vec{d}\cdot\vec{E_0} = \hbar\cos\Big(\vec{k}\cdot\vec{r_0} - \omega t\Big)\Big[\Omega_0\,|e\rangle\langle g| + \Omega_0^*\,|g\rangle\langle e|\,\Big]$$

where we have defined the *Rabi frequency* as

$$\boxed{\Omega_0 = -\frac{E_0}{\hbar}\hat{\epsilon}\cdot\ \langle e|\ \vec{d}\,|g\rangle} \tag{1.14}$$

Let us now write everything together:

$$H' = E_g\,|g\rangle\langle g| + E_e\,|e\rangle\langle e| + \hbar\Omega_0\cos\Big(\vec{k}\cdot\vec{r_0} - \omega t\Big)\,|e\rangle\langle g| + \hbar\Omega_0^*\cos\Big(\vec{k}\cdot\vec{r_0} - \omega t\Big)\,|g\rangle\langle e|\,.$$

Without loss of generality, we can set $E_g = 0$, such that $E_e = \hbar\omega_0$ [according to Eq. (1.10)], and then

$$H' = \hbar\omega_0\,|e\rangle\langle e| + \hbar\cos\Big(\vec{k}\cdot\vec{r_0} - \omega t\Big)\Big[\Omega_0\,|e\rangle\langle g| + \Omega_0^*\,|g\rangle\langle e|\,\Big].$$

This Hamiltonian is *time-dependent*, which makes the corresponding Schrödinger equa-

tion a bit harder to solve (although possible!). In order to eliminate this time-dependence we perform yet another unitary transformation, which reads

$$U = |g\rangle\langle g| + e^{i\omega t} |e\rangle\langle e| . \tag{1.15}$$

This transformation is just a change into a *rotating frame*, i.e. we go into a frame of reference that oscillates with the frequency of the laser. The change is done the same way as before, i.e., we look for the Hamiltonian of the Schrödinger equation for the new wave function $|\psi''\rangle = U |\psi'\rangle$, i.e.,

$$H' |\psi'\rangle = i\hbar \frac{\partial |\psi'\rangle}{\partial t} \rightarrow H'' |\psi''\rangle = i\hbar \frac{\partial |\psi''\rangle}{\partial t}$$

such that

$$\begin{aligned} i\hbar \frac{\partial |\psi''\rangle}{\partial t} &= i\hbar \frac{\partial U |\psi'\rangle}{\partial t} = i\hbar \frac{\partial U}{\partial t} |\psi'\rangle + i\hbar U \frac{\partial |\psi'\rangle}{\partial t} \\ &= i\hbar \frac{\partial U}{\partial t} U^\dagger |\psi''\rangle + U H' U^\dagger |\psi''\rangle \\ &= \underbrace{\left(U H' U^\dagger + i\hbar \frac{\partial U}{\partial t} U^\dagger \right)}_{H''} |\psi''\rangle . \end{aligned}$$

For the unitary operation (1.15) we obtain (*)

$$\begin{aligned} H'' &= \hbar\omega_0 |e\rangle\langle e| + \hbar \cos\left(\vec{k} \cdot \vec{r_0} - \omega t\right) \left[\Omega_0 e^{+i\omega t} |e\rangle\langle g| + \Omega_0^* e^{-i\omega t} |g\rangle\langle e| \right] - \hbar\omega |e\rangle\langle e| \\ &\overset{(1.11)}{=} \hbar\Delta |e\rangle\langle e| + \hbar \frac{\Omega_0}{2} \left[e^{i\vec{k}\cdot\vec{r_0}} + e^{-i\vec{k}\cdot\vec{r_0}} e^{2i\omega t} \right] |e\rangle\langle g| \\ &+ \hbar \frac{\Omega_0^*}{2} \left[e^{i\vec{k}\cdot\vec{r_0}} e^{-2i\omega t} + e^{-i\vec{k}\cdot\vec{r_0}} \right] |g\rangle\langle e| \end{aligned}$$

This Hamiltonian still depends on time. But we now perform the so-called *Rotating Wave Approximation*. This approximation consists on neglecting the terms that rotate with frequency 2ω, i.e. the terms above. This is well justified since ω is a very high frequency (typically in the THz order) compared with Ω_0 (kHz − MHz). We are not interested in changes in the dynamics on such small timescales (order $1/\omega$). After

this, the final Hamiltonian reads

$$H'' = \hbar\Delta \left|e\right\rangle\!\left\langle e\right| + \frac{\hbar\Omega_0}{2} e^{i\vec{k}\cdot\vec{r_0}} \left|e\right\rangle\!\left\langle g\right| + \frac{\hbar\Omega_0^*}{2} e^{-i\vec{k}\cdot\vec{r_0}} \left|g\right\rangle\!\left\langle e\right|$$

Now that we have the Hamiltonian we can solve the Schrödinger equation and hence obtain the dynamics of any observable in the system. To do so, we write the wave function as

$$\left|\psi''(t)\right\rangle = c_g(t)\left|g\right\rangle + c_e(t)\left|e\right\rangle$$

where c_g and c_e are the probability amplitudes of the atom to be in the ground and excited state, respectively. Hence, the Schrödinger equation yields

- $i\hbar\frac{\partial|\psi''\rangle}{\partial t} = i\hbar\frac{\partial c_g(t)}{\partial t}\left|g\right\rangle + i\hbar\frac{\partial c_e(t)}{\partial t}\left|e\right\rangle$
- $H''\left|\psi''\right\rangle = c_g(t)\frac{\hbar\Omega_0}{2}e^{i\vec{k}\cdot\vec{r_0}}\left|e\right\rangle + \hbar\Delta c_e(t)\left|e\right\rangle + c_e(t)\frac{\hbar\Omega_0^*}{2}e^{-i\vec{k}\cdot\vec{r_0}}\left|g\right\rangle$

Multiplying each equation on the left by $\langle g|$ and $\langle e|$, we obtain two coupled equations

$$\rightarrow i\hbar\frac{\partial c_g}{\partial t} = \frac{\hbar\Omega_0^*}{2}e^{-i\vec{k}\cdot\vec{r_0}}c_e \tag{a}$$

$$\rightarrow i\hbar\frac{\partial c_e}{\partial t} = \frac{\hbar\Omega_0}{2}e^{i\vec{k}\cdot\vec{r_0}}c_g + \hbar\Delta c_e. \tag{b}$$

We can uncouple the equations by obtaining c_e and $\frac{\partial c_e}{\partial t}$ from (a), subbing in (b), so that

$$\rightarrow \frac{\partial^2 c_g}{\partial t^2} + i\Delta\frac{\partial c_g}{\partial t} + \frac{|\Omega_0|^2}{4}c_g = 0$$

$$\rightarrow \frac{\partial^2 c_e}{\partial t^2} + i\Delta\frac{\partial c_e}{\partial t} + \frac{|\Omega_0|^2}{4}c_e = 0.$$

Note that here, for simplicity, we have assumed that $\Omega_0 = \Omega_0^*$. To solve the dynamics we only need now the initial conditions. For example, we can take that $c_e(0) = 0$, $c_g(0) = 1$, i.e. the atom is at $t = 0$ in the ground state (one can take others, just think that $|c_g(t)|^2 + |c_e(t)|^2 = 1 \quad \forall t$). With these initial conditions the solution is

$$c_e(t) = -i\frac{\Omega_0}{\Omega}\sin\left(\frac{\Omega t}{2}\right)e^{-i\frac{\Delta}{2}t}$$

$$c_g(t) = \left[\cos\left(\frac{\Omega t}{2}\right) + \frac{i\Delta}{\Omega}\sin\left(\frac{\Omega t}{2}\right)\right]e^{-i\frac{\Delta}{2}t},$$

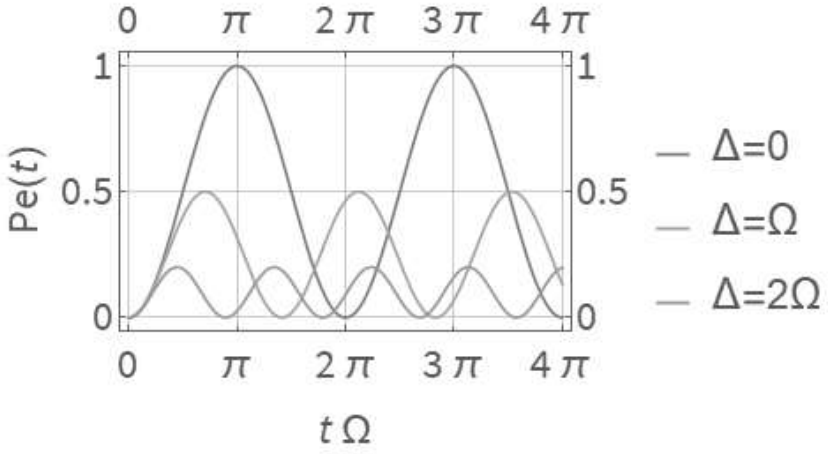
where we have introduced $\Omega = \sqrt{\Omega_0^2 + \Delta^2}$.

Rabi oscillations

Now we are in position calculate any observable we want. For example, the population of the ground and excited states is given, by $|c_g(t)|^2$ and $|c_e(t)|^2$, respectively, where

$$|c_g(t)|^2 + |c_e(t)|^2 = 1 \quad \forall t.$$

Let us then look into the probability of the atom being in the excited state. $P_e(t) \equiv |c_e(t)|^2$ for various situations:



On resonance ($\Delta = 0$):

The population simply oscillates between 0 and 1 with frequency Ω_0:

- When $\Omega_0 t = \pi$ the atom is on the excited state (π- pulse).
- When $\Omega_0 t = \pi/2$, the state of the atom becomes:

$$\left|\Psi''\left(\frac{\pi}{2\Omega_0}\right)\right\rangle = \frac{1}{\sqrt{2}}\left[|g\rangle - i\,|e\rangle\right] \ .$$

Not on resonance $\Delta \neq 0$:

The frequency of the oscillation is the modified $\Omega = \sqrt{\Omega_0^2 + \Delta^2}$, i.e. it is a faster oscillation, but the excited state population reaches a maximum

$$P_{e,max} = \frac{\Omega_0^2}{\Omega_0^2 + \Delta^2} \ .$$

Light shifts

Let us now consider how the energies of the atom change when the light field is present. Originally, when there is no light field, the eigenenergies are simply $E_g = 0$ and $E_e = \hbar\Delta$ (in the rotating frame). When the light field is present, we need to diagonalize the Hamiltonian

$$H'' = \hbar\Delta \left|e\right\rangle\!\left\langle e\right| + \frac{\hbar\Omega_0}{2} e^{i\vec{k}\cdot\vec{r_0}} \left|e\right\rangle\!\left\langle g\right| + \frac{\hbar\Omega_0^\dagger}{2} e^{-i\vec{k}\cdot\vec{r_0}} \left|g\right\rangle\!\left\langle e\right|$$

in order to obtain the eigenenergies of the system, which read

$$E_\pm = \frac{\hbar\Delta}{2} \pm \frac{\hbar\Omega}{2},$$

i.e., the energies are shifted due to the presence of the field as

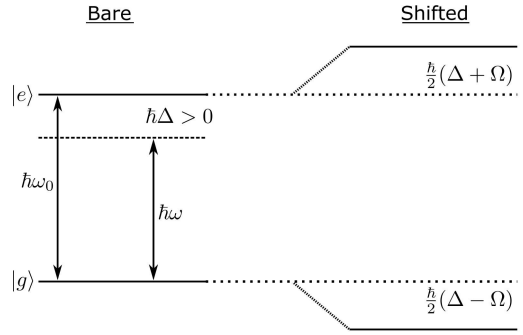


Figure 1: Red-detuned laser

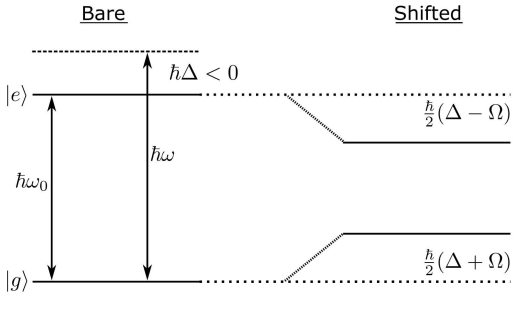
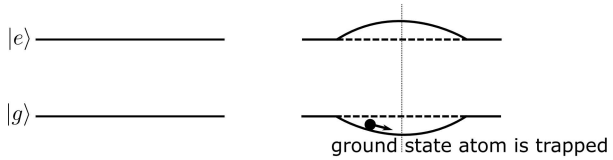


Figure 2: Blue-detuned laser

An interesting limit to consider is when $|\Delta| \gg \Omega$. Here, we can use second-order perturbation theory to obtain the eigenenergies and states. We find that the eigenstates are simply the ground and excited dressed with properties of the other one, and the energies read

$$E_g = -\frac{\hbar\Omega_0^2}{4\Delta} \quad \text{and} \quad E_e = \hbar\Delta + \frac{\hbar\Omega_0^2}{4\Delta}.$$

This is the mechanism used to trap atoms in a so-called dipole trap. There, the field is not homogenous, but a standing wave (in practice created by two counterpropagating laser beams), such that $\Omega_0^2 \to \Omega_0^2 \sin^2(|k|R)$. The light shift for a red-detuned laser becomes:



1.3 Interaction of a two-level atom with a quantum field: radiative decay

In this section, we will again start from the Hamiltonian (1.8) to describe the dynamics of a single atom (again a two-level system), this time interacting with a quantum field. In particular, we will aim to find the equation that describes the dynamics of the internal degrees of freedom of the atom when it is in contact with the full electromagnetic field. At the end of the section, we will find the *Master equation* for an open quantum system, which describes the decay of the electron from $|e\rangle$ to $|g\rangle$ with a rate γ.

The Hamiltonian here is again similar to (1.8)

$$H' = H_0 + H_F - \vec{d} \cdot \vec{E},$$

where $H_0 = \hbar\omega_0 \, |e\rangle\langle e|$. We have also now the field Hamiltonian H_F, which accounts for the energy of the photons in the electromagnetic field, and reads

$$H_F = \sum_{\vec{k}} \hbar\nu_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}}.$$

Here, $a^\dagger_{\vec{k}}$ and $a_{\vec{k}}$ are bosonic operators that represent the creation and annihilation, respectively, of a photon with momentum $\vec{k}$ and energy $\hbar\nu_{\vec{k}}$. They satisfy the bosonic commutation relation $\left[a_{\vec{k}}, a^\dagger_{\vec{k}'}\right] = \delta_{\vec{k},\vec{k}'}$. Finally, we have the term that describes the interaction between the atom and the field. Here, the electric field can be written as an operator that –evaluated at the position of the atom, which we consider here to be the origin– reads

$$\vec{E} = \sum_{\vec{k}} \hat{\epsilon}_{\vec{k}} \mathcal{E}_{\vec{k}} \left(a_{\vec{k}} + a^\dagger_{\vec{k}}\right)$$

where

$$\mathcal{E}_{\vec{k}} = \sqrt{\frac{\hbar\nu_{\vec{k}}}{2\epsilon_0 V}}$$

with ϵ_0 being the free space permittivity, and V the quantization volume. $\hat{\epsilon}_{\vec{k}}$ is the unit vector in the direction of the polarization, such that

$$\vec{k} \cdot \hat{\epsilon}_{\vec{k}} = 0 \ .$$

We have considered for simplicity polarization vector to be real (linear polarization basis).

With these definitions, we end up with a Hamiltonian that reads

$$H' = \hbar\omega_0\sigma^\dagger\sigma + \sum_{\vec{k}} \hbar\nu_k a^\dagger_{\vec{k}} a_{\vec{k}} + \underbrace{\hbar \sum_{\vec{k}} g_{\vec{k}} \left(\sigma^\dagger + \sigma\right) \left(a_{\vec{k}} + a^\dagger_{\vec{k}}\right)}_{H_{int}}$$

with

$$g_{\vec{k}} = -\frac{\langle g|\vec{d}|e\rangle \cdot \hat{\epsilon}_{\vec{k}} \mathcal{E}_{\vec{k}}}{\hbar}$$

and where we have defined the ladder operators

$$\sigma = |g\rangle\langle e| \qquad \sigma^\dagger = |e\rangle\langle g| \ .$$

It is convenient to work in the interaction picture, which means to perform again a unitary transformation, here given by

$$U = e^{i(H_0+H_F)t/\hbar}$$

which leads to a modified Hamiltonian: (*)

$$\begin{aligned} H'' &= e^{i(H_0+H_F)t/\hbar} H_{int} e^{-i(H_0+H_F)t/\hbar} \\ &= \sum_{\vec{k}} \hbar g_{\vec{k}} e^{i\omega_0\sigma^\dagger\sigma t} \left(\sigma^\dagger + \sigma\right) e^{-i\omega_0\sigma^\dagger\sigma t} e^{i\nu_k a^\dagger_{\vec{k}} a_{\vec{k}} t} \left(a_{\vec{k}} + a^\dagger_{\vec{k}}\right) e^{-i\nu_k a^\dagger_{\vec{k}} a_{\vec{k}} t} \end{aligned}$$

To go any further, we need the Baker–Campbell–Hausdorff formula

$$e^{\alpha A} B e^{-\alpha A} = B + \alpha\,[A,B] + \frac{\alpha^2}{2!}\,[A,[A,B]] + \dots$$

such that (*)

- $e^{i\omega_0 t\sigma^\dagger\sigma}\sigma^\dagger e^{-i\omega_0 t\sigma^\dagger\sigma} = \sigma^\dagger + i\omega_0 t \overbrace{\left[\sigma^\dagger\sigma, \sigma^\dagger\right]}^{\sigma^\dagger} - \frac{\omega_0^2 t^2}{2} \overbrace{\left[\sigma^\dagger\sigma, \left[\sigma^\dagger\sigma, \sigma^\dagger\right]\right]}^{\sigma^\dagger} + \dots$
  $= \sigma^\dagger \left(1 + i\omega_0 t - \frac{\omega_0^2 t^2}{2} + \dots\right) = \sigma^\dagger e^{i\omega_0 t}$
- $e^{i\omega_0 t\sigma^\dagger\sigma}\sigma e^{-i\omega_0 t\sigma^\dagger\sigma} = \sigma e^{-i\omega_0 t}$
- $e^{i\nu_k t a^\dagger_{\vec{k}} a_{\vec{k}}} a_{\vec{k}} e^{-i\nu_k t a^\dagger_{\vec{k}} a_{\vec{k}}} = a_{\vec{k}} e^{-i\nu_k t}$
- $e^{i\nu_k t a^\dagger_{\vec{k}} a_{\vec{k}}} a^\dagger_{\vec{k}} e^{-i\nu_k t a^\dagger_{\vec{k}} a_{\vec{k}}} = a^\dagger_{\vec{k}} e^{i\nu_k t}$

and then

$$H'' = \sum_{\vec{k}} \hbar g_{\vec{k}} \left[e^{i(\omega_0-\nu_k)t}\sigma^\dagger a_{\vec{k}} + e^{-i(\omega_0-\nu_k)t}\sigma a^\dagger_{\vec{k}} + e^{i(\omega_0+\nu_k)t}\sigma^\dagger a^\dagger_{\vec{k}} + e^{-i(\omega_0+\nu_k)t}\sigma a_{\vec{k}} \right]$$

Again, these terms rotate very fast, and under the rotating wave approximation they disappear. The final Hamiltonian reads

$$H'' = \sum_{\vec{k}} \hbar g_{\vec{k}} \left[e^{i(\omega_0-\nu_k)t}\sigma^\dagger a_{\vec{k}} + e^{-i(\omega_0-\nu_k)t}\sigma a^\dagger_{\vec{k}} \right] \tag{1.16}$$

which will be used in the following to describe the dynamics of the system.

1.3.1 A quick introduction to open quantum systems

The *density operator*, is defined as

$$\rho = \sum_{\Psi} P_\Psi \left|\Psi\right\rangle\!\left\langle\Psi\right|$$

and it is introduced to describe a physical situation where we know that the system is in the state $|\Psi\rangle$ with probability P_Ψ. If all P_Ψ are zero but one, the system is in a *pure state*. Otherwise, the state is *mixed*. The density matrix possesses the following properties:

- $\mathrm{tr}(\rho) = 1$ (conservation of probability)
- $\rho^\dagger = \rho$ (Hermitian)
- Positive semi-definite

For pure states, moreover, $\mathrm{tr}(\rho^2) = 1$, while for mixed states $\mathrm{tr}(\rho^2) < 1$. Starting from the Schrödinger equation

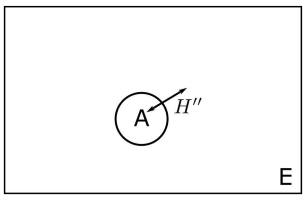
$$\frac{\partial \left|\Psi\right\rangle}{\partial t} = -\frac{i}{\hbar} H \left|\Psi\right\rangle$$

one can obtain the equation obeyed by ρ as

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= \sum_{\Psi} P_{\Psi} \left[\frac{\partial \left|\Psi\right\rangle}{\partial t} \left\langle\Psi\right| + \left|\Psi\right\rangle \frac{\partial \left\langle\Psi\right|}{\partial t} \right] \\ &= -\frac{i}{\hbar} \sum_{\Psi} P_{\Psi} \left[H \left|\Psi\right\rangle\!\left\langle\Psi\right| - \left|\Psi\right\rangle\!\left\langle\Psi\right| H \right] \\ &= -\frac{i}{\hbar} \left[H, \rho \right],\end{aligned}$$

usually referred to as the *Liouville or Von Neumann equation.*

Let us now go back to our problem. Our starting point is the equation of motion for the atom (A) and the electromagnetic field (E) which is determined by the von Neumann equation for the density matrix ρ_{AE} under the action of the time-dependent Hamiltonian H'', such that



$$\dot{\rho}_{AE} = -\frac{i}{\hbar} \left[H''(t), \rho_{AE} \right]. \tag{1.17}$$

Actually, we want to find the dynamics of the atomic degrees of freedom only. These are encoded in the reduced density matrix

$$\rho = \mathrm{tr}_E(\rho_{AE}) \tag{1.18}$$

where tr_E represents the trace over all degrees of freedom of the electromagnetic field. In order to obtain such equation, we follow a number of steps:

1. **Formal integration.** In this step we simply integrate the von Neumann equation from 0 to t, such that

   $$\rho_{AE}(t) = \rho_{AE}(0) - \frac{i}{\hbar} \int_0^t \left[H''(t'), \rho_{AE}(t') \right] dt'.$$

   Substituting this solution back into the von Neumann eq. (1.17) gives

   $$\dot{\rho}_{AE} = -\frac{i}{\hbar} \left[H''(t), \rho_{AE}(0) \right] - \frac{1}{\hbar^2} \int_0^t \left[H''(t), \left[H''(t'), \rho_{AE}(t') \right] \right] dt'. \tag{1.19}$$

2. **Weak coupling approximation (I).** We assume here that the coupling between the atom and the field, determined by H'' is weak, and hence we are looking for a

solution of the dynamics that satisfies

$$\rho_{AE}(t) = \rho(t) \otimes \rho_E(t) + \rho_c(t)$$

with

$$\mathrm{tr}_E(\rho_c(t)) = 0 \ ,$$

such that (1.18) is satisfied.

3. **Trace over E.** We now take the trace over the degrees of freedom of the electromagnetic field in equation (1.19). We then obtain

$$\dot{\rho} = -\frac{i}{\hbar}\,\mathrm{tr}_E\left[H''(t), \rho(0) \otimes \rho_E(0)\right] - \frac{1}{\hbar^2}\,\mathrm{tr}_E \int_0^t \left[H''(t), \left[H''(t'), \rho(t') \otimes \rho_E(t')\right]\right] dt', \tag{1.20}$$

where we have used already that $\mathrm{tr}_E(\rho_c(t)) = 0$.

4. **Equilibrium state.** Here we will assume that the reservoir (the electromagnetic field) starts the evolution (at time $t = 0$) in its equilibrium state (e.g. thermal equilibrium at temperature T). Since we have assumed before that the coupling is weak, we may assume that the system and the environment are non-correlated during all the time evolution, and hence $\rho_E(t') = \rho_E(0)$. However, note that this is just an approximation, as in general correlations will build up during the time evolution. This assumption is only valid if the time scales of correlation and relaxation of the environment are much smaller than the typical system time scale.

5. **Weak coupling approximation (II).** Formally integrating (1.20) between t and t' we obtain that

$$\rho(t') - \rho(t) = \mathcal{O}(H'').$$

If we were to substitute this result back inside the integral in (1.20), we would realize that the result would be

$$\dot{\rho} = -\frac{i}{\hbar}\,\mathrm{tr}_E\left[H''(t), \rho(0) \otimes \rho_E(0)\right] \tag{1.21}$$

$$- \frac{1}{\hbar^2}\,\mathrm{tr}_E \int_0^t \left[H''(t), \left[H''(t'), \rho(t) \otimes \rho_E(0)\right]\right] dt' + \mathcal{O}\left(H''^3\right). \tag{1.22}$$

However, we have assumed before that the coupling is weak. We choose here to keep terms in this equation only up to order $\mathcal{O}\left(H''^2\right)$. Note that effectively we

have substituted then $\rho(t') \to \rho(t)$.

6. **Markov approximation.** In this last step, we assume that the kernel in the integration (given by $H''(t)H''(t')$) decays very fast. This is ensured by a reservoir (in our case the electromagnetic field) which has a very large number of degrees of freedom, and hence leads to a kernel which is almost a delta function $\delta(t'-t)$. This also allows us to extend the upper limit of the integration from t to infinity with no real change in the outcome.

After all of these steps, we have the equation

$$\begin{aligned}\dot{\rho} = &-\frac{i}{\hbar}\,\mathrm{tr}_E\left[H''(t), \rho(0)\otimes\rho_E(0)\right] \\ &-\frac{1}{\hbar^2}\,\mathrm{tr}_E\int_0^\infty \left[H''(t),\left[H''(t'),\rho(t)\otimes\rho_E(0)\right]\right]dt',\end{aligned}$$

where we are now in position to substitute our Hamiltonian

$$H''(t) = \sum_{\vec{k}} \hbar g_{\vec{k}}\left[e^{i(\omega_0-\nu_k)t}\sigma^\dagger a_{\vec{k}} + e^{-i(\omega_0-\nu_k)t}\sigma a^\dagger_{\vec{k}}\right] \ .$$

The result is (*)

$$\begin{aligned}\dot{\rho} = &-i\sum_{\vec{k}} g_{\vec{k}}\left\langle a_{\vec{k}}\right\rangle\left[\sigma^\dagger,\rho(0)\right]e^{i(\omega_0-\nu_k)t} \\ &-\int_0^\infty dt'\sum_{\vec{k}\vec{k}'} g_{\vec{k}}g_{\vec{k}'}\cdot\left\{\left[\sigma\sigma\rho - 2\sigma\rho\sigma + \rho\sigma\sigma\right]e^{-i(\omega_0-\nu_k)t-i(\omega_0-\nu_{k'}t')}\left\langle a^\dagger_{\vec{k}}a^\dagger_{\vec{k}'}\right\rangle\right\} \\ &+\left[\sigma\sigma^\dagger\rho - \sigma^\dagger\rho\sigma\right]e^{-i(\omega_0-\nu_k)t+i(\omega_0-\nu_{k'})t'}\left\langle a^\dagger_{\vec{k}}a_{\vec{k}'}\right\rangle \\ &+\left[\sigma^\dagger\sigma\rho - \sigma\rho\sigma^\dagger\right]e^{i(\omega_0-\nu_k)t-i(\omega_0-\nu_{k'})t'}\left\langle a_{\vec{k}}a^\dagger_{\vec{k}'}\right\rangle + \text{H.c.}\ ,\end{aligned}$$

where we have used the definition of an expectation value of an operator O composed of field operators

$$\langle O\rangle = \mathrm{tr}_E(\rho_E O) = \mathrm{tr}_E(O\rho_E).$$

We can further simplify the resulting equation by choosing a particular equilibrium state of the field. As we said before, we choose this to be the thermal equilibrium state

$$\rho_E = \prod_{\vec{k}}\left[1 - e^{-\frac{\hbar\nu_k}{k_BT}}\right]e^{-\frac{\hbar\nu_k}{k_BT}a^\dagger_{\vec{k}}a_{\vec{k}}}, \tag{1.23}$$

such that

- $\left\langle a_{\vec{k}} \right\rangle = \left\langle a^\dagger_{\vec{k}} \right\rangle = 0$
- $\left\langle a_{\vec{k}} a_{\vec{k}'} \right\rangle = \left\langle a^\dagger_{\vec{k}} a^\dagger_{\vec{k}'} \right\rangle = 0$
- $\left\langle a^\dagger_{\vec{k}} a_{\vec{k}'} \right\rangle = \bar{n}_{\vec{k}} \delta_{\vec{k},\vec{k}'}$
- $\left\langle a_{\vec{k}} a^\dagger_{\vec{k}'} \right\rangle = (\bar{n}_{\vec{k}} + 1)\delta_{\vec{k},\vec{k}'}$,

where the thermal average boson number is given by

$$\bar{n}_{\vec{k}} = \frac{1}{e^{\frac{\hbar\nu_k}{k_B T}} - 1}. \tag{1.24}$$

In particular, if we choose the state at zero temperature we obtain $\bar{n}_{\vec{k}} = 0$, and thus

- $\left\langle a^\dagger_{\vec{k}} a_{\vec{k}'} \right\rangle = 0$
- $\left\langle a_{\vec{k}} a^\dagger_{\vec{k}'} \right\rangle = \delta_{\vec{k},\vec{k}'}$

such that the equation of motion reads

$$\dot{\rho} = -\int_0^\infty dt' \sum_{\vec{k}} g^2_{\vec{k}} \left\{ e^{i(\omega_0 - \nu_k)(t-t\prime)} \left[\sigma^\dagger \sigma \rho - \sigma \rho \sigma^\dagger\right] + e^{-i(\omega_0 - \nu_k)(t-t')} \left[\rho \sigma^\dagger \sigma - \sigma \rho \sigma^\dagger\right] \right\}$$

The next step is to substitute the sum over $\vec{k}$ by an integral, as we can assume a continuum of photon energies. In particular:

$$\sum_{\vec{k}} \to \overbrace{2}^{\text{polarizations}} \underbrace{\frac{V}{(2\pi)^3}}_{\text{Volume of each mode}} \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \int_0^\infty dk k^2 \ .$$

Using that

$$g^2_{\vec{k}} = \left| d_{ge} \cdot \hat{\epsilon}_{\vec{k}} \right|^2 \frac{\nu_k}{2\hbar\epsilon_0 V} \quad \text{with} \quad \nu_k = kc$$

and defining the azimuthal angle θ to be the one formed by the two vectors: $\vec{d}_{ge} \cdot \hat{\epsilon}_{\vec{k}} =$

$\left|\vec{d}_{ge}\right| \cos\theta$, we obtain

$$\int_0^\infty dt' \sum_{\vec{k}} g_{\vec{k}}^2 e^{i(\omega_0-\nu_k)(t-t')} = \frac{\left|\vec{d}_{ge}\right|^2}{(2\pi)^3\hbar\epsilon_0} \overbrace{\int_0^{2\pi} d\varphi}^{=2\pi} \overbrace{\int_0^{\pi} d\theta \sin\theta\cos^2\theta}^{=2/3} \frac{1}{c^3} \int_0^\infty d\nu_k \nu_k^3 \overbrace{\int_0^\infty dt' e^{i(\omega_0-\nu_k)(t-t')}}^{=\delta(\nu_k-\omega_0)\cdot\pi}$$

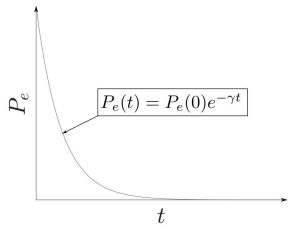
$$= \frac{\left|\vec{d}_{ge}\right|^2 \omega_0^3}{6\pi\hbar\epsilon_0 c^3} \equiv \frac{\gamma}{2}.$$

The *markovian Lindblad master equation* (or Gorini-Kossakowski-Sudarshan-Lindblad master equation) is finally given by

$$\boxed{\dot{\rho} = \gamma\left[\sigma\rho\sigma^\dagger - \frac{1}{2}\left\{\sigma^\dagger\sigma, \rho\right\}\right]}$$

Let us now interpret this equation by, for example, obtaining $P_e(t) \equiv \langle e|\rho|e\rangle$ (the occupation of the excited state), as we did in the case of the interaction with a laser field. Here, our initial state is the atom in the excited state, i.e. $P_e(0) = 1$, and the evolution yields (*)

$$\left.\begin{array}{rl} \dot{P}_e & = -\gamma P_e \\ \dot{P}_g & = \gamma P_e \\ P_e + P_g & = 1 \end{array}\right\}$$



which is why γ is called the *decay rate* of the excited state. An atom in $|e\rangle$ in contact with the radiation field will eventually decay to the ground state.

As a final note, one can actually describe the two-level system interacting with both fields via the master equation

$$\dot{\rho} = -\frac{i}{\hbar}\left[H_L, \rho\right] + \gamma\left[\sigma\rho\sigma^\dagger - \frac{1}{2}\left\{\sigma^\dagger\sigma, \rho\right\}\right]$$

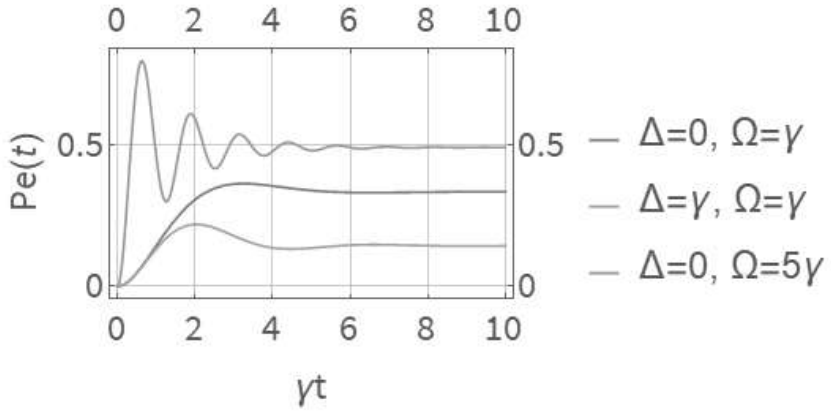
with

$$H_L = \hbar\Delta \overbrace{\sigma^\dagger\sigma}^{|e\rangle\langle e|} + \frac{\hbar\Omega_0}{2}\left(\overbrace{\sigma}^{|g\rangle\langle e|} + \overbrace{\sigma^\dagger}^{|e\rangle\langle g|}\right).$$

If we now solve again the equation of motion, for the probability $P_e(t)$, we can see that it presents damped oscillations towards a stationary state given by

$$P_e(t \to \infty) = \frac{\Omega^2}{\gamma^2 + 4\Delta^2 + 2\Omega^2}$$

as one can see in the figure below.



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