Lecture notes on laser spectroscopy and laser cooling

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Contents

Chapter 1

Review of quantum electrodynamics

In this chapter we review the basic laws of electrodynamics and formulate them in the Lagrangian formalism using Coulomb gauge. We aim at deriving the minimal coupling Hamiltonian and performing quantization in the canonical manner. This approach establishes the ground to define atoms and to describe their interaction with the electromagnetic radiation field in the next chapters.

1.1 The coupled system of electromagnetic fields and charges

In this section, starting from the fundamental Maxwell equations, we will identify the independent degrees of freedom that are the real dynamical variables in the general system of electromagnetic fields interacting with sources. It is very convenient to describe the independent degrees of freedom in terms of the vector and scalar potentials.

1.1.1 The Lorentz-Maxwell equations

The electromagnetic field is described in terms of the real electric $\mathbf{E}(\mathbf{r},t)$ and magnetic $\mathbf{B}(\mathbf{r},t)$ vector fields. Their evolution is governed by coupled partial differential equations, i.e., the Maxwell equations,

$$\nabla\mathbf{E}(\mathbf{r},t) = \frac{1}{\epsilon_0}\rho(\mathbf{r},t)\ , \tag{1.1a}$$

$$\nabla\mathbf{B}(\mathbf{r},t) = 0\ , \tag{1.1b}$$

$$\nabla\times\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)\ , \tag{1.1c}$$

$$\nabla\times\mathbf{B}(\mathbf{r},t) = \frac{\partial}{c^2\partial t}\mathbf{E}(\mathbf{r},t) + \frac{1}{\epsilon_0 c^2}\mathbf{j}(\mathbf{r},t)\ . \tag{1.1d}$$

These equations contain source terms, that is, the electromagnetic field is generated by charge and current densities, $\rho(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$, respectively. If the material component is a set of charges q_ν ($\nu = 1,2,\ldots$) in the positions $\mathbf{r}_\nu$ moving with velocities $\mathbf{v}_\nu(t)$ then

$$\rho(\mathbf{r},t) = \sum_\nu q_\nu\delta(\mathbf{r}-\mathbf{r}_\nu(t))\ , \tag{1.2a}$$

$$\mathbf{j}(\mathbf{r},t) = \sum_\nu q_\nu\mathbf{v}_\nu\delta(\mathbf{r}-\mathbf{r}_\nu(t))\ . \tag{1.2b}$$

Having separated the elements of a four-vector, with this definition of the densities the formalism will not be relativistically covariant. Let us check that

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t) = \sum_\nu q_\nu \left(-\nabla\delta(\mathbf{r}-\mathbf{r}_\nu(t))\right)\dot{\mathbf{r}}_\nu(t) = -\sum_\nu q_\nu \mathbf{v}_\nu \nabla\delta(\mathbf{r}-\mathbf{r}_\nu(t)) \;, \tag{1.3a}$$

$$\nabla\mathbf{j}(\mathbf{r},t) = \sum_\nu q_\nu \mathbf{v}_\nu \nabla\delta(\mathbf{r}-\mathbf{r}_\nu(t)) \;, \tag{1.3b}$$

so that the continuity equation is obeyed,

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t) + \nabla\mathbf{j}(\mathbf{r},t) = 0 \;, \tag{1.3c}$$

which, in general, expresses the conservation of charges. Moreover, in Eq. (1.2), the charge and current density is defined by labeling given charges, hence the possibility of pair creation is excluded. Therefore the theory deviates from the non-relativistic quantum electrodynamics that is to be used for high energy physics.

Moving charges generate the electromagnetic field, at the same time, the charges move under the effect of the force exerted by the electromagnetic field, i.e., the Lorentz force,

$$m_\nu \frac{d^2}{dt^2}\mathbf{r}_\nu(t) = q_\nu \left(\mathbf{E}(\mathbf{r}_\nu,t) + \mathbf{v}_\nu(t)\times\mathbf{B}(\mathbf{r}_\nu,t)\right) \;. \tag{1.4}$$

The theory of the coupled system of charges and the electromagnetic field is completely given by the coupled Lorentz-Maxwell equations. The dynamical variables are the real electric and magnetic fields (6 real vector components in each space point) and the position and velocity vectors associated with the charges (six real numbers for each charge particle ν). One needs the initial conditions for the variables

$$\{\mathbf{E}(\mathbf{r},t_0), \mathbf{B}(\mathbf{r},t_0), \mathbf{r}_\nu(t_0), \mathbf{v}_\nu(t_0)\} \;. \tag{1.5}$$

However, there are relations between these variables and the number of genuine degrees of freedom is less. This is what we are going to determine in the following.

1.1.2 The Maxwell equations in reciprocal space

Let us consider the vector fields in reciprocal-space, which is defined by the Fourier transformation

$$\mathcal{E}(\mathbf{k},t) = \frac{1}{(2\pi)^{3/2}}\int d^3\mathbf{r}\,\mathbf{E}(\mathbf{r},t)e^{-i\mathbf{k}\mathbf{r}} \;. \tag{1.6}$$

The vector fields in reciprocal space are complex, however, the property that the fields are real in real space implies

$$\mathcal{E}^*(\mathbf{k},t) = \mathcal{E}(-\mathbf{k},t) \;. \tag{1.7}$$

Some transformation rules to be noted follows:

$$\frac{1}{4\pi r} \leftrightarrow \frac{1}{(2\pi)^{3/2}}\frac{1}{k^2} \;, \tag{1.8a}$$

$$\frac{\mathbf{r}}{4\pi r^3} \leftrightarrow \frac{1}{(2\pi)^{3/2}}\frac{-i\mathbf{k}}{k^2} \;, \tag{1.8b}$$

$$\delta(\mathbf{r}-\mathbf{r}_\nu) \leftrightarrow \frac{1}{(2\pi)^{3/2}}e^{-i\mathbf{k}\mathbf{r}_\nu} \;. \tag{1.8c}$$

The main reason to transform the problem into reciprocal space is that the Maxwell equations become *local*,

$$i\mathbf{k}\mathcal{E}(\mathbf{k},t) = \frac{1}{\epsilon_0}\rho(\mathbf{k},t) \ , \tag{1.9a}$$

$$i\mathbf{k}\mathcal{B}(\mathbf{k},t) = 0 \ , \tag{1.9b}$$

$$i\mathbf{k}\times\mathcal{E}(\mathbf{k},t) = -\frac{\partial}{\partial t}\mathcal{B}(\mathbf{k},t) \ , \tag{1.9c}$$

$$i\mathbf{k}\times\mathcal{B}(\mathbf{k},t) = \frac{\partial}{c^2\partial t}\mathcal{E}(\mathbf{k},t) + \frac{1}{\epsilon_0 c^2}\mathbf{j}(\mathbf{k},t) \ . \tag{1.9d}$$

This is a very useful, pragmatic representation of the fields in free space which will be the case for most of the systems to be studied in this course. When one considers a problem in a finite volume enclosed by boundaries, e.g., cavity quantum electrodynamics, the reciprocal space is not necessarily a suitable representation for the calculation. However, the Fourier transform approach makes electrodynamics conceptually simple, in general.

1.1.2.1 Longitudinal and transverse vector fields

Any vector field $\mathbf{V}(\mathbf{r})$ can be composed of the sum of a longitudinal and a transverse vector field, which are defined by

$$\nabla\times\mathbf{V}_\parallel(\mathbf{r}) = 0 \quad\leftrightarrow\quad \mathbf{k}\times\mathcal{V}_\parallel = 0 \ , \tag{1.10a}$$

$$\nabla\mathbf{V}_\perp(\mathbf{r}) = 0 \quad\leftrightarrow\quad \mathbf{k}\mathcal{V}_\perp = 0 \ , \tag{1.10b}$$

for all $\mathbf{r}$ and $\mathbf{k}$. For example, for the electric field $\nabla\mathbf{E} = q_\nu\delta(\mathbf{r}-\mathbf{r}_\nu)$, i.e., the divergence vanishes except in the single point of the charge position, but the field is clearly not transverse since $\mathbf{k}\mathcal{E}(\mathbf{k}) \propto \exp(-i\mathbf{k}\mathbf{r}_\nu) \neq 0$.

The decomposition can be made in reciprocal space,

$$\mathcal{V}_\parallel(\mathbf{k}) = \frac{1}{k^2}\mathbf{k}\left(\mathbf{k}\mathcal{V}(\mathbf{k})\right) \ , \tag{1.11a}$$

$$\mathcal{V}_\perp(\mathbf{k}) = \mathcal{V}(\mathbf{k}) - \mathcal{V}_\parallel(\mathbf{k}) \ , \tag{1.11b}$$

where it is a local relation. This is not the case in real space, for example,

$$V_{\perp i}(\mathbf{r}) = \sum_j \int d^3\mathbf{r}'\delta^\perp_{ij}(\mathbf{r}-\mathbf{r}')V_j(\mathbf{r}') \ , \tag{1.12}$$

where the transverse Dirac-delta is obtained from the definition as

$$\delta^\perp_{ij}(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi)^3}\int d^3\mathbf{k}e^{i\mathbf{k}\mathbf{r}}\left(\delta_{ij} - \frac{k_ik_j}{k^2}\right) = \delta_{ij}\delta(\mathbf{r}) + \frac{1}{4\pi}\frac{\partial^2}{\partial r_i\partial r_j}\frac{1}{r} \ . \tag{1.13}$$

1.1.2.2 Longitudinal and transverse electric and magnetic fields

From the Maxwell equation (1.9b) it follows immediately that the magnetic field is purely transverse, i.e.,

$$\mathcal{B}_\parallel(\mathbf{k},t) = 0 \ . \tag{1.14a}$$

For the longitudinal electric field the Eq. (1.9a) can be directly solved,

$$\mathcal{E}_{\parallel}(\mathbf{k},t)=\frac{1}{k^2}\mathbf{k}\left(\mathbf{k}\mathcal{E}(\mathbf{k})\right)=-i\frac{\mathbf{k}}{\epsilon_0 k^2}\rho(\mathbf{k},t)\ . \tag{1.14b}$$

By performing the inverse Fourier transformation and using the rules (1.8), one gets the electric field

$$\mathbf{E}_{\parallel}(\mathbf{r},t)=\frac{1}{4\pi\epsilon_0}\int d^3\mathbf{r}'\rho(\mathbf{r}',t)\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}=\frac{1}{4\pi\epsilon_0}\sum_{\nu}q_\nu\frac{\mathbf{r}-\mathbf{r}_\nu(t)}{|\mathbf{r}-\mathbf{r}_\nu(t)|^3}\ . \tag{1.14c}$$

The longitudinal component of the electric field is the Coulomb field associated with the distribution of charges at the same instant t. Since the longitudinal field can be expressed as a function of the position of charges $\mathbf{r}_\nu(t)$, it is not a true dynamical variable.

The transverse fields are the real dynamical variables and obey

$$i\mathbf{k}\times\mathcal{E}_{\perp}(\mathbf{k},t)=-\frac{\partial}{\partial t}\mathcal{B}(\mathbf{k},t)\ , \tag{1.15a}$$

$$i\mathbf{k}\times\mathcal{B}(\mathbf{k},t)=\frac{\partial}{c^2\partial t}\mathcal{E}_{\perp}(\mathbf{k},t)+\frac{1}{\epsilon_0 c^2}\mathbf{j}_{\perp}(\mathbf{k},t)\ . \tag{1.15b}$$

For the magnetic field we did not explicitly mark the transverse character here, as it is always transverse. To summarize, the independent field variables are the altogether four complex components of the transverse electric and magnetic field vectors in each point of the positive half of the reciprocal space ($\mathbf{k}>0$, because $\mathcal{E}_{\perp}(\mathbf{k})$ and $\mathcal{E}_{\perp}(-\mathbf{k})$ are not independent).

The longitudinal part of Eq. (1.9d), which we did not use so far, has a vanishing left-hand-side and is equivalent with the continuity equation.

It follows from Eq. (1.14c) that the effect of any displacement of the charges is instantaneously transmitted as a change of the field $E_{\parallel}$ at remote positions. One can conclude then that the transverse field $E_{\perp}$ must also have an instantaneous term which compensates the instantaneous effect of the longitudinal field so that the total electric field obeys causality. The instantaneous component of $E_{\perp}$ and $B_{\perp}$ is generated by the low frequency current $j_{\perp}$ in the limit $\partial/\partial t\to i\omega\to 0$. The longitudinal and transverse components of the field, separately, violate then the causality. Nevertheless, as we will see later, this separation offers an approximately good physical interpretation of atoms as being charge clusters held together by the longitudinal electric field.

1.1.3 Vector and scalar potentials

The electric and magnetic field vectors can be expressed in terms of the so-called vector potential $\mathbf{A}(\mathbf{r},t)$ and the scalar potential $U(\mathbf{r},t)$ fields,

$$\mathbf{E}(\mathbf{r},t)=-\nabla U(\mathbf{r},t)-\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t)\ , \tag{1.16a}$$

$$\mathbf{B}(\mathbf{r},t)=\nabla\times\mathbf{A}(\mathbf{r},t)\ . \tag{1.16b}$$

With this definition, the Maxwell equations (1.1b,c) are automatically satisfied, and the other two equations lead to

$$\Delta U(\mathbf{r},t) = -\frac{1}{\epsilon_0}\rho(\mathbf{r},t) - \frac{\partial}{\partial t}\nabla\mathbf{A}(\mathbf{r},t)\ , \tag{1.17a}$$

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta\right)\mathbf{A}(\mathbf{r},t) = \frac{1}{\epsilon_0 c^2}\mathbf{j}(\mathbf{r},t) - \nabla\left(\nabla\mathbf{A}(\mathbf{r},t) + \frac{1}{c^2}\frac{\partial}{\partial t}U(\mathbf{r},t)\right)\ . \tag{1.17b}$$

The physically relevant fields, $\mathbf{E}$ and $\mathbf{B}$, are invariant under the *gauge transformation* of the potentials associated with the scalar field $F(\mathbf{r},t)$,

$$U(\mathbf{r},t) \to U(\mathbf{r},t) - \frac{\partial}{\partial t}F(\mathbf{r},t)\ , \tag{1.18a}$$

$$\mathbf{A}(\mathbf{r},t) \to \mathbf{A}(\mathbf{r},t) + \nabla F(\mathbf{r},t)\ . \tag{1.18b}$$

In reciprocal space, the gauge transformation is

$$\mathcal{U}(\mathbf{k},t) \to \mathcal{U}(\mathbf{k},t) - \frac{\partial}{\partial t}\mathcal{F}(\mathbf{k},t)\ , \tag{1.19a}$$

$$\mathcal{A}(\mathbf{k},t) \to \mathcal{A}(\mathbf{k},t) + i\mathbf{k}\mathcal{F}(\mathbf{k},t)\ . \tag{1.19b}$$

It follows that an arbitrary function can be added to the longitudinal part of the vector potential. We will use this freedom to choose $\mathcal{F}(\mathbf{k},t)$ such that the vector potential becomes a pure transverse field,

$$\mathcal{A}_\parallel(\mathbf{k},t) = 0\,,\ \mathcal{A}(\mathbf{k},t) \equiv \mathcal{A}_\perp(\mathbf{k},t) \tag{1.20}$$

This is called the *Coulomb gauge*. Note that the transverse part of the vector potential does not vary with the gauge transformation. This is in accordance with that $\mathbf{A}_\perp$ determines the gauge-invariant magnetic field vector. To summarize, in the Coulomb gauge, the longitudinal and transverse electric fields and the magnetic field are expressed as

$$\mathbf{E}_\parallel(\mathbf{r},t) = -\nabla U(\mathbf{r},t)\ , \tag{1.21a}$$

$$\mathbf{E}_\perp(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t)\ , \tag{1.21b}$$

$$\mathbf{B}(\mathbf{r},t) = \nabla\times\mathbf{A}(\mathbf{r},t)\ , \tag{1.21c}$$

respectively. As we saw previously, the longitudinal vector field is not a true dynamical variable. From the above equations it directly follows that the same holds for the scalar potential, and it can be readily obtained as a function of the charge coordinates

$$U(\mathbf{r},t) = \frac{1}{4\pi\epsilon_0}\int d^3\mathbf{r}'\rho(\mathbf{r}',t)\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{4\pi\epsilon_0}\sum_\nu q_\nu\frac{1}{|\mathbf{r}-\mathbf{r}_\nu(t)|}\ . \tag{1.22}$$

It is easy to check that the gradient of this scalar potential yields the longitudinal electric field given by Eq. (1.14c). The vector potential obeys the wave equation

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta\right)\mathbf{A}(\mathbf{r},t) = \frac{1}{\epsilon_0 c^2}\mathbf{j}(\mathbf{r},t)\ , \tag{1.23}$$

which can be obtained from Eq. (1.15). This is a second order differential equation with respect to the time, therefore the initial condition must contain the values $\mathbf{A}(\mathbf{r}, t_0)$ and also their velocities, $\dot{\mathbf{A}}(\mathbf{r}, t_0)$. The dynamical variables are then

$$\left\{ \mathbf{A}(\mathbf{r}, t), \dot{\mathbf{A}}(\mathbf{r}, t), \mathbf{r}_\nu(t), \dot{\mathbf{r}}_\nu(t) \right\} \ , \tag{1.24}$$

which amounts to four real field vector components in each point of the real space.

1.2 The Lagrangian of electrodynamics in the Coulomb gauge

Let us recall first the basic elements of the Lagrangian formalism. The Lagrangian is a function of the coordinates x_i in the configurational space ($i = 1 \dots N$) and their velocities $\dot{x}_i$ such that its integral,

$$S = \int_{t_1}^{t_2} L(x_i, \dot{x}_i, t) dt \ , \tag{1.25}$$

called the *action*, has an extremum along the real path of the system $x_i(t)$, given the initial and final points, $x_i(t_1)$ and $x_i(t_2)$, respectively. This is the principle of least action. Equations of motion can be derived from this principle by a variational method, which leads to the Euler-Lagrange equations,

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} = \frac{\partial L}{\partial x_i} \ . \tag{1.26}$$

When the system has a continuum of degrees of freedom, i.e., this is the case for a field $\mathbf{A}(\mathbf{r})$, the Lagrangian is replaced by a Lagrangian density $\mathcal{L}$,

$$S = \int_{t_1}^{t_2} \int d^3\mathbf{r} \mathcal{L}(A_i(\mathbf{r}), \dot{A}_i(\mathbf{r}), \partial_j A_i(\mathbf{r})) dt \ , \qquad i, j = 1, 2, 3 \ , \tag{1.27}$$

which depends on the spatial derivatives of the field, too. The Euler-Lagrange equations derive from this density functional as

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{A}_j} = \frac{\partial \mathcal{L}}{\partial A_j} - \sum_{i=x,y,z} \frac{\partial}{\partial r_i} \frac{\partial \mathcal{L}}{\partial \left(\partial_i A_j\right)} \ . \tag{1.28}$$

Note that a full time derivative and a divergence can be added to the Lagrange density,

$$\mathcal{L}' = \mathcal{L} + \frac{d}{dt} f_0(A_i(\mathbf{r}), \mathbf{r}, t) + \nabla \mathbf{f}(A_i(\mathbf{r}), \mathbf{r}, t) \ , \tag{1.29}$$

keeping the action S invariant. Therefore, the Lagrangian density $\mathcal{L}'$ defines the same dynamics as $\mathcal{L}$.

The Lagrangian of electrodynamics in the Coulomb gauge is given by

$$L = \sum_\nu \frac{1}{2} m_\nu \dot{\mathbf{r}}_\nu^2 - V_{\text{Coul}} + \int d^3\mathbf{r} \mathcal{L}_F + \sum_\nu q_\nu \dot{\mathbf{r}}_\nu \mathbf{A}(\mathbf{r}_\nu) \ , \tag{1.30}$$

where ν labels the charges. The free field Lagrangian density reads

$$\mathcal{L}_F = \frac{\epsilon_0}{2}\left(\dot{\mathbf{A}}^2(\mathbf{r},t) - c^2\left(\nabla\times\mathbf{A}(\mathbf{r},t)\right)^2\right) = \frac{\epsilon_0}{2}\left({\mathbf{E}_\perp}^2(\mathbf{r},t) - c^2\mathbf{B}^2(\mathbf{r},t)\right) \ . \tag{1.31}$$

Remarkably, it can be expressed in terms of the transverse electric and magnetic fields, $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$. The effect of the longitudinal electric field appears in the Coulomb term which is composed of a self-interaction of charges and the instantaneous Coulomb interaction between different charges, that is,

$$V_{\rm Coul} = E_\nu^{(\rm self)} + \frac{1}{8\pi\epsilon_0}\sum_{\nu\neq\mu}\frac{q_\nu q_\mu}{|\mathbf{r}_\nu - \mathbf{r}_\mu|} \ , \tag{1.32}$$

where the Coulomb self-interaction of charges can be expressed in momentum space,

$$E_\nu^{(\rm self)} = \sum_\nu \frac{q_\nu^2}{2\epsilon_0(2\pi)^3}\int d^3\mathbf{k}\frac{1}{k^2} \ . \tag{1.33}$$

Without a momentum cutoff this integral is divergent. However, this term does not imply any kind of coupling between the dynamical degrees of freedom, in fact, it can be eliminated by renormalizing the rest mass of the charge carriers. The coupling of sources to the radiation field is accounted for by the last term in (1.30). In a more general form this coupling term can be written also as a spatial integral of a Lagrangian density,

$$L_c = \int d^3\mathbf{r}\,\mathcal{L}_c \equiv \int d^3\mathbf{r}\,\mathbf{j}(\mathbf{r},t)\mathbf{A}(\mathbf{r},t) \ , \tag{1.34}$$

which, by using the definition (1.2b) of the current density, reduces to the form given in (1.30). In any way, the coupling of currents and radiation demands the use of the vector potential in order to describe the electrodynamics within the Lagrangian formalism. Note that this Lagrangian form assumes that the Coulomb gauge is used and thus

$$\nabla\mathbf{A}(\mathbf{r},t) = 0 \ . \tag{1.35}$$

The Lagrangian (1.30) can be verified by showing the equivalence of the corresponding Euler-Lagrange equations with the Maxwell-Lorentz equations. In the first step, let us derive the equation of motion for the motion of charges. The *canonical momentum* associated with the position $\mathbf{r}_\nu$ is defined by

$$\mathbf{p}_\nu = \frac{\partial L}{\partial\dot{\mathbf{r}}_\nu} = m_\nu\dot{\mathbf{r}}_\nu + q_\nu\mathbf{A}(\mathbf{r}_\nu,t) \ . \tag{1.36}$$

One can show that the term in addition to the kinetic momentum $m_\nu\dot{\mathbf{r}}_\nu$ is just the momentum associated with the longitudinal electric field generated by a charge q_ν in the position $\mathbf{r}_\nu$, i.e.,

$$\epsilon_0\int d^3\mathbf{r}\,\mathbf{E}_\parallel(\mathbf{r},t)\times\mathbf{B}(\mathbf{r},t) = q_\nu\mathbf{A}(\mathbf{r}_\nu,t) \ . \tag{1.37}$$

Note that the canonical momentum differs from the kinetic momentum $m_\nu\dot{\mathbf{r}}_\nu$ of the particles. The total time derivative is

$$\dot{\mathbf{p}}_\nu = m_\nu\ddot{\mathbf{r}}_\nu + q_\nu\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r}_\nu,t) + (\dot{\mathbf{r}}_\nu\nabla)\mathbf{A}(\mathbf{r}_\nu,t) \ , \tag{1.38}$$

which must equal to

$$\frac{\partial L}{\partial \mathbf{r}_\nu} = q_\nu \frac{\partial}{\partial \mathbf{r}_\nu}\left(-\sum_\mu \frac{q_\mu}{4\pi\epsilon_0\,|\mathbf{r}_\nu - \mathbf{r}_\mu|} + \dot{\mathbf{r}}_\nu \mathbf{A}(\mathbf{r}_\nu, t)\right)$$
$$= -q_\nu \nabla U(\mathbf{r}_\nu) + q_\nu(\dot{\mathbf{r}}_\nu \nabla)\mathbf{A}(\mathbf{r}_\nu, t) + q_\nu \dot{\mathbf{r}}_\nu \times (\nabla \times \mathbf{A})(\mathbf{r}_\nu, t)) \ , \quad (1.39)$$

from which follows

$$m_\nu \ddot{\mathbf{r}}_\nu = -q_\nu\left(\nabla U(\mathbf{r}_\nu) + \frac{\partial}{\partial t}\mathbf{A}(\mathbf{r}_\nu, t)\right) + q_\nu \dot{\mathbf{r}}_\nu \times (\nabla \times \mathbf{A}(\mathbf{r}_\nu, t)) = q_\nu(\mathbf{E} + v_\nu \times \mathbf{B}) \ , \quad (1.40)$$

that is, the Lorentz force acting on charges is recovered. In the second step, let's derive the wave equation for the vector potential. The canonically conjugate variable associated with the vector potential components $A_i(\mathbf{r}, t)$ is defined by

$$\Pi_i = \frac{\partial L}{\partial \dot{A}_i} = \epsilon_0 \dot{A}_i = \epsilon_0 E_\perp \ . \quad (1.41)$$

The right-hand side of the Euler-Lagrange equation (1.28) involves a differentiation with respect to the spatial derivatives of the vector potential, which appear in the term

$$(\nabla \times \mathbf{A})^2 = (\partial_2 A_3 - \partial_3 A_2)^2 + (\partial_3 A_1 - \partial_1 A_3)^2 + (\partial_1 A_2 - \partial_2 A_1)^2 \ . \quad (1.42)$$

It follows that

$$\frac{\partial \mathcal{L}}{\partial(\partial_j A_i)} = 2(\partial_j A_i - \partial_i A_j) \ . \quad (1.43)$$

On assembling the terms of the equation (1.28), one obtains

$$\epsilon_0 \ddot{A}_i = j_i + \frac{\epsilon_0 c^2}{2}\sum_j \partial_j 2(\partial_j A_i - \partial_i A_j) = j_i + \epsilon_0 c^2 \Delta A_i \ , \quad (1.44)$$

which gives the same wave equation for the vector potential as we got in Eq. (1.23).

1.2.1 Gauge transformations of the Lagrangian

Finally, for the sake of completeness, we present that gauge transformations of electrodynamics (1.18) can be translated into the transformation of the Lagrangian $\mathcal{L}' = \mathcal{L} + \mathcal{L}_1$ with

$$\mathcal{L}_1 = \mathbf{j}(\mathbf{r}, t)\nabla F(\mathbf{r}, t) + \rho(\mathbf{r}, t)\frac{\partial F(\mathbf{r}, t)}{\partial t} \ , \quad (1.45)$$

which is

$$\mathcal{L}_1 = \nabla\left(\mathbf{j}(\mathbf{r}, t)F(\mathbf{r}, t)\right) + \frac{\partial}{\partial t}\left(\rho(\mathbf{r}, t)F(\mathbf{r}, t)\right) - \left(\nabla \mathbf{j}(\mathbf{r}, t) + \frac{\partial \rho(\mathbf{r}, t)}{\partial t}\right)F(\mathbf{r}, t) \ , \quad (1.46)$$

the some of a full divergence and a time derivative since the last term vanishes by the continuity equation.

1.3 The minimal coupling Hamiltonian

The independent degrees of freedom cannot be readily seized in the previous picture based on the Lagrangian in real space. The reason is the relation $\nabla \mathbf{A} = 0$ which leads to a constraint among the components of the vector potential in adjacent positions. One has to move into the reciprocal space where the Coulomb gauge condition is local, $\mathbf{k}\mathcal{A} = 0$. The Fourier transform of the Lagrangian gives

$$L = \sum_\nu \frac{1}{2} m_\nu \dot{\mathbf{r}}_\nu^2 - \int_{k>0} d^3\mathbf{k} \frac{\rho^* \rho}{\epsilon_0 k^2} + \epsilon_0 \int_{k>0} d^3\mathbf{k} \left[\dot{\mathcal{A}}^* \cdot \dot{\mathcal{A}} - c^2 \, k^2 \, \mathcal{A}^* \cdot \mathcal{A} \right] + \int_{k>0} d^3\mathbf{k} \left[\mathcal{A}^* \cdot \mathbf{j} + \mathbf{j}^* \cdot \mathcal{A} \right] \ . \quad (1.47)$$

For each point $\mathbf{k}$ in the reciprocal space, there are two independent components $\mathcal{A}_\lambda(\mathbf{k})$ of the vector potential $\mathcal{A}(\mathbf{k})$. The corresponding directions $\mathbf{e}_\lambda(\mathbf{k})$, being called the *polarization*, are mutually orthogonal and both are perpendicular to the local vector $\mathbf{k}$. With each of the independent variables $\mathcal{A}_\lambda(\mathbf{k})$, where $\lambda = 1, 2$ and $\mathbf{k}$ is in the positive half space, one can associate a canonical momentum

$$\Pi_\lambda(\mathbf{k}) = \epsilon_0 \dot{\mathcal{A}}_\lambda(\mathbf{k}) \ . \quad (1.48)$$

Going back to vector notation, $\Pi(\mathbf{k}) = \sum_{\lambda=1,2} \mathbf{e}_\lambda(\mathbf{k}) \Pi_\lambda(\mathbf{k})$.

Now, the Hamiltonian can be obtained by the Legendre transformation,

$$H = \sum_\nu \mathbf{p}_\nu \dot{\mathbf{r}}_\nu + \int_{k>0} d^3\mathbf{k} \left[\Pi \dot{\mathcal{A}}^* + \Pi^* \dot{\mathcal{A}} \right] - L \ , \quad (1.49)$$

and by eliminating the velocities. This canonical method leads to the so-called *minimal coupling Hamiltonian*,

$$H = \sum_\nu \frac{1}{2m_\nu} \left[\mathbf{p}_\nu - q_\nu \mathbf{A}(\mathbf{r}_\nu) \right]^2 + V_{\text{Coul}} + H_F \ , \quad (1.50a)$$

where the radiation field Hamiltonian is

$$H_F = \epsilon_0 \int_{k>0} d^3\mathbf{k} \left[\frac{\Pi^* \cdot \Pi}{\epsilon_0^2} + c^2 \, k^2 \, \mathcal{A}^* \cdot \mathcal{A} \right] = \frac{\epsilon_0}{2} \int d^3\mathbf{r} \ \left[\mathbf{E}_\perp^2(\mathbf{r}) + c^2 \, \mathbf{B}^2(\mathbf{r}) \right] \ , \quad (1.50b)$$

and the Coulomb interaction is given by Eq. (1.32). This Hamiltonian, describing electrodynamics in the presence of sources without approximations, is the main result of this chapter.

The quantum theory can now be formulated by the canonical quantization procedure which amounts to imposing the commutation relations on the canonically conjugate variable pairs,

$$[\hat{r}_{\nu,i}, \hat{p}_{\nu',j}] = i\hbar \delta_{\nu,\nu'} \, \delta_{ij} \quad (1.51a)$$

and for the field

$$\left[\hat{\mathcal{A}}_\lambda(\mathbf{k}), \hat{\Pi}_{\lambda'}(\mathbf{k}') \right] = 0 \ , \quad (1.51b)$$

$$\left[\hat{\mathcal{A}}_\lambda(\mathbf{k}), \hat{\Pi}_{\lambda'}^\dagger(\mathbf{k}') \right] = i\hbar \, \delta_{\lambda,\lambda'} \delta(\mathbf{k} - \mathbf{k}') \ . \quad (1.51c)$$

1.4 QED with normal variables

In this last section we introduce the normal variables which allow for the most compact description of the fields and for the most suitable representation for calculations.

The normal coordinates of the fields can be defined as a linear combination of the canonically conjugate variables,

$$\alpha_\lambda(\mathbf{k}) = \frac{1}{2\mathcal{N}(\mathbf{k})}\left[\omega\mathcal{A}_\lambda(\mathbf{k}) + \frac{i}{\epsilon_0}\Pi_\lambda(\mathbf{k})\right] , \tag{1.52a}$$

$$\alpha^*_\lambda(-\mathbf{k}) = \frac{1}{2\mathcal{N}(\mathbf{k})}\left[\omega\mathcal{A}_\lambda(\mathbf{k}) - \frac{i}{\epsilon_0}\Pi_\lambda(\mathbf{k})\right] , \tag{1.52b}$$

where $\omega = ck$, and $\mathcal{N}(\mathbf{k})$ is a normalization constant uninteresting at this stage. There are two independent linear combinations of the two variables and, as one can check, there is no complex conjugation relationship between $\alpha_\lambda(\mathbf{k})$ and $\alpha_\lambda(-\mathbf{k})$. Therefore, the $\alpha_\lambda(\mathbf{k})$ are independent variables in the full reciprocal space. From the Hamiltonian equations of motion for the variables $\mathcal{A}_\lambda(\mathbf{k})$ and $\Pi_\lambda(\mathbf{k})$, one can deduce the equation of motion for the normal variable[1]

$$\dot{\alpha}_\lambda(\mathbf{k},t) + i\omega\alpha_\lambda(\mathbf{k},t) = \frac{i}{2\epsilon_0\mathcal{N}(\mathbf{k})}\mathbf{e}_\lambda\mathbf{j}(\mathbf{k},t) . \tag{1.53}$$

This equation of motion reveals the significance of the normal variables of the radiation field: each of them corresponds to a harmonic oscillator with angular frequency ω, which is driven by the current.

The normal variables of the corresponding quantum theory derive from Eq. (1.52) by substituting the vector potential and its canonical momentum by the respective operators,

$$\hat{a}_\lambda(\mathbf{k}) = \sqrt{\frac{\epsilon_0}{2\hbar\omega}}\left[\omega\hat{\mathcal{A}}_\lambda(\mathbf{k}) + \frac{i}{\epsilon_0}\hat{\Pi}_\lambda(\mathbf{k})\right] , \tag{1.54a}$$

$$\hat{a}^\dagger_\lambda(\mathbf{k}) = \sqrt{\frac{\epsilon_0}{2\hbar\omega}}\left[\omega\hat{\mathcal{A}}^\dagger_\lambda(\mathbf{k}) - \frac{i}{\epsilon_0}\hat{\Pi}^\dagger_\lambda(\mathbf{k})\right] , \tag{1.54b}$$

which is the pair of bosonic annihilation and creation operators associated with each of the normal mode harmonic oscillators. The normalization was set, for later convenience, as

$$\mathcal{N}(\mathbf{k}) = \sqrt{\frac{\hbar\omega}{2\epsilon_0}} . \tag{1.55}$$

which leads to a simple commutation relation between the quantized normal variables.

[1] The derivation requires the quantity $\partial\mathbf{A}(\mathbf{r}_\nu)/\partial\mathcal{A}^*_\lambda(\mathbf{k})$, which can be read out from the expansion

$$\mathbf{A}(\mathbf{r}_\nu) = \frac{1}{(2\pi)^{3/2}}\sum_{\lambda=1,2}\mathbf{e}_\lambda\int_{k>0} d^3\mathbf{k}\left(\mathcal{A}_\lambda(\mathbf{k})e^{i\mathbf{k}\mathbf{r}_\nu} + \mathcal{A}^*_\lambda(\mathbf{k})e^{-i\mathbf{k}\mathbf{r}_\nu}\right) ,$$

and $\mathbf{j}(\mathbf{k}) = 1/(2\pi)^{3/2}\, q_\nu\dot{\mathbf{r}}_\nu\, e^{-i\mathbf{k}\mathbf{r}_\nu}$.

From the canonical commutation relation Eqs. (1.51b) follows that

$$[\hat{a}_\lambda(\mathbf{k}), \hat{a}_{\lambda'}(\mathbf{k}')] = 0 \,, \tag{1.56a}$$

$$\left[\hat{a}^\dagger_\lambda(\mathbf{k}), \hat{a}^\dagger_{\lambda'}(\mathbf{k}')\right] = 0 \,, \tag{1.56b}$$

$$\left[\hat{a}_\lambda(\mathbf{k}), \hat{a}^\dagger_{\lambda'}(\mathbf{k}')\right] = \delta_{\lambda,\lambda'}\delta(\mathbf{k}-\mathbf{k}') \,. \tag{1.56c}$$

The inverse of Eq. (Eq. (1.52)) can be carried out and then the Fourier transform leads to the vector potential in real space,

$$\hat{\mathbf{A}}(\mathbf{r},t) = \frac{1}{(2\pi)^{3/2}} \int d^3\mathbf{k} \sum_{\lambda=1,2} \sqrt{\frac{\hbar}{2\epsilon_0\omega}} \mathbf{e}_\lambda \left(\hat{a}_\lambda(\mathbf{k},t)e^{i\mathbf{kr}} + \hat{a}^\dagger_\lambda(\mathbf{k},t)e^{-i\mathbf{kr}}\right) \,. \tag{1.57}$$

1.4.1 Discretization of the space

Instead of using a continuum of modes, it is convenient to introduce a fictitious boundary box with finite volume (L^3) and impose periodic boundary conditions on the mode functions so that to discretize the Fourier expansion. Physically, this construction does not lead to any noticeable modification of the results provided the minimum frequency $\omega_{\min} = 2\pi c/L$ is much smaller than the resolution of the detectors in the actual physical setup under consideration. Then we can introduce a discrete set of normal variables

$$\hat{a}_{\mathbf{k},\lambda} = \left(\frac{2\pi}{L}\right)^{3/2} \hat{a}(\mathbf{k},\lambda) \,. \tag{1.58}$$

The discretized bosonic annihilation and creation operators $\hat{a}_{\mathbf{k},\lambda}$ and $\hat{a}^\dagger_{\mathbf{k},\lambda}$ obey the commutation relations

$$\left[\hat{a}_{\mathbf{k},\lambda}, \hat{a}^\dagger_{\mathbf{k}',\lambda'}\right] = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\lambda,\lambda'} \tag{1.59a}$$

$$[\hat{a}_{\mathbf{k},\lambda}, \hat{a}_{\mathbf{k}',\lambda'}] = \left[\hat{a}^\dagger_{\mathbf{k},\lambda}, \hat{a}^\dagger_{\mathbf{k}',\lambda'}\right] = 0 \,. \tag{1.59b}$$

The quantized vector potential, electric and magnetic fields read

$$\hat{\mathbf{A}}(\mathbf{r},t) = \sum_{\mathbf{k},\lambda} \sqrt{\frac{\hbar}{2\epsilon_0\omega L^3}} \mathbf{e}_\lambda \left(\hat{a}_{\mathbf{k},\lambda}(t)e^{i\mathbf{kr}} + \hat{a}^\dagger_{\mathbf{k},\lambda}(t)e^{-i\mathbf{kr}}\right) \,, \tag{1.60a}$$

$$\hat{\mathbf{E}}_\perp(\mathbf{r},t) = i\sum_{\mathbf{k},\lambda} \sqrt{\frac{\hbar\omega}{2\epsilon_0 L^3}} \mathbf{e}_\lambda \left(\hat{a}_{\mathbf{k},\lambda}(t)e^{i\mathbf{kr}} - \hat{a}^\dagger_{\mathbf{k},\lambda}(t)e^{-i\mathbf{kr}}\right) \,, \tag{1.60b}$$

$$\hat{\mathbf{B}}(\mathbf{r},t) = i\sum_{\mathbf{k},\lambda} \sqrt{\frac{\hbar\omega}{2\epsilon_0 L^3}} \frac{\mathbf{k}}{ck} \times \mathbf{e}_\lambda \left(\hat{a}_{\mathbf{k},\lambda}(t)e^{i\mathbf{kr}} - \hat{a}^\dagger_{\mathbf{k},\lambda}(t)e^{-i\mathbf{kr}}\right) \,. \tag{1.60c}$$

The energy associated with the transverse field Eq. (1.50b) can be expressed as

$$\mathcal{H}_{\mathrm{F}} = \frac{1}{2}\sum_{\mathbf{k},\lambda} \hbar\omega \left(\hat{a}_{\mathbf{k},\lambda}\hat{a}^\dagger_{\mathbf{k},\lambda} + \hat{a}^\dagger_{\mathbf{k},\lambda}\hat{a}_{\mathbf{k},\lambda}\right) = \sum_{\mathbf{k},\lambda} \hbar\omega \left(\hat{a}^\dagger_{\mathbf{k},\lambda}\hat{a}_{\mathbf{k},\lambda} + \frac{1}{2}\right) \,. \tag{1.61}$$

The $1/2$ is the zero-point energy and is an uninteresting shift of the energy in the forthcoming theory. One can check that the Heisenberg equation of motion for the field amplitude operator $\hat{a}_{\mathbf{k},\lambda}$ renders the free evolution part of Eq. (1.53),

$$\frac{d}{dt}\hat{a}_{\mathbf{k},\lambda} = \frac{1}{i\hbar}\left[\hat{a}_{\mathbf{k},\lambda}, \mathcal{H}_{\mathrm{F}}\right] = -i\omega\hat{a}_{\mathbf{k},\lambda} \ . \tag{1.62}$$

Chapter 2

Atom model and dipole interaction with the field

In the previous chapter the canonical quantization procedure has been performed, and we arrived at the minimal coupling Hamiltonian without any approximation (apart from the labeling of charges which is not appropriate in general for quantum fields representing the charge carriers).

2.1 Dipole approximation

By "atom" we will mean a cluster of charges kept together by the Coulomb attraction between the nucleus and the electrons. To label the charges, in the following, we will split the index ν to two parts: $\nu \to A, i_A$, where (i) A labels which atom the charge belongs to, and (ii) i_A labels the charge within the atom A. Then, we will assume that the size of the atom (being in the range of the Bohr radius, 0.5 A) is much smaller than the characteristic length scale on which the vector potential varies noticeably, i.e., is much smaller than the typical wavelength of the excited normal modes (the radiation wavelength, 100 nm... 1μm in optics). Therefore, in each clusters, the vector potential will be considered in the position of the atom $\mathbf{r}_a$ (center-of-mass position of the charges in the cluster). This is the *dipole approximation*. The minimal coupling Hamiltonian is approximated by

$$H = \sum_A \left\{ \sum_{i_A} \frac{\mathbf{p}_{i_A}^2}{2m_{i_A}} + \sum_{i_A \neq j_A} \frac{1}{8\pi\epsilon_0} \frac{q_{i_A} q_{j_A}}{|\mathbf{r}_{i_A} - \mathbf{r}_{j_A}|} + \sum_{i_A} E_{i_A}^{\text{self}} \right\} - \sum_A \left\{ \sum_{i_A} \frac{q_{i_A}}{m_{i_A}} \mathbf{p}_{i_A} \mathbf{A}(\mathbf{r}_A) + \sum_{i_A} \frac{q_{i_A}^2}{2m_{i_A}} \mathbf{A}^2(\mathbf{r}_A) \right\} + \sum_{A \neq B} \sum_{i_A, j_B} \frac{1}{4\pi\epsilon_0} \frac{q_{i_A} q_{j_B}}{|\mathbf{r}_{i_A} - \mathbf{r}_{j_B}|} + H_{\text{F}} \ , \quad (2.1)$$

where the field Hamiltonian is

$$H_{\text{F}} = \sum_{\mathbf{k},\lambda} \hbar\omega \left(\hat{a}_{\mathbf{k},\lambda}^\dagger \hat{a}_{\mathbf{k},\lambda} + \frac{1}{2} \right) \ , \quad (2.2)$$

and the vector potential is

$$\hat{\mathbf{A}}(\mathbf{r}_A,t)=\sum_{\mathbf{k},\lambda}\sqrt{\frac{\hbar}{2\epsilon_0\omega L^3}}\mathbf{e}_\lambda\left(\hat{a}_{\mathbf{k},\lambda}(t)e^{i\mathbf{k}\mathbf{r}_A}+\hat{a}^\dagger_{\mathbf{k},\lambda}(t)e^{-i\mathbf{k}\mathbf{r}_A}\right)\ . \tag{2.3}$$

The expression in the first line seems to properly define an atomic Hamiltonian. However, there are several problems with this approach. First, when separating the canonical momentum associated with the center-of-mass position r_A, one gets the canonical momentum instead of the kinetic one which is the observable quantity in the laboratory. Moreover, there is a potential acting on the center-of-mass motion represented by the second term of the second line, which exhibits a weird behaviour: its mean value does not vanish in vacuum, it is even divergent without a cutoff in momentum space. Finally, the last line contains the scalar potential which amounts to an instantaneous dipole-dipole-type Coulomb interaction between remote atoms.

2.1.1 Unitary transformation into the length gauge

In order to properly define the atomic part of the Hamiltonian, we will transform into a gauge other than the Coulomb gauge. This is the *electric dipole gauge* (sometimes called the "length gauge"), which is connected to the Coulomb gauge and to the minimal coupling Hamiltonian by the unitary transformation

$$T=\exp\left\{-\frac{i}{\hbar}\sum_A\mathbf{d}_A\mathbf{A}(\mathbf{r}_A)\right\}=\exp\left\{\sum_A\sum_{\mathbf{k},\lambda}\beta^*_{\mathbf{k},\lambda,A}\hat{a}_{\mathbf{k},\lambda}-\beta_{\mathbf{k},\lambda,A}\hat{a}^\dagger_{\mathbf{k},\lambda}\right\}\ , \tag{2.4}$$

where we have introduced the atomic dipole moment operator

$$\hat{\mathbf{d}}_A=\sum_{i_A}q_{i_A}\hat{\mathbf{r}}_{i_A}(t)\ , \tag{2.5}$$

and the shorthands

$$\beta_{\mathbf{k},\lambda,A}=i\frac{\mathbf{e}_{\mathbf{k},\lambda}\mathbf{d}_A}{\sqrt{2\epsilon_0\hbar\omega_k L^3}}e^{-i\mathbf{k}\mathbf{r}_A}\ ,\ \text{and}\ \beta_{\mathbf{k},\lambda}=\sum_A\beta_{\mathbf{k},\lambda,A}\ . \tag{2.6}$$

All operators $\hat{O}$ associated with a physical quantity have to be transformed as $\hat{O}'=T\hat{O}T^\dagger$ and, simultaneously, the states $|\psi\rangle$ of the system have to be transformed as $T|\psi\rangle$, then we get an equivalent formulation of the problem giving the same measurable quantities. Let us survey how the physical quantities relevant to the electrodynamics problem transform. With regards to the charged particles, note that T contains only position operators $\mathbf{r}_{i_A}$, therefore it commutes with all the positions and $\hat{\mathbf{r}}'_{i_A}=\hat{\mathbf{r}}_{i_A}$. The same applies for the transform of the vector potential, $\mathbf{A}'(\mathbf{r})=\mathbf{A}(\mathbf{r})$, since $\mathbf{A}(\mathbf{r})$ commutes with $\mathbf{A}(\mathbf{r}_A)$ everywhere in the real space.

For the momentum operators, the effect of the similarity transformation is a displacement, i.e.,

$$\hat{\mathbf{p}}'_{i_A}=e^{-\frac{i}{\hbar}q_{i_A}\hat{\mathbf{r}}_{i_A}\mathbf{A}(\mathbf{r}_A)}\hat{\mathbf{p}}_{i_A}e^{\frac{i}{\hbar}q_{i_A}\hat{\mathbf{r}}_{i_A}\mathbf{A}(\mathbf{r}_A)}=\hat{\mathbf{p}}_{i_A}+q_{i_A}\mathbf{A}(\mathbf{r}_A)\ . \tag{2.7}$$

The velocities transform as

$$\hat{\mathbf{v}}'_{i_A} = T\,\hat{\mathbf{v}}_{i_A}\,T^\dagger = \frac{1}{m_{i_A}} T\,\left[\hat{\mathbf{p}}_{i_A} - q_{i_A}\mathbf{A}(\mathbf{r}_A)\right]\,T^\dagger = \frac{\hat{\mathbf{p}}_{i_A}}{m_{i_A}}\,, \tag{2.8}$$

that is, the canonical momentum $\mathbf{p}_{i_A}$ coincides with the kinetic momentum in the length gauge.

The bosonic operators are also displaced,

$$\hat{a}'_{\mathbf{k},\lambda} = T\,\hat{a}_{\mathbf{k},\lambda}\,T^\dagger = \hat{a}_{\mathbf{k},\lambda} + \beta_{\mathbf{k},\lambda}\,, \tag{2.9}$$

$$\hat{a}^{\dagger\prime}_{\mathbf{k},\lambda} = T\,\hat{a}^\dagger_{\mathbf{k},\lambda}\,T^\dagger = \hat{a}^\dagger_{\mathbf{k},\lambda} + \beta^\dagger_{\mathbf{k},\lambda}\,, \tag{2.10}$$

where $\beta_{\mathbf{k},\lambda} = \sum_A \beta_{\mathbf{k},\lambda,A}$. As we mentioned the vector potential is invariant, so is the magnetic field because

$$\mathbf{B}'(\mathbf{r},t) = \nabla\times\mathbf{A}'(\mathbf{r},t) = \nabla\times\mathbf{A}(\mathbf{r},t) = \mathbf{B}(\mathbf{r},t)\,. \tag{2.11}$$

On the other hand, the transverse electric field vector transforms non-trivially,

$$\begin{aligned}
\mathbf{E}'_\perp(\mathbf{r},t) &= i\sum_{\mathbf{k},\lambda}\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\mathbf{e}_{\mathbf{k},\lambda}\left[(\hat{a}_{\mathbf{k},\lambda}+\beta_{\mathbf{k},\lambda})e^{i\mathbf{k}\mathbf{r}} - (\hat{a}^\dagger_{\mathbf{k},\lambda}+\beta^\dagger_{\mathbf{k},\lambda})e^{-i\mathbf{k}\mathbf{r}}\right]\\
&= \mathbf{E}_\perp(\mathbf{r},t) - \sum_A\sum_{\mathbf{k},\lambda}\frac{1}{2\epsilon_0 V}\mathbf{e}_{\mathbf{k},\lambda}(\mathbf{e}_{\mathbf{k},\lambda}\mathbf{d}_A)\left[e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}_A)} + e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}_A)}\right]\\
&= \mathbf{E}_\perp(\mathbf{r},t) - \frac{V}{(2\pi)^3}\int d^3\mathbf{k}\,\left(1-\frac{\mathbf{k}\circ\mathbf{k}}{k^2}\right)\frac{1}{2\epsilon_0 V}\left[\sum_A \mathbf{d}_A(t)e^{-i\mathbf{k}\mathbf{r}_A(t)}e^{i\mathbf{k}\mathbf{r}} + \text{c.c.}\right]\\
&= \mathbf{E}_\perp(\mathbf{r},t) - \frac{1}{\epsilon_0}\sum_A \delta_\perp(\mathbf{r}-\mathbf{r}_A(t))\mathbf{d}_A(t)\,,
\end{aligned} \tag{2.12}$$

where we used the definition in Eq. (1.13). The physical meaning of the transformed transverse electric field can be revealed by introducing the charge density in the dipole approximation. The charge density, starting from its definition, can be approximated as

$$\begin{aligned}
\rho(\mathbf{r},t) &= \sum_A\sum_{i_A} q_{i_A}\delta(\mathbf{r}-\mathbf{r}_{i_A}(t)-\mathbf{r}_A(t))\\
&\approx -\sum_A\sum_{i_A} q_{i_A}\mathbf{r}_{i_A}(t)\nabla\delta(\mathbf{r}-\mathbf{r}_A(t)) = -\nabla\sum_A \mathbf{d}_A\delta(\mathbf{r}-\mathbf{r}_A(t))\,,
\end{aligned} \tag{2.13}$$

where we assumed that the coordinates $\mathbf{r}_{i_A}$ are taken with respect to the origin defined by the center-of-mass coordinate $\mathbf{r}_A$ and are thus small. The above approximation can be performed, for example, in the reciprocal space,

$$\begin{aligned}
\rho(\mathbf{k},t) &= \frac{1}{(2\pi)^{3/2}}\int d^3\mathbf{r}\,\rho(\mathbf{r},t)e^{-i\mathbf{k}\mathbf{r}} = \sum_A\sum_{i_A} q_{i_A}\frac{1}{(2\pi)^{3/2}}e^{-i\mathbf{k}(\mathbf{r}_{i_A}+\mathbf{r}_A)}\\
&\approx \sum_A\sum_{i_A} q_{i_A}\frac{1}{(2\pi)^{3/2}}(1-i\mathbf{k}\mathbf{r}_{i_A})e^{-i\mathbf{k}\mathbf{r}_A} = -\sum_A\frac{1}{(2\pi)^{3/2}}i\mathbf{k}\mathbf{d}_A e^{-i\mathbf{k}\mathbf{r}_A}
\end{aligned} \tag{2.14}$$

One can thus introduce the polarization density within the dipole approximation of atoms,

$$\mathbf{P}(\mathbf{r},t) = \sum_A \mathbf{d}_A(t)\delta(\mathbf{r}-\mathbf{r}_A(t)) \;, \tag{2.15}$$

or its Fourier transform

$$\mathcal{P}(\mathbf{k},t) = \sum_A \frac{1}{(2\pi)^{3/2}}\mathbf{d}_A(t)e^{-i\mathbf{k}\mathbf{r}_A(t)} \;. \tag{2.16}$$

The charge density fixes only the longitudinal part of the polarization field, however, with this choice the last expression in Eq. (2.12) can be recognized being equal to

$$\mathbf{E}'_\perp(\mathbf{r},t) = \mathbf{E}_\perp(\mathbf{r},t) - \frac{1}{\epsilon_0}P_\perp(\mathbf{r},t) \;. \tag{2.17}$$

With this result, one can find the transform of the displacement field,

$$\begin{aligned}\mathbf{D}'_\perp(\mathbf{r},t) = T\,\mathbf{D}_\perp(\mathbf{r},t)\,T^\dagger = \epsilon_0 T\,\mathbf{E}_\perp(\mathbf{r},t)\,T^\dagger + T\,\mathbf{P}_\perp(\mathbf{r},t)\,T^\dagger = \mathbf{E}_\perp(\mathbf{r},t) \\ = i\sum_{\mathbf{k},\lambda}\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\mathbf{e}_{\mathbf{k},\lambda}\left[\hat{a}_{\mathbf{k},\lambda}e^{i\mathbf{k}\mathbf{r}} - \hat{a}^\dagger_{\mathbf{k},\lambda}e^{-i\mathbf{k}\mathbf{r}}\right] \;,\end{aligned} \tag{2.18}$$

that is, in the electric dipole gauge the displacement field is the canonical conjugate momentum to the vector potential. The displacement vector is a purely transverse vector field

$$\nabla\mathbf{D}(\mathbf{r},t) = \nabla(\epsilon_0\mathbf{E}(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t)) = \rho(\mathbf{r},t) - \rho(\mathbf{r},t) = 0 \;, \tag{2.19}$$

i.e., there are no free charges other than those composing the atoms.

2.1.2 The dipole Hamiltonian

After having calculated the unitary transform of the relevant physical quantities, now we can find the Hamiltonian in the new gauge, and express it in terms of the same variables $\left\{\hat{a}_{\mathbf{k},\lambda}, \hat{a}^\dagger_{\mathbf{k},\lambda}, \mathbf{r}_{i_A}, \mathbf{p}_{i_A}\right\}$. The Hamiltonian transforms differently from the other physical quantities, $H' = THT^\dagger + i\hbar\frac{\partial T}{\partial t}T^\dagger$, so that the Schrödinger equation remains invariant in the new picture. However, the unitary transformation T in Eq. (2.4) does not depend explicitly on the time, so this last term vanishes.

As we saw previously, the kinetic energy term of the Hamiltonian transforms as

$$\frac{1}{2m_{i_A}}\left(\mathbf{p}_{i_A} - q_{i_A}\mathbf{A}(r_A)\right)^2 \longrightarrow \frac{\mathbf{p}^2_{i_A}}{2m_{i_A}} \;. \tag{2.20}$$

The Coulomb interaction, depending only on the position of charges, is invariant. The radiation field Hamiltonian, on the other hand, transforms essentially:

$$\begin{aligned}H'_{\mathrm{F}} = T\,H_{\mathrm{F}}\,T^\dagger = \sum_{\mathbf{k},\lambda}\hbar\omega_k\left[\left(\hat{a}^\dagger_{\mathbf{k},\lambda} + \beta^\dagger_{\mathbf{k},\lambda}\right)\left(\hat{a}_{\mathbf{k},\lambda} + \beta_{\mathbf{k},\lambda}\right) + \frac{1}{2}\right] \\ = \sum_{\mathbf{k},\lambda}\hbar\omega\left(\hat{a}^\dagger_{\mathbf{k},\lambda}\hat{a}_{\mathbf{k},\lambda} + \frac{1}{2}\right) + \sum_A i\sum_{\mathbf{k},\lambda}\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\mathbf{e}_{\mathbf{k},\lambda}\mathbf{d}_A\left[\hat{a}_{\mathbf{k},\lambda}e^{i\mathbf{k}\mathbf{r}_A} - \hat{a}^\dagger_{\mathbf{k},\lambda}e^{-i\mathbf{k}\mathbf{r}_A}\right] \\ + \sum_{A,A'}\sum_{\mathbf{k},\lambda}\hbar\omega_k\beta^\dagger_{\mathbf{k},\lambda}\beta_{\mathbf{k},\lambda} \;.\end{aligned} \tag{2.21}$$

The first term counts the photons of the radiation field, the second term describes the interaction between the atomic dipoles and the radiation field, and it can be written in terms of physical quantities as

$$H_{\rm dip} = \sum_A \mathbf{d}_A \mathbf{D}'_\perp(\mathbf{r}_A, t) \ . \tag{2.22}$$

The last term, when $A = A'$, gives rise to a dipole self-energy of the atoms, analogously the Coulomb self-energy of charges. The remaining summation over the pairs $A \neq A'$ can be further transformed as

$$\begin{aligned}
&\sum_{\mathbf{k},\lambda} \hbar\omega_k \frac{(\mathbf{e}_{\mathbf{k},\lambda}\mathbf{d}_A)(\mathbf{e}_{\mathbf{k},\lambda}\mathbf{d}_{A'})}{2\epsilon_0\hbar\omega_k V} e^{i\mathbf{k}(\mathbf{r}_A - \mathbf{r}_{A'})} \\
&\qquad = \frac{1}{2\epsilon_0(2\pi)^3} \int d^3\mathbf{k} \left(\sum_{i_A} q_{i_A}\mathbf{r}_{i_A}\right)\left(1 - \frac{\mathbf{k}\circ\mathbf{k}}{k^2}\right)\left(\sum_{i_{A'}} q_{i_{A'}}\mathbf{r}_{i_{A'}}\right) e^{i\mathbf{k}(\mathbf{r}_A - \mathbf{r}_{A'})} \\
&= \frac{1}{2\epsilon_0}\frac{1}{(2\pi)^{3/2}}\left[\mathbf{d}_A\mathbf{d}_{A'}\,\delta(\mathbf{r}_A - \mathbf{r}_{A'}) - \sum_{i_A}\sum_{i_{A'}} q_{i_A}q_{i_{A'}} \int d^3\mathbf{k}\, \frac{e^{i\mathbf{k}\left[(\mathbf{r}_A + \mathbf{r}_{i_A}) - (\mathbf{r}_{A'} + \mathbf{r}_{i_{A'}})\right]}}{k^2}\right] \\
&\qquad = \frac{1}{2\epsilon_0}\frac{1}{(2\pi)^{3/2}}\mathbf{d}_A\mathbf{d}_{A'}\,\delta(\mathbf{r}_A - \mathbf{r}_{A'}) - \sum_{i_A}\sum_{i_{A'}} \frac{q_{i_A}q_{i_{A'}}}{4\pi\epsilon_0\left|(\mathbf{r}_A + \mathbf{r}_{i_A}) - (\mathbf{r}_{A'} + \mathbf{r}_{i_{A'}})\right|}
\end{aligned} \tag{2.23}$$

On passing from the second to the third line, we made use of the neutrality of atoms, $\sum_{i_A} q_{i_A} = 0$. In the final result, the second term cancels the part of the Coulomb interaction $V_{\rm Coul}$ which describes the instantaneous Coulomb interaction between charges in different clusters. Therefore, the only remaining interaction between remote atoms is the one mediated by the transverse displacement field which coincides with the transverse electric field outside the charge clusters. Therefore, the interaction between atoms in this new picture manifestly obeys the causality. The first term is non-vanishing only if the atoms overlap, and it is called the contact interaction between atoms.

In summary, the dipole Hamiltonian in the length gauge is obtained,

$$\begin{aligned}
H = &\sum_A \left[\frac{\mathbf{p}_{i_A}^2}{2m_{i_A}} + \sum_{i_A < j_A} \frac{q_{i_A}q_{j_A}}{4\pi\epsilon_0\left|\mathbf{r}_{i_A} - \mathbf{r}_{j_A}\right|} + \sum_{i_A} E_{i_A}^{\rm self} + E_{\rm dip}^{\rm self}\right] \\
&+ \sum_{\mathbf{k},\lambda} \hbar\omega\left(\hat{a}^\dagger_{\mathbf{k},\lambda}\hat{a}_{\mathbf{k},\lambda} + \frac{1}{2}\right) + \sum_A \mathbf{d}_A\mathbf{D}'_\perp(\mathbf{r}_A, t) + \sum_{A<A'} \frac{1}{\epsilon_0}\frac{1}{(2\pi)^{3/2}}\mathbf{d}_A\mathbf{d}_{A'}\,\delta(\mathbf{r}_A - \mathbf{r}_{A'}) \ .
\end{aligned} \tag{2.24}$$

The argument of the first summation is what we call "the atom". We will not need the detailed description of it since, in the following, we will use only a phenomenological description of the atom based on obeservables quantities, such as the resonance frequencies, the linewidths, etc.

2.2 Two-level atom

Let us assume that only two energy eigenstates are relevant in the system. The internal dynamics of the atom can be restricted to the subspace spanned by the 'ground' state

$|g\rangle$ and the excited state $|e\rangle$. These energy levels are separated by the energy $E_e - E_g = \hbar\omega_A$. The internal structure of the atom appears in the coupling to the electromagnetic field via the dipole moment which is projected onto the reduced electronic space as follows,

$$\begin{aligned}\hat{\mathbf{d}} &= (|g\rangle\langle g| + |e\rangle\langle e|)\,\hat{\mathbf{d}}\,(|g\rangle\langle g| + |e\rangle\langle e|) \\ &= \langle g|\hat{\mathbf{d}}|g\rangle\,|g\rangle\langle g| + \langle e|\hat{\mathbf{d}}|e\rangle\,|e\rangle\langle e| + \langle g|\hat{\mathbf{d}}|e\rangle\,|g\rangle\langle e| + \langle e|\hat{\mathbf{d}}|g\rangle\,|e\rangle\langle g| \end{aligned} \quad (2.25)$$

The matrix elements can be evaluated in coordinate representation,

$$\mathbf{d}_{ij} \equiv \langle i|\hat{\mathbf{d}}|j\rangle = -e\int d^3\mathbf{r}\psi_i^*(\mathbf{r})\mathbf{r}\psi_j(\mathbf{r})\ , \quad (2.26)$$

where, for simplicity, we considered a single electron atom. Since the inversion is a symmetry of the atomic Hamiltonian, the energy eigenfunctions have either even parity, $\psi_i(\mathbf{r}) = \psi_i(-\mathbf{r})$, or odd parity, $\psi_i(\mathbf{r}) = -\psi_i(-\mathbf{r})$. In either case they obey $|\psi_i(\mathbf{r})|^2 = |\psi_i(-\mathbf{r})|^2$. Therefore, for the diagonal elements $i = j$, changing the integral variable $\mathbf{r}$ to $-\mathbf{r}$ in Eq. (2.26) leads to a change of the sign of the integral. This is a volume integral which must be independent of such a change of the variable, that is, the integral is zero. *Dipole transition can exist only between states with different parity*. The corresponding matrix element, the *induced* or *transition dipole moment*, $\mathbf{d}_{eg} \equiv \langle e|\hat{\mathbf{d}}|g\rangle$, describes the transition strength, and can be derived from the theoretical energy eigenstates of the atom, according to Eq. (2.26). It can be chosen real, i.e., $\mathbf{d}_{eg} = \mathbf{d}_{ge}$, by properly adjusting the phase of one of the electronic states. Later we will express the transition dipole moment in terms of the natural linewidth of the given transition, which is an experimentally observable quantity.

2.2.1 Pauli spin operators

There are four operators forming a closed algebra in the space of the atomic internal degree of freedom: $|g\rangle\langle g|$, $|e\rangle\langle e|$, $|g\rangle\langle e|$, and $|e\rangle\langle g|$. Note that $|g\rangle\langle g| + |e\rangle\langle e| = 1$, expressing that we consider only the two-level subspace. It is convenient to introduce the Pauli operators,

$$\begin{aligned}\sigma &= |g\rangle\langle e|\ , \\ \sigma^\dagger &= |e\rangle\langle g|\ , \\ \sigma_z &= \frac{1}{2}\left(|e\rangle\langle e| - |g\rangle\langle g|\right)\ , \end{aligned} \quad (2.27)$$

which obey the commutation relations,

$$\left[\sigma, \sigma^\dagger\right] = -2\sigma_z \quad (2.28a)$$

$$[\sigma, \sigma_z] = \sigma \quad (2.28b)$$

$$\left[\sigma^\dagger, \sigma_z\right] = -\sigma^\dagger \quad (2.28c)$$

This is the same algebra as that of a spin-$\frac{1}{2}$ particle. The operator σ is referred to as the *polarization*, and σ_z as the *population inversion*, or briefly, as the population. The

Hamiltonian associated with the internal degree of freedom of the atom is given by

$$\mathcal{H}_A = \hbar\omega_A \sigma_z = \hbar\omega_A \sigma^\dagger \sigma - \frac{\hbar\omega_A}{2} \ , \tag{2.29}$$

where the last constant can be safely neglected.

Dipole coupling

The dipole moment operator can be expressed as

$$\hat{\mathbf{d}} = \mathbf{d}_{eg} \left(\sigma + \sigma^\dagger\right) \ . \tag{2.30}$$

The dipole interaction term of the Hamiltonian takes on the simple form

$$\mathcal{H}_{\text{int}} = i\hbar \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(a^\dagger_{\mathbf{k},\lambda} e^{i\mathbf{k}\mathbf{R}_A} - a_{\mathbf{k},\lambda} e^{-i\mathbf{k}\mathbf{R}_A} \right) \left(\sigma + \sigma^\dagger\right) \ . \tag{2.31}$$

with the coupling constant

$$g_{\mathbf{k},\lambda} = \sqrt{\frac{\omega}{2\hbar\epsilon_0 L^3}} \mathbf{e}_\lambda \mathbf{d}_{eg} \ . \tag{2.32}$$

The free field mode and the free atom evolves at a frequency ω and ω_A, respectively. The coupling is significant if these frequencies are nearly resonant. That is, both frequencies fall in the optical range of the electromagnetic spectrum, $\omega \sim 2\pi\, 10^{15}$ s^{-1}. By contrast, their interaction yields the atom-field coupling strength $g_{\mathbf{k},\lambda}$ which is typically around 10^6 s^{-1}, much less than the optical frequencies. Two of the terms in Eq. (**??**) oscillate with angular frequency $\omega - \omega_A$, the other two oscillate with $\omega + \omega_A$. While the former can be comparable with the frequency characteristic of the atom-field coupling, the latter is definitely many orders of magnitude larger. The corresponding *counter-rotating* terms, $\sigma^\dagger \hat{a}^\dagger_{\mathbf{k},\lambda}$ and $\sigma \hat{a}_{\mathbf{k},\lambda}$, strongly oscillate during the period of time needed for the atom-field coupling to result in a noticeable evolution, and averages out. Neglecting these terms oscillating with the double of the optical frequency is the *rotating wave approximation* (RWA). The final form of the interaction Hamiltonian is then

$$\mathcal{H}^{\text{RWA}}_{\text{int}} = i\hbar \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(a^\dagger_{\mathbf{k},\lambda} \sigma e^{i\mathbf{k}\mathbf{R}_A} - \sigma^\dagger a_{\mathbf{k},\lambda} e^{-i\mathbf{k}\mathbf{R}_A} \right) \ . \tag{2.33}$$

The physical meaning of the two terms is obvious: the first term describes the emission of a photon while the atom jumps from the state $|e\rangle$ to the state $|g\rangle$; and the second term corresponds to the absorption of a photon while the atom jumps up from $|g\rangle$ to $|e\rangle$. One can check that the dipole potential in Eq. (**??**) leads to the same interaction Hamiltonian as in Eq. (2.33) in the rotating wave approximation.

One might think that the fast counter-rotating terms express unphysical processes, such as the atom emits a photon while stepping from the ground to the excited state, and reversely. These processes, though strongly suppressed by the large energy mismatch, are real and manifest themselves in observable effects, such as the van der Waals interaction between two ground state atoms. It is a fourth-order process involving two times co-rotating and two-times counter-rotating interaction terms.

Chapter 3

Spontaneous emission

In this chapter we will discuss the interaction of a two-level atom with the entire set of electromagnetic radiation modes being in vacuum state. This interaction is fundamental and cannot be eliminated from the system. In principle, the vacuum state should be replaced by the thermal state, however, at room temperature the population in the modes with optical frequency is practically zero: $k_B T/\hbar\omega \approx 10^{-2}$.

The atom will be assumed immobile, and due to the translational symmetry of the system, its position can be assumed the origin, $\mathbf{R}_A = 0$. The Hamiltonian of the system is

$$\mathcal{H} = \hbar\omega_A \sigma_z + \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k},\lambda} a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} + i\hbar \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(a^\dagger_{\mathbf{k},\lambda} \sigma - \sigma^\dagger a_{\mathbf{k},\lambda} \right) . \tag{3.1}$$

Let us go into interaction picture with respect to the free atom and free field Hamiltonians $\mathcal{H}_A$ and $\mathcal{H}_{trans}$, respectively. The fast oscillation is separated,

$$\begin{aligned} a_{\mathbf{k},\lambda}(t) &= \tilde{a}_{\mathbf{k},\lambda}(t) e^{-i\omega_{\mathbf{k},\lambda} t} \\ \sigma(t) &= \tilde{\sigma}(t) e^{-i\omega_A t} , \end{aligned}$$

and σ_z is the same in both pictures. In the following we will drop the subscript of $\omega_{\mathbf{k},\lambda}$ and we will tacitly mean by ω the angular frequency derived from usual dispersion relation $\omega = c|\mathbf{k}|$. The Hamiltonian in interaction picture

$$\mathcal{H}_I = i\hbar \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(\tilde{a}^\dagger_{\mathbf{k},\lambda} \tilde{\sigma} e^{i(\omega-\omega_A)t} - \tilde{\sigma}^\dagger \tilde{a}_{\mathbf{k},\lambda} e^{-i(\omega-\omega_A)t} \right) . \tag{3.2}$$

The equations of motion for the system variables derive from

$$\frac{d}{dt}\tilde{\mathcal{O}} = \frac{1}{i\hbar} \left[\tilde{O}, \mathcal{H}_I, \right] ,$$

and read

$$\frac{d}{dt}\tilde{a}_{\mathbf{k},\lambda} = g_{\mathbf{k},\lambda} \tilde{\sigma} e^{i(\omega-\omega_A)t} , \tag{3.3a}$$

$$\frac{d}{dt}\tilde{\sigma} = \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} 2\sigma_z \tilde{a}_{\mathbf{k},\lambda} e^{-i(\omega-\omega_A)t} , \tag{3.3b}$$

$$\frac{d}{dt}\sigma_z = -\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(\tilde{a}^\dagger_{\mathbf{k},\lambda} \tilde{\sigma} e^{i(\omega-\omega_A)t} + \tilde{\sigma}^\dagger \tilde{a}_{\mathbf{k},\lambda} e^{-i(\omega-\omega_A)t} \right) . \tag{3.3c}$$

The equation for $\tilde{\sigma}^\dagger$ is obviously the Hermitian adjoint of that of the operator $\tilde{\sigma}$. This is a set of coupled, nonlinear equations which cannot be directly solved.

3.1 Free field and source term in normal order

The first equation of Eq. (3.3) can formally be integrated,

$$\begin{aligned}\tilde{a}_{\mathbf{k},\lambda}(t) &= \tilde{a}_{\mathbf{k},\lambda}(t_0) + \int_{t_0}^{t} g_{\mathbf{k},\lambda}\tilde{\sigma}(t')e^{i(\omega-\omega_A)t'}dt' \\ &= \tilde{a}_{\mathbf{k},\lambda}(t_0) + \int_{0}^{t-t_0} g_{\mathbf{k},\lambda}\tilde{\sigma}(t-\tau)e^{i(\omega-\omega_A)(t-\tau)}d\tau \ . \end{aligned} \tag{3.4}$$

The first term is the solution for the free radiation field, the second one corresponds to the field radiated by the atomic dipole. Note that, although $\tilde{a}_{\mathbf{k},\lambda}(t)$ commutes with the operators σ, the above terms, separately, do not. One must be very careful with operator ordering when the above formal solution is substituted into $\tilde{a}_{\mathbf{k},\lambda}(t)$. In the following we will chose the so-called normal ordering, in which creation operators ($\sigma^\dagger$, $a^\dagger$) stand on the far most left, and annihilation operators (σ, a) stand on the far most right. This is a good choice since the field state is in vacuum, and the effect of the operator $\tilde{a}_{\mathbf{k},\lambda}(t_0)$ on the state $|0\rangle$ can evaluated: it gives zero. Similarly, $\langle 0|\,\tilde{a}^\dagger_{\mathbf{k},\lambda}(t_0) = 0$.

3.2 Markov-approximation

Let us use the formal solution in Eq. (3.4) to rewrite the equations of motion for the atomic operators:

$$\begin{aligned}\frac{d}{dt}\tilde{\sigma} = \sum_{\mathbf{k},\lambda} g^2_{\mathbf{k},\lambda}\int_0^{t-t_0} \mathrm{d}\tau\, 2\sigma_z(t)\tilde{\sigma}(t-\tau)\, e^{-i(\omega-\omega_A)\tau} \\ + \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}\, 2\sigma_z(t)\tilde{a}_{\mathbf{k},\lambda}(t_0)e^{-i(\omega-\omega_A)t} \ , \end{aligned} \tag{3.5a}$$

$$\begin{aligned}\frac{d}{dt}\sigma_z = -\sum_{\mathbf{k},\lambda} g^2_{\mathbf{k},\lambda}\int_0^{t-t_0} \mathrm{d}\tau\, \left(\tilde{\sigma}^\dagger(t)\tilde{\sigma}(t-\tau)\, e^{-i(\omega-\omega_A)\tau} + \tilde{\sigma}^\dagger(t-\tau)\tilde{\sigma}(t)\, e^{i(\omega-\omega_A)\tau}\right) \\ - \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}\, \left(\tilde{\sigma}^\dagger(t)\tilde{a}(t_0)\, e^{-i(\omega-\omega_A)t} + \tilde{a}^\dagger(t_0)\tilde{\sigma}(t)\, e^{i(\omega-\omega_A)t}\right) \ . \end{aligned} \tag{3.5b}$$

In both equations, the first line expresses the effect of the electromagnetic field radiated by the dipole back on itself. We will invoke the *Markov approximation* to simplify these terms. In the second lines the terms have a zero mean, since the operator $\tilde{a}_{\mathbf{k},\lambda}(t_0)$ on the far most right, or the operator $\tilde{a}^\dagger_{\mathbf{k},\lambda}(t_0)$ on the far most left, acts on the vacuum state. These are *quantum noise* terms

$$\xi(t) = \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}\, 2\sigma_z(t)\tilde{a}_{\mathbf{k},\lambda}(t_0)e^{-i(\omega-\omega_A)t} \ , \tag{3.6a}$$

$$\xi_z(t) = -\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(\tilde{\sigma}^\dagger(t)\tilde{a}(t_0)\, e^{-i(\omega-\omega_A)t} + \tilde{a}^\dagger(t_0)\tilde{\sigma}(t)\, e^{i(\omega-\omega_A)t} \right) , \tag{3.6b}$$

originating from the vacuum field surrounding the atom, and their properties will be discussed below.

For calculating the first terms, it is convenient to replace the summation by an integral

$$\sum_{\mathbf{k},\lambda} \to \left(\frac{L}{2\pi}\right)^3 \int \mathrm{d}\mathbf{k}^3 \sum_\lambda = \left(\frac{L}{2\pi c}\right)^3 \int_0^\infty \mathrm{d}\omega\omega^2 \int_0^{2\pi} \mathrm{d}\phi \int_0^\pi \mathrm{d}\theta \sin\theta \sum_\lambda$$

$$\sum_{\mathbf{k},\lambda} g^2_{\mathbf{k},\lambda} \to \frac{1}{16\pi^3\epsilon_0 c^3\hbar^3} \int_0^\infty \mathrm{d}\omega\omega^3 \int_0^{2\pi} \mathrm{d}\phi \int_0^\pi \mathrm{d}\theta \sin\theta \sum_\lambda \left(\mathbf{e}_\lambda \mathbf{d}_{eg}\right)^2 , \tag{3.7}$$

where θ and ϕ are the usual Euler angles of the wave vector $\mathbf{k}$. The sum over the polarization can be eliminated by using the relation

$$d^2_{eg} = \sum_\lambda \left(\mathbf{e}_\lambda \mathbf{d}_{eg}\right)^2 + \left(\mathbf{k}\mathbf{d}_{eg}\right)^2 / k^2 \Longrightarrow \sum_\lambda \left(\mathbf{e}_\lambda \mathbf{d}_{eg}\right)^2 = d^2_{eg}(1-\cos^2\theta) . \tag{3.8}$$

Note that if the argument in the summation a function depending only on the modulus of $\mathbf{k}$, i.e., $|\mathbf{k}| = c\omega$, but not on its direction, the angular integrals can also be evaluated, which results in

$$\sum_{\mathbf{k},\lambda} g^2_{\mathbf{k},\lambda} f(\omega) = \frac{d^2_{eg}}{16\pi^3\epsilon_0 c^3\hbar^3} \int_0^\infty \mathrm{d}\omega\omega^3 f(\omega) . \tag{3.9}$$

Now we can see that the first terms in Eq. (3.5) contain an integral over the field mode frequency ω, and a temporal integral accounting for the dipole polarization in times prior to the actual time t. On changing the order of the integrals, one gets a broadband frequency integral,

$$\int_0^\infty \mathrm{d}\omega\, \omega^3\, e^{\pm i(\omega-\omega_A)\tau} \approx 0 \quad \text{for any } \tau \neq 0 . \tag{3.10}$$

More precisely, one can introduce the notion of *reservoir bandwidth* Ω into the integral,

$$\int_{-\Omega}^{\Omega} \mathrm{d}\omega' \left(\omega_A + \omega'\right)^3 e^{\pm i\omega'\tau} = 2\Omega \left(\omega_A - i\frac{\partial}{\partial\tau}\right)^3 \frac{\sin\Omega\tau}{\Omega\tau} , \tag{3.11}$$

which has a finite support of the size $\tau_c \approx \Omega^{-1}$. Since the reservoir bandwidth is far larger than any other dynamical frequencies of the system in interaction picture, τ_c amounts to a too short time scale for the system variables to noticeably change. Therefore, the double integral has contribution only from a very small vicinity of $\tau \approx 0$. The Markov approximation consists in neglecting the variation of the system variables $\sigma(t)$, $\sigma_z(t)$ in this short period of time around t, and replacing the upper bound of the integral, $t - t_0$ by ∞. Then the system variables can be taken out of the integrand, and

$$\frac{d}{dt}\tilde{\sigma} = \sum_{\mathbf{k},\lambda} g^2_{\mathbf{k},\lambda}\, 2\sigma_z(t)\tilde{\sigma}(t) \int_0^\infty \mathrm{d}\tau\, e^{-i(\omega-\omega_A)\tau} + \xi(t) , \tag{3.12a}$$

$$\frac{d}{dt}\sigma_z = -\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2 \left(\tilde{\sigma}^\dagger(t)\tilde{\sigma}(t) \left(\int_0^\infty \mathrm{d}\tau e^{-i(\omega-\omega_A)\tau} \right) + \tilde{\sigma}^\dagger(t)\tilde{\sigma}(t) \left(\int_0^\infty \mathrm{d}\tau e^{i(\omega-\omega_A)\tau} \right) \right)$$
$$- \left(\sigma_z(t) + \frac{1}{2} \right) \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2 \left(\int_{-\infty}^\infty \mathrm{d}\tau e^{-i(\omega-\omega_A)\tau} \right) + \xi_z(t) \ . \quad (3.12b)$$

In these equations the system variables occur only at the actual time t, i.e., there is no memory effect, and this is why the name 'Markov' approximation. In fact, the radiation field modes store the history of the evolution for an extremely short time, which is called the reservoir correlation time scale (τ_c).

The τ integral can be carried out by using the identity for distributions:

$$\int_0^\infty \mathrm{d}\tau e^{-i(\omega-\omega_A)\tau} = -i\mathrm{P}\frac{1}{\omega-\omega_A} + \pi\delta(\omega-\omega_A) \ , \quad (3.13)$$

where $\mathrm{P}\frac{1}{\omega-\omega_A}$ denotes the principal value integral.

In the Markov approximation, the equations of motion for the atomic operators can finally be expressed as

$$\frac{d}{dt}\tilde{\sigma} = (-i\Delta - \gamma)\tilde{\sigma} + \xi \ , \quad (3.14a)$$

$$\frac{d}{dt}\sigma_z = -2\gamma \left(\sigma_z + \frac{1}{2} \right) + \xi_z \ , \quad (3.14b)$$

where

$$\gamma = \pi \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2 \delta(\omega-\omega_A) \ , \quad (3.15a)$$

$$\Delta = \mathrm{P} \sum_{\mathbf{k},\lambda} \frac{g_{\mathbf{k},\lambda}^2}{\omega-\omega_A} \ , \quad (3.15b)$$

the natural linewidth (half width at half of the maximum) and the vacuum-induced light shift, respectively. This latter is an uninteresting shift of the frequency since the physically observable frequency of an atomic transition already contains the vacuum shift. That is, the bare atom frequency ω_A should be renormalized so that it incorporates Δ and provides the real, measurable frequency[1].

3.3 Spontaneous emission rate

The parameter γ, besides expressing the natural linewidth, gives the rate of spontaneous emission of an excited atom into the vacuum. On taking the quantum mechanical average of Eq. (3.14b),

$$\frac{d}{dt}\langle\sigma_z\rangle = -2\gamma \left(\langle\sigma_z\rangle + \frac{1}{2} \right) \ , \quad (3.16)$$

[1]The vacuum induced light shift is manifested in the atomic spectrum when considering the difference in the shifts of different excited states. For example, the lift of the degeneracy of the $2s$ and $2p$ states in hydrogen, the *Lamb-shift*, is an important QED effect.

and considering an excited atom as the initial condition, $\langle\sigma_z(t_0)\rangle = 1/2$, the solution is

$$\langle\sigma_z(t)\rangle = -\frac{1}{2} + e^{-2\gamma(t-t_0)} \,, \tag{3.17}$$

which is an exponential decay to the ground state $\langle\sigma_z(\infty)\rangle = -1/2$. The decay rate γ, defined in Eq. (3.15), can be evaluated by using the integral form in Eq. (3.7),

$$\gamma = \pi \frac{\omega_A^2 d_{eg}^2}{16\pi^3\epsilon_0 c^3\hbar^3} \int_0^\infty \mathrm{d}\omega\omega \int_0^{2\pi} \mathrm{d}\phi \int_0^\pi \mathrm{d}\theta \sin\theta(1-\cos^2\theta)\delta(\omega-\omega_A) \tag{3.18}$$

which leads to

$$\boxed{\gamma = \frac{\omega_A^3 d_{eg}^2}{6\pi c^3\epsilon_0\hbar} \,.} \tag{3.19}$$

This is one of the fundamental results of quantum electrodynamics. Note that this expression permits us to express the transition dipole moment d_{eg} in terms of the experimentally observable natural linewidth γ.

3.4 Quantum noise correlation

The operator equations in Eq. (3.14) include dissipation, i.e., the terms associated with spontaneous emission, and quantum fluctuations. These latter can be characterized by the two-time correlation functions $\left\langle \xi(t_1)\xi^\dagger(t_2)\right\rangle$. We can directly calculate them from the definition,

$$\begin{aligned}
\left\langle \xi(t_1)\xi^\dagger(t_2)\right\rangle &= \sum_{\mathbf{k},\lambda}\sum_{\mathbf{k}',\lambda'} g_{\mathbf{k},\lambda}g_{\mathbf{k}',\lambda'} e^{-i(\omega-\omega_A)t_1} e^{i(\omega'-\omega_A)t_2} 4\langle\sigma_z(t_1)\tilde{a}_{\mathbf{k},\lambda}(t_0)\tilde{a}^\dagger_{\mathbf{k}',\lambda'}(t_0)\sigma_z(t_2)\rangle \\
&= \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2 e^{-i(\omega-\omega_A)(t_1-t_2)} 4\langle\sigma_z(t_1)\sigma_z(t_2)\rangle \\
&+ \sum_{\mathbf{k},\lambda}\sum_{\mathbf{k}',\lambda'} g_{\mathbf{k},\lambda}g_{\mathbf{k}',\lambda'} e^{-i(\omega-\omega_A)t_1} e^{i(\omega'-\omega_A)t_2} 4\langle\sigma_z(t_1)\tilde{a}^\dagger_{\mathbf{k}',\lambda'}(t_0)\tilde{a}_{\mathbf{k},\lambda}(t_0)\sigma_z(t_2)\rangle \\
&= 4\gamma\langle\sigma_z(t_1)\sigma_z(t_2)\rangle\delta(t_1-t_2) \\
&+ \sum_{\mathbf{k},\lambda}\sum_{\mathbf{k}',\lambda'} g_{\mathbf{k},\lambda}g_{\mathbf{k}',\lambda'} e^{-i(\omega-\omega_A)t_1} e^{i(\omega'-\omega_A)t_2} 4\langle\Big[\sigma_z(t_1), \tilde{a}^\dagger_{\mathbf{k}',\lambda'}(t_0)\Big]\,[\tilde{a}_{\mathbf{k},\lambda}(t_0), \sigma_z(t_2)]\rangle
\end{aligned} \tag{3.20}$$

The evaluation of the commutators in the last line is not trivial because the operators are taken at different times. We can express $\tilde{a}_{\mathbf{k},\lambda}(t_0)$ in terms of the field amplitude at time t_2 by using the formal result Eq. (3.4) 'backward':

$$\begin{aligned}
&\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} e^{-i(\omega-\omega_A)t_1}\,[\tilde{a}_{\mathbf{k},\lambda}(t_0), \sigma_z(t_2)] = \\
&\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} e^{-i(\omega-\omega_A)t_1} \left([\tilde{a}_{\mathbf{k},\lambda}(t_2), \sigma_z(t_2)] - \int_0^{t_2-t_0} g_{\mathbf{k},\lambda}\,[\tilde{\sigma}(t_2-\tau), \sigma_z(t_2)]\, e^{i(\omega-\omega_A)(t_2-\tau)} d\tau \right) \,.
\end{aligned} \tag{3.21}$$

The first, equal-time commutator vanishes, the second term leads to

$$-\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2 \int_0^{t_2-t_0} e^{i(\omega-\omega_A)(t_2-t_1-\tau)} \left[\tilde{\sigma}(t_2-\tau), \sigma_z(t_2)\right] d\tau = \\ -\gamma \left[\tilde{\sigma}(t_1), \sigma_z(t_2)\right] \Theta(t_2-t_1) \ . \quad (3.22)$$

This result can be inserted into the correlation function above,

$$\left\langle \xi(t_1)\xi^\dagger(t_2)\right\rangle = \gamma\delta(t_1-t_2) + \gamma^2\Theta(t_2-t_1)\Theta(t_1-t_2) \ . \quad (3.23)$$

The second term is negligible since the support of the δ-function is the reservoir correlation time, τ_c, and $1/\tau_c \gg \gamma$.

Chapter 4

Dipole radiation

In the previous chapter we discussed the back action of the field radiated by the atomic dipole on the evolution of the dipole itself. This effect was incorporated in a simple decay process within the Markov approximation, which leads to a differential equation for the atomic operators that are independent of the electric field. In the following, we will calculate the radiated electric field and how this field interacts with an other dipole.

4.1 Electric field of a dipole source

From Eq. (1.60), the quantized electric field is

$$\hat{\mathbf{E}}_{\perp}(\mathbf{R},t) = i\sum_{\mathbf{k},\lambda}\sqrt{\frac{\hbar\omega}{2\epsilon_0 L^3}}\mathbf{e}_{\lambda}\left(\hat{a}_{\mathbf{k},\lambda}(t)e^{i\mathbf{k}\mathbf{R}} - \text{H. c.}\right) \ , \tag{4.1}$$

which can be separated to free field and dipole radiated field components, according to Eq. (3.4). The dipole radiated field mode amplitudes are

$$a^{(\text{dip})}_{\mathbf{k},\lambda} = e^{-i\omega_A t}g_{\mathbf{k},\lambda}\int_0^t \mathrm{d}t'\tilde{\sigma}(t')e^{i(\omega_A-\omega)(t-t')} \ , \tag{4.2}$$

where we transformed back from interaction to normal (Heisenberg) picture, and the time origin is $t_0 = 0$ for simplicity. The positive frequency part of the dipole radiated electric field is

$$\hat{\mathbf{E}}^{(+)}_{\text{dip}}(\mathbf{R},t) = \frac{i\,e^{-i\omega_A t}}{2\epsilon_0(2\pi c)^3}\int_0^{\infty}\mathrm{d}\omega\,\omega^3\int\mathrm{d}\Omega\left(1-\frac{\mathbf{k}\circ\mathbf{k}}{k^2}\right)\mathbf{d}_{eg}e^{i\mathbf{k}\mathbf{R}}\int_0^t\mathrm{d}t'\tilde{\sigma}(t')e^{i(\omega_A-\omega)(t-t')} \ , \tag{4.3}$$

where the summation over the polarization is performed by means of the identity

$$\sum_{\lambda}\mathbf{e}_{\mathbf{k},\lambda}(\mathbf{e}_{\mathbf{k},\lambda}\mathbf{u}) = \sum_{\lambda}(\mathbf{e}_{\mathbf{k},\lambda}\circ\mathbf{e}_{\mathbf{k},\lambda})\mathbf{u} = \left(1-\frac{\mathbf{k}\circ\mathbf{k}}{k^2}\right)\mathbf{u} \ , \tag{4.4}$$

for arbitrary vector $\mathbf{u}$. Fixing the z axis into the direction of the position $\mathbf{R}$, and using the usual Euler angles θ, ϕ for the wave vector $\mathbf{k}$, the above projector can be written

into the matrix form in cartesian basis

$$1-\frac{\mathbf{k}\circ\mathbf{k}}{k^2}=\begin{pmatrix}1-\sin^2\theta\cos^2\phi & -\sin^2\theta\cos\phi\sin\phi & -\sin\theta\cos\theta\cos\phi\\ -\sin^2\theta\cos\phi\sin\phi & 1-\sin^2\theta\sin^2\phi & -\sin\theta\cos\theta\sin\phi\\ -\sin\theta\cos\theta\cos\phi & \sin\theta\cos\theta\sin\phi & 1-\cos^2\theta\end{pmatrix} \tag{4.5}$$

The angular integral $\int_0^{2\pi}\mathrm{d}\phi$ diminishes all the matrix elements containing $\cos\phi$ and $\sin\phi$ in the first power. Only the diagonal elements survive, however, the matrix is not isotrope. The zz element can be picked with the operator $\hat{\mathbf{R}}\circ\hat{\mathbf{R}}$, where $\hat{\mathbf{R}}$ is the unit vector in the direction of $\mathbf{R}$. Similarly, the xx and yy elements are taken out by the operator $(1-\hat{\mathbf{R}}\circ\hat{\mathbf{R}})$. Thus, one obtains

$$\begin{aligned}\hat{\mathbf{E}}^{(+)}_{\rm dip}(\mathbf{R},t)&=\frac{i\,e^{-i\omega_A t}}{2\epsilon_0(2\pi)^2c^3}\int_0^\infty\mathrm{d}\omega\,\omega^3\int_{-1}^1\mathrm{d}(\cos\theta)\\ &\left[(1-\hat{\mathbf{R}}\circ\hat{\mathbf{R}})\left(\frac{1}{2}+\frac{1}{2}\cos^2\theta\right)+\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\left(1-\cos^2\theta\right)\right]\mathbf{d}_{eg}e^{ikR\cos\theta}\int_0^t\mathrm{d}t'(\ldots)\\ &=\frac{i\,e^{-i\omega_A t}}{4\epsilon_0(2\pi)^2c^3}\int_0^\infty\mathrm{d}\omega\,\omega^3\int_{-1}^1\mathrm{d}(\cos\theta)\\ &\qquad\left[\left(1+\cos^2\theta\right)+\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\left(1-3\cos^2\theta\right)\right]\mathbf{d}_{eg}e^{ikR\cos\theta}\int_0^t\mathrm{d}t'(\ldots)\\ &=\frac{i\,e^{-i\omega_A t}}{4\epsilon_0(2\pi)^2c^3}\int_0^\infty\mathrm{d}\omega\,\omega^3\\ &\times\left[\left(1+\frac{\partial^2}{\partial(ikR)^2}\right)+\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\left(1-3\frac{\partial^2}{\partial(ikR)^2}\right)\right]\mathbf{d}_{eg}\frac{e^{ikR}-e^{-ikR}}{ikR}\int_0^t\mathrm{d}t'(\ldots)\,,\end{aligned} \tag{4.6}$$

where the differentiation with respect to ikR appeared to substitute $\cos\theta$ in the polynomials. The broadband frequency integral includes an exponential function,

$$\int_0^\infty\mathrm{d}\omega\omega e^{i(\omega_A-\omega)(t-t'\pm R/c)}\propto\delta(t-t'\pm R/c)\,, \tag{4.7}$$

in accordance with Eq. (3.10). Since $t'<t$, only the $-$ sign gives non-zero contribution. The differentiation is performed as

$$\frac{\partial^2}{\partial x^2}\frac{e^x}{x}=\frac{e^x}{x}\left(1-\frac{2}{x}+\frac{2}{x^2}\right)\,, \tag{4.8}$$

with $x=ikR$. Continuing the above transformations,

$$\begin{aligned}\hat{\mathbf{E}}^{(+)}_{\rm dip}(\mathbf{R},t)&=\frac{e^{-i\omega_A t}}{4\epsilon_0(2\pi)^2c^2R}\int_0^\infty\mathrm{d}\omega\,\omega^2\Big[1+\left(1-\frac{2}{ikR}+\frac{2}{(ikR)^2}\right)\\ &\qquad+\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\left(1-3\left(1-\frac{2}{ikR}+\frac{2}{(ikR)^2}\right)\right)\Big]\mathbf{d}_{eg}\\ &\qquad\times\int_0^t\mathrm{d}t'\tilde{\sigma}(t')e^{i(\omega_A-\omega)(t-t'-R/c)}e^{i\omega_A R/c}\\ &=\frac{e^{-i\omega_A(t-R/c)}}{2\epsilon_0(2\pi)^2c^2R}\int_0^\infty\mathrm{d}\omega\,\omega^2\,\tilde{\sigma}(t-R/c)2\pi\delta(\omega_A-\omega)\\ &\left[\left(1-\frac{1}{ikR}+\frac{1}{(ikR)^2}\right)-\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\left(1-\frac{3}{ikR}+\frac{3}{(ikR)^2}\right)\right]\mathbf{d}_{eg}\end{aligned} \tag{4.9}$$

In this step we have used the Markov approximation to evaluate the double integral $\int_0^\infty \mathrm{d}\omega \int_0^t \mathrm{d}t'$. According to Eq. (4.7), the variation of $\tilde{\sigma}$ in the time integral can be neglected. $\tilde{\sigma}(t - R/c)$ can be taken out of the time integral and the remaining integral can be carried out. Because of the retardation, the relevant time $t' = t - R/c$ is now well within the integral range $[0, t]$. Therefore, dislike Eq. (3.13) no imaginary part appears and the real part, the Dirac-delta, is doubled. Note that $\tilde{\sigma}(t - R/c)e^{-i\omega_A(t-R/c)} = \sigma(t-R/c)$, i.e., the exponential factor just transforms back into normal picture from the interaction one.

The final result for the positive frequency part of the electric field (the total field is twice the real part of this)

$$\hat{\mathbf{E}}^{(+)}_{\mathrm{dip}}(\mathbf{R}, t) = \frac{1}{\epsilon_0}\underline{\mathbf{G}}(\mathbf{R}, 0, t)\mathbf{P}^{(+)}(0, t - R/c) \;, \tag{4.10a}$$

where $\mathbf{P}^{(+)}(\mathbf{r}, t) = \mathbf{d}_{eg}\sigma(t)$ is the atomic dipole at the position $\mathbf{r}$, being the source of radiation, and the Green-function was obtained as

$$\underline{\mathbf{G}}(\mathbf{R}, 0, t) = \frac{k_A^2 e^{ik_A R}}{4\pi R}\left[\left(1 - \hat{\mathbf{R}} \circ \hat{\mathbf{R}}\right)\left(1 - \frac{1}{ikR} + \frac{1}{(ikR)^2}\right) + 2\hat{\mathbf{R}} \circ \hat{\mathbf{R}}\left(\frac{1}{ikR} - \frac{1}{(ikR)^2}\right)\right] , \tag{4.10b}$$

where $k_A = \omega_A/c$. The first term in the square bracket presents the tangentially polarised part of the field (it is in the xy plane, perpendicular to the axis of propagation), and the second term gives the radially polarised part of the field. This latter is purely a near-field decaying fast with the distance kR. The tangential part also has near-field components present in a few-wavelength vicinity of the dipole source. The propagating field is a purely transverse spherical wave, and the $\left(1 - \hat{\mathbf{R}} \circ \hat{\mathbf{R}}\right)\mathbf{d}_{eg}$ leads to the well-known $\sin^2\theta$ pattern of the dipole radiation field in the far-field limit.

The Green-function has an $1/R^3$ singularity in the origin. Its volume integral in the full space, however, can be calculated provided the angular part is integrated first,

$$\begin{aligned}\int \mathrm{d}\mathbf{R}^3 \underline{\mathbf{G}}(\mathbf{R}, 0) &= \frac{k_A^2}{4\pi}\int \mathrm{d}R\, R e^{ik_A R} \\ &\quad \left[4\pi\left(1 - \frac{1}{ikR} + \frac{1}{(ikR)^2}\right) - 2\pi\frac{2}{3}\left(1 - \frac{3}{ikR} + \frac{3}{(ikR)^2}\right)\right] \\ &= \frac{2}{3}\int_0^\infty \mathrm{d}(k_A R)\, k_A R e^{ik_A R} = \frac{2}{3}\left\{[xe^{ix}]_0^{(1+i\epsilon)\infty} - \frac{1}{i}\int_0^{(1+i\epsilon)\infty} \mathrm{d}x e^{ix}\right\} \\ &= -\frac{2}{3}\,. \end{aligned} \tag{4.11}$$

When processes in the vicinity of the atom are of importance (and using a gauge better describing the atomic length scale), the Green-function, derived above, is complemented by $2/3\,\delta(\mathbf{R})$ so that the total integral vanish.

4.2 The resonant dipole-dipole interaction

Let us consider the Hamiltonian describing the interaction of many atomic dipoles with the electromagnetic vacuum

$$\mathcal{H} = \sum_i \hbar\omega_A \sigma_z^{(i)} + \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k},\lambda} a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} + i\hbar \sum_i \sum_{\mathbf{k},\lambda} g^{(i)}_{\mathbf{k},\lambda} \left(a^\dagger_{\mathbf{k},\lambda} \sigma_i e^{-i\mathbf{k}\mathbf{R}_i} - \sigma_i^\dagger a_{\mathbf{k},\lambda} e^{i\mathbf{k}\mathbf{R}_i} \right) . \quad (4.12)$$

In interaction picture

$$\mathcal{H}_I = i\hbar \sum_i \sum_{\mathbf{k},\lambda} g^{(i)}_{\mathbf{k},\lambda} \left(a^\dagger_{\mathbf{k},\lambda} \sigma_i e^{-i\mathbf{k}\mathbf{R}_i} e^{i(\omega-\omega_A)t} - \sigma_i^\dagger a_{\mathbf{k},\lambda} e^{i\mathbf{k}\mathbf{R}_i} e^{-i(\omega-\omega_A)t} \right) . \quad (4.13)$$

Take an arbitrary physical quantity $\mathcal{Q}$ which depends on the atomic operators σ. Its Heisenberg-equation of motion in the interaction picture reads

$$\dot{\mathcal{Q}} = \frac{1}{i\hbar} [\mathcal{Q}, \mathcal{H}_I] = \sum_i \sum_{\mathbf{k},\lambda} g^{(i)}_{\mathbf{k},\lambda} \left(a^\dagger_{\mathbf{k},\lambda} e^{-i\mathbf{k}\mathbf{R}_i} e^{i(\omega-\omega_A)t} [\mathcal{Q}, \sigma_i] - \left[\mathcal{Q}, \sigma_i^\dagger\right] a_{\mathbf{k},\lambda} e^{i\mathbf{k}\mathbf{R}_i} e^{-i(\omega-\omega_A)t} \right) . \quad (4.14)$$

Substituting the form of $a_{\mathbf{k},\lambda}(t)$ in which the free and the radiated fields are separated into the equation of motion leads to

$$\begin{aligned} \dot{\mathcal{Q}} = \sum_i \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(a^\dagger_{\mathbf{k},\lambda}(0)\, e^{-i\mathbf{k}\mathbf{R}_i} [\mathcal{Q}, \sigma_i] - \left[\mathcal{Q}, \sigma_i^\dagger\right] a_{\mathbf{k},\lambda}(0)\, e^{i\mathbf{k}\mathbf{R}_i} \right) \\ + \sum_{i,j} \sum_{\mathbf{k},\lambda} g^{(i)}_{\mathbf{k},\lambda} g^{(j)}_{\mathbf{k},\lambda} \Bigg(e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R_j})} \int_0^t \mathrm{d}t' \tilde{\sigma}_j^\dagger(t') e^{i(\omega-\omega_A)(t-t')} [\mathcal{Q}, \sigma_i] \\ - e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R_j})} \left[\mathcal{Q}, \sigma_i^\dagger\right] \int_0^t \mathrm{d}t' \tilde{\sigma}_j(t') e^{-i(\omega-\omega_A)(t-t')} \Bigg) . \end{aligned} \quad (4.15)$$

The first term is noise and we do not consider it here. We will deal with only the second term in the double sum over (i, j), since the evaluation of the first one follows analogously.

$$\begin{aligned} - \sum_{i,j} \left[\mathcal{Q}, \sigma_i^\dagger\right] \frac{1}{2\epsilon_0 \hbar L^3} \frac{L^3}{(2\pi\, c)^3} \int \mathrm{d}\omega \omega^3 \int \mathrm{d}\Omega \sum_\lambda (\mathbf{e}_{\mathbf{k},\lambda} \mathbf{d}^{(i)})(\mathbf{e}_{\mathbf{k},\lambda} \mathbf{d}^{(j)}) e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R_j})} \\ \int_0^t \mathrm{d}t' \tilde{\sigma}_j(t') e^{-i(\omega-\omega_A)(t-t')} \\ = - \sum_{i,j} \left[\mathcal{Q}, \sigma_i^\dagger\right] \mathbf{d}^{(i)} \frac{1}{2\epsilon_0 \hbar (2\pi\, c)^3} \int \mathrm{d}\omega\, \omega^3 \int \mathrm{d}\Omega \left(1 - \frac{\mathbf{k} \circ \mathbf{k}}{k^2} \right) \mathbf{d}^{(j)} e^{i\mathbf{k}\mathbf{R}} \\ \int_0^t \mathrm{d}t' \tilde{\sigma}_j(t') e^{-i(\omega-\omega_A)(t-t')} , \end{aligned} \quad (4.16)$$

where $\mathbf{R} = \mathbf{R}_i - \mathbf{R_j}$. This is very similar to the form of the electric dipole radiation field given in Eq. (4.3), since here the effect of the source field originating from the dipole $\tilde{\sigma}_j$ is calculated on the remote dipole $\tilde{\sigma}_i^\dagger$. Next, we follow the steps of Eq. (4.6). In the

reference frame with $\mathbf{R}$ pointing in the $\hat{z}$ direction, we can first perform the azimuthal part of the angular integral. Then using the derivative with respect to ikR to replace $\cos\theta$, the remaining $\cos\theta$ dependence can be integrated out. We get

$$-\sum_{i,j}\left[\mathcal{Q},\sigma_i^\dagger\right]\mathbf{d}^{(i)}\frac{1}{4\epsilon_0\hbar(2\pi)^2\,c^3}\int \mathrm{d}\omega\,\omega^3$$
$$\left[\left(1+\frac{\partial^2}{\partial(ikR)^2}\right)+\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\left(1-3\frac{\partial^2}{\partial(ikR)^2}\right)\right]\mathbf{d}^{(j)}\frac{e^{ikR}-e^{-ikR}}{ikR}\int_0^t \mathrm{d}t'\tilde{\sigma}_j(t')e^{-i(\omega-\omega_A)(t-t')}\,. \tag{4.17}$$

Here we deviate from the derivation that led us to the dipole radiation pattern through the approximation in Eq. (4.9). There, we assumed large enough kR which pushed the relevant contribution of the double frequency and time integrals from $t'\approx t$ to $t'\approx t-R/c$, indicating a significant retardation effect. Here the atoms can sit close enough that during the reservoir correlation time (the inverse of the bandwidth) the light travels much longer than the interatomic distance. Therefore we need to keep both $e^{\pm ikR}$ terms, and we perform first the time integral. It is still true that non-vanishing contribution to the double integral over the frequency space and over the time domain originates from the region $t'\approx t\pm kR$. Of course, the variation of $\tilde{\sigma}(t')$ can safely be neglected during this very short time and, in the spirit of the Markoff-approximation, it can be extracted from the integral:

$$\int_0^t \mathrm{d}t'\tilde{\sigma}_j(t')e^{-i(\omega-\omega_A)(t-t')}\approx\tilde{\sigma}_j(t)\left(-i\mathrm{P}\frac{1}{\omega-\omega_A}+\pi\delta(\omega-\omega_A)\right)\,. \tag{4.18}$$

The differentiation rule Eq. (4.8) leads us to

$$-\frac{3\gamma}{2\pi\omega_A^3}\sum_{i,j}\left[\mathcal{Q},\sigma_i^\dagger\right]\left(\mathbf{d}^{(i)}/d\right)\int \mathrm{d}\omega\,\omega^3\left(-i\mathrm{P}\frac{1}{\omega-\omega_A}+\pi\delta(\omega-\omega_A)\right)$$
$$\left[\left(\frac{\sin kR}{kR}+\frac{\cos kR}{(kR)^2}-\frac{\sin kR}{(kR)^3}\right)-\left(\frac{\sin kR}{kR}+3\frac{\cos kR}{(kR)^2}-3\frac{\sin kR}{(kR)^3}\right)\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\right]\left(\mathbf{d}^{(j)}/d\right)\,, \tag{4.19}$$

where we use $\gamma=\omega_A^3d^2/(6\epsilon_0\pi\hbar c^2)$, half of the spontaneous emission rate, and d is the dipole moment modulus. The complicated expression in the square bracket accounts for the geometry (the direction and distance between the two atoms (i) and (j)) and the polarizations. After integrating over ω, one gets the form

$$\gamma\sum_{i,j}\left[\mathcal{Q},\sigma_i^\dagger\right]\sigma_j\mathbf{d}^{(i)}/d\left(i\overleftrightarrow{\beta}(\mathbf{R})-\overleftrightarrow{\alpha}(\mathbf{R})\right)\mathbf{d}^{(j)}/d\,. \tag{4.20}$$

The first term in the double sum of Eq. (4.15) results, after interchanging the summation indices i,j, in

$$-\gamma\sum_{i,j}\sigma_i^\dagger\left[\mathcal{Q},\sigma_j\right]\mathbf{d}^{(i)}/d\left(i\overleftrightarrow{\beta}(\mathbf{R})-\overleftrightarrow{\alpha}(\mathbf{R})\right)\mathbf{d}^{(j)}/d\,. \tag{4.21}$$

On combining these two terms, the evolution of the quantum average of the quantity $\mathcal{Q}$ is given by

$$\dot{\mathcal{Q}} = -\gamma \sum_{i,j} \Bigg(\left(\mathcal{Q}\sigma_i^\dagger \sigma_j + \sigma_i^\dagger \sigma_j \mathcal{Q} - 2\sigma_i^\dagger \mathcal{Q} \sigma_j \right) \frac{\mathbf{d}^{(i)}}{d} \overleftrightarrow{\alpha}(\mathbf{R}) \frac{\mathbf{d}^{(j)}}{d} \\ - i \left(\mathcal{Q}\sigma_i^\dagger \sigma_j - \sigma_i^\dagger \sigma_j \mathcal{Q} \right) \frac{\mathbf{d}^{(i)}}{d} \overleftrightarrow{\beta}(\mathbf{R}) \frac{\mathbf{d}^{(j)}}{d} \Bigg) . \quad (4.22)$$

We took the average so that to get rid of the noise terms involving the free field amplitudes $a_{\mathbf{k},\lambda}(t_0)$. The first part descibes dissipation by means of the usual terms in a quantum Master-equation. These terms cannot be embedded into a Hamiltonian formalism; they inherently correspond to the irreversible dissipation in the system. It is interesting to note that the atoms do not feel independent reservoirs. If they are close enough, i.e., within a wavelength, the decay process is collective. This is the basis for the effect of superradiance, for example. The dissipative part α belongs to the Dirac-$\delta(\omega - \omega_A)$, and can be readily obtained

$$\overleftrightarrow{\alpha}(\mathbf{R}) = \frac{3}{2} \left[\left(1 - \hat{\mathbf{R}} \circ \hat{\mathbf{R}} \right) \frac{\sin k_A R}{k_A R} + \left(1 - 3\hat{\mathbf{R}} \circ \hat{\mathbf{R}} \right) \left(\frac{\cos k_A R}{(k_A R)^2} - \frac{\sin k_A R}{(k_A R)^3} \right) \right] . \quad (4.23)$$

The electromagnetic field in vacuum state mediates another type of interaction between atoms, this is represented by the second part of Eq. (4.22), which can be well incorporated into an effective Hamiltonian:

$$V_{\mathrm{dip-dip}} = -\gamma \sum_{i,j} \sigma_i^\dagger \frac{\mathbf{d}^{(i)}}{d} \overleftrightarrow{\beta}(\mathbf{R}) \frac{\mathbf{d}^{(j)}}{d} \sigma_j . \quad (4.24)$$

The conservative potential part originates from the principal value integral. Let us see how to perform integrals like

$$\mathrm{P} \int \mathrm{d}\omega \frac{\sin kR}{\omega - \omega_A} f(\omega) = \frac{1}{2i} \mathrm{P} \int \mathrm{d}x \frac{e^{ix} - e^{-ix}}{x - x_A} \tilde{f}(x) \\ = \frac{e^{ix_A}}{2i} \mathrm{P} \int \mathrm{d}x \frac{e^{ix}}{x} \tilde{f}(x) - \frac{e^{-ix_A}}{2i} \mathrm{P} \int \mathrm{d}x \frac{e^{-ix}}{x} \tilde{f}(x) , \quad (4.25)$$

where $f(\omega)$ is an analytic function of ω (a power functions ω, ω^2, and ω^3 in the specific cases). Using analytic continuation in the complex plane,

$$\mathrm{P} \int \mathrm{d}x \frac{e^{ix}}{x} = \lim_{R\to\infty, \epsilon\to 0} \left(\oint - \int_S - \int_{S'} \right) \mathrm{d}z \frac{e^{iz}}{z} \tilde{f}(z) \\ = 0 - 0 - \lim_{\epsilon\to 0} i \int_\pi^0 \mathrm{d}\varphi \exp\left\{ i\epsilon e^{i\varphi} \right\} \tilde{f}(\epsilon e^{i\varphi}) = i\pi \tilde{f}(0) . \quad (4.26)$$

The other term contains the complex conjugate, from which follows

$$\mathrm{P} \int \mathrm{d}\omega \frac{\sin kR}{\omega - \omega_A} f(\omega) = \pi \cos k_A R f(\omega_A) . \quad (4.27a)$$

Similarly,

$$\mathrm{P}\int \mathrm{d}\omega \frac{\cos kR}{\omega-\omega_A} f(\omega) = \pi \sin k_A R f(\omega_A)\ . \tag{4.27b}$$

After transforming all terms, the final result is

$$\overleftrightarrow{\beta}(\mathbf{R}) = \frac{3}{2}\left[\left(1-\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\right)\frac{\cos k_A R}{k_A R} - \left(1-3\hat{\mathbf{R}}\circ\hat{\mathbf{R}}\right)\left(\frac{\sin k_A R}{(k_A R)^2}+\frac{\cos k_A R}{(k_A R)^3}\right)\right]\ . \tag{4.28}$$

Chapter 5

The optical Bloch equations

Let us consider a single immobile atom in the free electromagnetic radiation field. The atom is driven by a quasi-resonant, single-mode laser field. The laser field amplitude is not a dynamic variable but a fixed complex number (intensity and phase). The system Hamiltonian reads

$$H = H_0 + H_L + H_{\mathrm{AF}} \ , \tag{5.1a}$$

$$H_0 = H_A + H_F = \hbar\omega_A \sigma^\dagger\sigma + \sum_{\mathbf{k},\lambda} \hbar\omega a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} \ , \tag{5.1b}$$

$$H_{\mathrm{AF}} = -i\hbar \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(\sigma^\dagger a_{\mathbf{k},\lambda} e^{-i\mathbf{k}\mathbf{R}_A} - a^\dagger_{\mathbf{k},\lambda} \sigma e^{i\mathbf{k}\mathbf{R}_A} \right) \ , \tag{5.1c}$$

$$H_L = -\mathbf{d}\mathbf{E}_L(\mathbf{R}_A, t) \ . \tag{5.1d}$$

The laser electric field is

$$\mathbf{E}_L(\mathbf{R}, t) = \epsilon(\mathbf{R}) \mathcal{E}_L(\mathbf{R}) \cos\left(\omega_L t + \Phi(\mathbf{R})\right) \ , \tag{5.2}$$

where the polarization $\epsilon(\mathbf{R})$, the amplitude $\mathcal{E}_L(\mathbf{R})$, and the phase $\Phi(\mathbf{R})$ vary in space. This is a general description of a single-mode plane wave, including standing waves ($\mathcal{E}_L(\mathbf{R}) = \cos(\mathbf{k}\mathbf{R})$ and $\Phi(\mathbf{R}) = 0$) or propagating plane waves ($\mathcal{E}_L(\mathbf{R}) = 1$ and $\Phi(\mathbf{R}) = \mathbf{k}\mathbf{R}$). In the rotating wave approximation, the dipole coupling term can be written as

$$H_L = -\hbar\Omega(\mathbf{R}_A) \left(\sigma^\dagger e^{-i(\omega_L t + \Phi(\mathbf{R}_A))} + \sigma e^{i(\omega_L t + \Phi(\mathbf{R}_A))} \right) \ , \tag{5.3}$$

where the atom-laser interaction strength is described by the spatially dependent Rabi frequency

$$\Omega(\mathbf{R}_A) = \left(\epsilon(\mathbf{R}_A)\mathbf{d}_{eg}\right) \mathcal{E}_L(\mathbf{R}_A)/2\hbar \ . \tag{5.4}$$

A general laser mode, which is not necessarily a plane wave, e.g. they are frequently Gaussian modes in the lab, can easily included in this framework by properly defining the Rabi frequency. The coordinate system will be set to have its origin at the fixed position of the atom, $\mathbf{R}_A = 0$. We will denote $\Omega(\mathbf{R}_A = 0) = \Omega$ and $\Phi(\mathbf{R}_A = 0) = \Phi$.

The Heisenberg equations of motion are

$$\dot{a}_{\mathbf{k},\lambda} = -i\omega a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda}\sigma \ , \tag{5.5a}$$

$$\dot{\sigma} = -i\omega_A\sigma - i2\sigma_z\Omega e^{-i(\omega_L t+\Phi)} + 2\sigma_z\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}a_{\mathbf{k},\lambda} \ , \tag{5.5b}$$

$$\dot{\sigma}_z = i\Omega\left(\sigma^\dagger e^{-i(\omega_L t+\Phi)} - \sigma e^{i\omega t}\right) - \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}\left(\sigma^\dagger a_{\mathbf{k},\lambda} + a^\dagger_{\mathbf{k},\lambda}\sigma\right) \tag{5.5c}$$

The vacuum field contribution is eliminated from the dynamics and is incorporated into loss terms and fluctuations, as it was discussed in the previous courses. These latter disapper when taking the quantum mechanical average of the operators:

$$\langle\dot{\sigma}\rangle = -(i\omega_A+\gamma)\langle\sigma\rangle - 2i\Omega\langle\sigma_z\rangle e^{-i(\omega_L t+\Phi)} \ , \tag{5.6a}$$

$$\langle\dot{\sigma}_z\rangle = i\Omega\left(\left\langle\sigma^\dagger\right\rangle e^{-i(\omega_L t+\Phi)} - \langle\sigma\rangle e^{i(\omega_L t+\Phi)}\right) - 2\gamma\left(\langle\sigma_z\rangle + \frac{1}{2}\right) \ . \tag{5.6b}$$

Let us transform the variables into a frame rotating at the frequency ω_L of the driving laser in order to eliminate the fast oscillation. One gets the Bloch equations,

$$\left\langle\dot{\tilde{\sigma}}\right\rangle = (i\Delta_A-\gamma)\langle\tilde{\sigma}\rangle - 2i\Omega e^{-i\Phi}\langle\sigma_z\rangle \ , \tag{5.7a}$$

$$\langle\dot{\sigma}_z\rangle = i\Omega\left(\left\langle\tilde{\sigma}^\dagger\right\rangle e^{-i\Phi} - \langle\tilde{\sigma}\rangle e^{i\Phi}\right) - 2\gamma\left(\langle\sigma_z\rangle + \frac{1}{2}\right) \ , \tag{5.7b}$$

where the detuning is $\Delta_A = \omega_L - \omega_A$. These are first-order linear differential equations with constant coefficients, which can be easily solved. Note that the atomic polarization $\langle\tilde{\sigma}\rangle$ is coupled to the population $\langle\sigma_z\rangle$. This is the reason why, although the dynamics is given by first order differential equations, oscillatory solutions, so-called *Rabi oscillations*, occur.

There is a customary way of handling the Bloch equations in terms of real variables. Let us introduce the real and imaginary parts, u and v respectively, of the mean of the polarization operator σ in a frame

$$u = \frac{1}{2}(\langle\sigma\rangle e^{i(\omega_L t+\Phi)} + \left\langle\sigma^\dagger\right\rangle e^{-i(\omega_L t+\Phi)}) \ , \tag{5.8a}$$

$$v = \frac{1}{2i}(\langle\sigma\rangle e^{i(\omega_L t+\Phi)} - \left\langle\sigma^\dagger\right\rangle e^{-i(\omega_L t+\Phi)}) \ , \tag{5.8b}$$

$$w = \langle\sigma_z\rangle \ . \tag{5.8c}$$

One gets then

$$\dot{u} = -\Delta_A v - \gamma u \ , \tag{5.9a}$$

$$\dot{v} = \Delta_A u - \gamma v - 2\Omega w \ , \tag{5.9b}$$

$$\dot{w} = 2\Omega v - 2\gamma(w+1/2) \ . \tag{5.9c}$$

Note that the last term of the Eq. (5.9c) represents an inhomogeneous driving. Then the solution of the linear differential equation is the sum of the general solution of the homogeneous part and one special solution of the inhomogeneous part. For this latter,

a possible good choice is the *steady-state*, i.e., when $\dot{u} = \dot{v} = \dot{w} = 0$, and the variables u, v, w obey the remaining algebraic equation. There is a straightforward physical interpretation of this separation. The solution of the homogeneous part describes the transient oscillations, decaying with the rate about γ, and the system evolves into the steady state.

5.1 Transient Rabi oscillations

The homogeneous part combines two types of harmonic oscillations: (i) the one with frequency Δ_A due to the detuning between the laser and the atomic frequency, and (ii) the one with the Rabi frequency between the imaginary part of the polarization v and the population inversion w, which originates from the laser excitation. Subtracting the unit matrix times $-\gamma$ from the linear 3x3 Bloch-matrix, the remaining non-trivial part has the characteristic polinom

$$\lambda^3 + \gamma\lambda^2 + (\Omega^2 + \Delta_A^2)\lambda + \gamma\Delta_A^2 = 0 \; . \tag{5.10}$$

In order to extract the oscillation frequency of the transients, one can temporarily set the loss rate γ to zero (small). Then one gets

$$\lambda = \pm\sqrt{\Omega^2 + \Delta_A^2} \; , \quad 0 \; . \tag{5.11}$$

This is typically the frequency of the Rabi oscillations, i.e., that of the population oscillations of a two-level system driven by an external harmonic field. For non-vanishing but small γ, corrections to it can be derived systematically.

The general case is complicated mixing the Rabi frequency, the detuning and the loss rate in the real and imaginary parts of the eigenvalues. The equation can be cast in the form of $\lambda^3 + p\lambda + q$ with

$$p = \Omega^2 + \Delta_A^2 - \gamma^2/3 \text{ , and } q = \gamma/3(2\Delta_A^2 - \Omega^2 + 2\gamma^2/9) \; . \tag{5.12}$$

If $Q = (p/3)^3 + (q/2)^2 > 0$, then there is one real eigenvalue and one pair of complex conjugates.

Let us consider the special case of resonant driving, $\Delta_A = 0$. Then one of the eigenvalues is $-\gamma + 0$, the other two are

$$\lambda = -3\gamma/2 \pm \sqrt{(\gamma/2)^2 - \Omega^2} \approx -3\gamma/2 \pm i|\Omega| \; , \tag{5.13}$$

where the last transformation assumes $\Omega \gg \gamma$ (strong driving). This means three distinct frequencies, the central 'carrier' frequency itself, ω_L corresponding to $\lambda = 0$, and two sidebands $\pm\Omega$ away from the center. This is called the *Mollow-triplet*. Later we will discuss the measurable physical signal exhibiting these spectral components.

5.2 Steady-state solution

The steady-state plays a central role in processes slower than the decay rate γ. It follows straightforwardly that the population is

$$w_{\rm st} = \frac{-1/2}{1+s} \ , \tag{5.14}$$

where the *saturation* parameter is

$$s = \frac{2\Omega^2}{\Delta_A^2 + \gamma^2} \ . \tag{5.15}$$

For small saturation (weak laser intensity, $\Omega \ll \Delta_A^2 + \gamma^2$), the excited state population is about

$$\left\langle \sigma^\dagger \sigma \right\rangle = \langle \sigma_z \rangle + 1/2 \approx \frac{1}{2} - \frac{1}{2}(1-s) = \frac{s}{2} = \frac{\Omega^2}{\Delta_A^2 + \gamma^2} \ . \tag{5.16}$$

For high saturation, $s \to \infty$, the excited and ground state populations are equal. The steady-state polarization is

$$u_{\rm st} = \Omega \frac{-\Delta_A}{\Delta_A^2 + \gamma^2 + 2\Omega^2} \ , \tag{5.17a}$$

$$v_{\rm st} = \Omega \frac{\gamma}{\Delta_A^2 + \gamma^2 + 2\Omega^2} \ , \tag{5.17b}$$

The mean value of the dipole operator in the steady-state regime is given by

$$\begin{aligned} \langle \mathbf{d} \rangle = \mathbf{d}_{eg}(\langle \sigma \rangle + \left\langle \sigma^\dagger \right\rangle) &= \mathbf{d}_{eg} \left((u+iv) e^{-i(\omega_L t + \Phi)} + (u - iv) e^{i(\omega_L t + \Phi)} \right) \\ &= \frac{\mathbf{d}_{eg} \circ \mathbf{d}_{eg}}{\hbar} \Big(\frac{-\Delta_A}{\Delta_A^2 + \gamma^2 + 2\Omega^2} \epsilon \mathcal{E}_L \cos(\omega_L t + \Phi) + \\ &\quad \frac{\gamma}{\Delta_A^2 + \gamma^2 + 2\Omega^2} \epsilon \mathcal{E}_L \sin(\omega_L t + \Phi) \Big) \\ \frac{\mathbf{d}_{eg} \circ \mathbf{d}_{eg}}{\hbar} &\left(\frac{-\Delta_A}{\Delta_A^2 + \gamma^2 + 2\Omega^2} \mathbf{E}_L(\mathbf{R}_A, t) + \frac{\gamma}{\Delta_A^2 + \gamma^2 + 2\Omega^2} \mathbf{E}_L(\mathbf{R}_A, t - T/4) \right) \ , \end{aligned} \tag{5.18}$$

The atomic dipole has an in-phase and an out-of-phase component with respect to the temporal phase of the incident laser field. The proportionality factor is the susceptibility (for single atoms one often defines it as polarizability). Assuming a fixed polarization, the tensor character can be omitted and one gets

$$\chi(\omega_L) = \frac{d_{eg}^2}{\hbar \epsilon_0} \frac{\omega_A - \omega + i\gamma}{\Delta_A^2 + \gamma^2 + 2\Omega^2} \ . \tag{5.19}$$

This is not a linear susceptibility because of the Rabi frequency in the denominator. Assuming low excitation, $s \ll 1$, the susceptibility corresponds precisely to Lorentzian resonance asa function of the laser probe frequency. That is, the unsaturated atom can be considered a harmonic oscillator. For high excitation non-linear effects become important due to the saturation. Consequences of this nonlinearity will be studied in a following course.

The work done by the laser on the atom is

$$\mathcal{W}_L = \left(\frac{d}{dt}d\right)\mathbf{E}_L(\mathbf{R}_A,t) = \mathbf{d}_{eg}(\langle\dot{\sigma}\rangle + \langle\dot{\sigma^\dagger}\rangle)\mathbf{E}_L(\mathbf{R}_A,t) = \\ \mathbf{d}_{eg}\left[(\dot{u}+i\dot{v}-i\omega_L(u+iv))e^{-i(\omega_L t+\Phi)} + (\dot{u}-i\dot{v}+i\omega_L(u-iv))e^{i(\omega_L t+\Phi)}\right]\mathbf{E}_L(\mathbf{R}_A,t)\ , \tag{5.20}$$

where the time derivatives vanish in steady-state. Thus,

$$\mathcal{W}_L = \omega_L\left[2v_{\rm st}\cos(\omega_L t+\Phi) - 2i\,u_{\rm st}\sin(\omega_L t+\Phi)\right]2\hbar\Omega\cos(\omega_L t+\Phi)\ , \tag{5.21}$$

and time averaging over one optical period gives

$$\mathcal{W}_L = \hbar\omega_L\,2v\,\Omega = \hbar\omega_L\,2\gamma\,\frac{\Omega^2}{\Delta_A^2+\gamma^2+2\Omega^2} = \hbar\omega_L\,2\gamma\,\left\langle\sigma^\dagger\sigma\right\rangle \tag{5.22}$$

where the last approximation applies for the weak excitation limit (linear susceptibility). The clear physical meaning is that the work done by the laser on the atom is transmitted into the dipole radiation of the atom into the free electromagnetic modes.

5.3 Spectrum: intensity and spectral density

We will study the spectrum of the radiation field radiated by the atom into the free-space modes. As we have learned previously, the field has a dipole pattern and is given by

$$E^{(+)}(\mathbf{R},t) = \eta\sigma(t-R/c) + E_0^{(+)}(\mathbf{R},t)\ , \tag{5.23}$$

where the second term corresponds to the vacuum noise (from the initial condition), and the first atom-radiated term includes the Green-function

$$\eta = \frac{k_A^2 e^{ik_A R}}{4\pi\epsilon_0 R}\left[\left(1-\frac{\mathbf{R}\circ\mathbf{R}}{R^2}\right)\left(1-\frac{1}{ik_A R}+\frac{1}{(ik_A R)^2}\right)+2\frac{\mathbf{R}\circ\mathbf{R}}{R^2}\left(\frac{1}{ik_A R}-\frac{1}{(ik_A R)^2}\right)\right]\mathbf{d}_{eg} \tag{5.24}$$

The calculation of measurable spectral quantities involves the correlation function

$$C_1(t,\tau) = \left\langle E^{(-)}(\mathbf{R},t+\tau)E^{(+)}(\mathbf{R},t)\right\rangle \tag{5.25}$$

Thanks to working in normal order, $E_0^{(+)}(\mathbf{R},t)$ gives no contribution to the second-order correlation function C_1. We will consider two quantities, the mean intensity $I(t)$ and the spectral density $\mathcal{I}(\omega)$,

$$I(t) = C_1(t,0) \tag{5.26}$$

$$\mathcal{I}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau\, e^{-i\omega\tau}C_1(t,\tau)\ , \tag{5.27}$$

respectively.

In the steady-state, the correlation function does not depend on t. The intensity is simply $\eta^2\langle\sigma^\dagger\sigma\rangle$, which is proportional to the population in the excited state. It can be split into a coherent and an incoherent part:

$$I = \eta^2\left(\langle\sigma^\dagger\rangle\langle\sigma\rangle + \langle\delta\sigma^\dagger\,\delta\sigma\rangle\right) \tag{5.28}$$

where the coherent part is

$$\frac{1}{\eta^2} I_{\rm coh} = |\langle \sigma \rangle|^2 = |\langle (u_{\rm st} + i v_{\rm st}) \rangle|^2 = u_{\rm st}^2 + v_{\rm st}^2 = \frac{1}{2} \frac{s}{(1+s)^2} \, . \tag{5.29}$$

The incoherent part can be then expressed as

$$\frac{1}{\eta^2} I_{\rm incoh} = \langle \sigma^\dagger \sigma \rangle - \frac{1}{\eta^2} I_{\rm coh} = \frac{1}{2} \frac{s}{1+s} - \frac{1}{2} \frac{s}{(1+s)^2} = \frac{1}{2} \frac{s^2}{(1+s)^2} \, . \tag{5.30}$$

For low saturation, the scattering is dominantly coherent and the intensity of the dipole emission is proportional to the laser intensity, $I_L \propto \Omega^2$. For large saturation, the coherent part diminishes and the incoherent scattering is dominant. It saturates and becomes independent of the incoming intensity: half of the atomic population is in the excited state so that the absorption and induced emission are balanced. A photon can be scattered only after a spontaneous emission occurs.

The coherent part has the simple spectral distribution,

$$\mathcal{I}_{\rm coh}(\omega) = \frac{\eta^2}{2\pi} \int_{-\infty}^{\infty} d\tau \, e^{i(\omega_L - \omega)\tau} \, |\langle \sigma \rangle|^2 = I_{\rm coh} \delta(\omega - \omega_L) \, , \tag{5.31}$$

which reflects the spectrum of the incoming laser radiation. The incoherent part is

$$\begin{aligned} \mathcal{I}_{\rm incoh}(\omega) = \frac{\eta^2}{2\pi} \int_{-\infty}^{\infty} d\tau \, e^{i(\omega_L - \omega)\tau} \langle \delta\sigma^\dagger(\tau) \delta\sigma(0) \rangle \\ = \frac{\eta^2}{2\pi} \int_0^{\infty} d\tau \, e^{i(\omega_L - \omega)\tau} \langle \delta\sigma^\dagger(\tau) \delta\sigma(0) \rangle + \text{c.c.} \, . \end{aligned} \tag{5.32}$$

This form demands the calculation of two-time averages, which can be accomplished by using the *quantum regression theorem*. The Heisenberg–Langevin equations for the fluctuations of the atomic spin operators, $\delta\sigma_q \equiv \sigma_0 - \langle \sigma_q \rangle$, can be written in the compact form

$$\delta\dot{\sigma}_q(\tau) = \sum_{q'} \mathcal{B}_{qq'} \delta\sigma_{q'}(\tau) + \xi_q(\tau) \, , \tag{5.33}$$

where $\mathcal{B}_{qq'}$ is the Bloch-matrix, given in Eq. (5.7), and ξ is the Langevin noise. Now, for $\tau > 0$, the equation of motion for the two-time average follows,

$$\frac{d}{d\tau} \langle \delta\sigma_q(\tau) \delta\sigma(0) \rangle = \sum_{q'} \mathcal{B}_{qq'} \langle \delta\sigma_{q'}(\tau) \delta\sigma(0) \rangle \, , \tag{5.34}$$

since the correlation between a system operator and a noise operator, this latter being taken at a later time, $\langle \xi_q(\tau) \delta\sigma(0) \rangle$, vanishes. That is, the two-time correlation function has the same linear coupling as that appears in the Bloch equation. The difference is that the inhomogeneous term in Eq. (5.7) is missing here, and the initial conditions have to be recalculated, too. The quantum regression theorem finally leads to the incoherent spectrum, which contains the eigenfrequencies given by the characteristic polinomial Eq. (5.10). There are three lines with a finite broadening determined by the natural atomic linewidth γ, and the other system parameters Δ_A and Ω. One special case is the resonant driving which gives rise to the Mollow-triplet Eq. (5.13).

Chapter 6

Light force on an atom

In the following chapters we will set up a Langevin-equation for the motion of the atom, where the various force terms are derived from the quantum theory for the electronic degrees of freedom. This chapter is devoted to the general considerations that assist us in the course of a systematic derivation of the semiclassical Langevin-equations starting from an entirely quantized Hamiltonian problem. As a new feature with respect to the Bloch-equations discussed before, here we consider the center-of-mass motion of the atom with the canonically conjugate position and momentum variables $\hat{\mathbf{R}}_A$ and $\hat{\mathbf{P}}_A$,

$$H = \frac{\hat{\mathbf{P}}_A^2}{2M} + H_0 + H_L + H_{\mathrm{AF}} \ , \tag{6.1a}$$

$$H_0 = H_A + H_F = \hbar\omega_A \sigma^\dagger\sigma + \sum_{\mathbf{k},\lambda} \hbar\omega a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} \ , \tag{6.1b}$$

$$H_{\mathrm{AF}} = -i\hbar \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(\sigma^\dagger a_{\mathbf{k},\lambda} e^{-i\mathbf{k}\hat{\mathbf{R}}_A} - a^\dagger_{\mathbf{k},\lambda} \sigma e^{i\mathbf{k}\hat{\mathbf{R}}_A} \right) \ , \tag{6.1c}$$

$$H_L = -\hbar\Omega(\hat{\mathbf{R}}_A) \left(\sigma^\dagger e^{-i(\omega_L t + \Phi(\hat{\mathbf{R}}_A))} + \sigma e^{i(\omega_L t + \Phi(\hat{\mathbf{R}}_A))} \right) \ . \tag{6.1d}$$

Note that canonical momentum $\mathbf{P}_A$ coincides with the kinetic momentum $M\dot{\mathbf{R}}_A$ in this dipole coupling Hamiltonian. The Heisenberg-equation of motion for the position and momentum are

$$\dot{\mathbf{R}}_A = \frac{1}{i\hbar}\left[\mathbf{R}_A, \mathcal{H}\right] = \frac{\partial \mathcal{H}}{\partial \mathbf{P}_A} = \frac{\mathbf{P}_A}{M} \ , \tag{6.2a}$$

$$\dot{\mathbf{P}}_A = \frac{1}{i\hbar}\left[\mathbf{P}_A, \mathcal{H}\right] = -\frac{\partial \mathcal{H}}{\partial \mathbf{R}_A} = -\nabla\left(\mathcal{H}_L + \mathcal{H}_{\mathrm{AF}}\right) \equiv \hat{\mathbf{F}} \ . \tag{6.2b}$$

The force is defined as the rate of variation of the momentum. In our specific system, the force operator can be directly expressed from Eq. (6.1) as

$$\begin{aligned} F_L = {} & \hbar\nabla\Omega(\mathbf{R}_A)\left(\sigma^\dagger e^{-i(\omega_L t + \Phi(\mathbf{R}_A))} + \sigma e^{i(\omega_L t + \Phi(\mathbf{R}_A))}\right) \\ & - i\hbar\Omega(\mathbf{R}_A)\nabla\Phi(\mathbf{R}_A))\left(\sigma^\dagger e^{-i(\omega_L t + \Phi(\mathbf{R}_A))} - \sigma e^{i(\omega_L t + \Phi(\mathbf{R}_A))}\right) \ , \end{aligned} \tag{6.3a}$$

$$F_{\mathrm{AF}} = \hbar \sum_{\mathbf{k},\lambda} \mathbf{k} g_{\mathbf{k},\lambda} \left(\sigma^\dagger a_{\mathbf{k},\lambda} e^{-i\mathbf{k}\mathbf{R}_A} + a^\dagger_{\mathbf{k},\lambda} \sigma e^{i\mathbf{k}\mathbf{R}_A} \right) \tag{6.3b}$$

6.1 Semiclassical approximation

6.1.1 Time scales

Let us survey the different characteristic time scales of the full dynamics.

- Reservoir correlation time $\tau_c \lesssim 1/\omega_A$; This is the far smallest time scale, which allows for the elimination of the vacuum field modes in the frame of the Markovian approximation.
- Relaxation time of the atom $\tau_R \approx 1/\gamma$; The Rabi-frequency Ω and the detuning Δ_A are typically in the same order of magnitude. These are the characteristic time scales in the dynamics described by the Bloch-equations.
- Time scale of motion induced by laser photons $\tau_{\text{ext}} = 1/\omega_{\text{rec}} \equiv \left(\frac{\hbar k_L^2}{2M}\right)^{-1}$. This characteristic time stems from the kinetic energy gained by the atom in a single laser photon absorption process. Therefore, photon scattering induces transitions between quantized energy eigenstates separated by this quantity.

For Rubidium $\tau_{\text{ext}} = 40\mu$s, while $\tau_R = 0.05\mu$s. That is the internal dynamics is much faster than the translational motion:

$$\tau_{\text{ext}} \gg \tau_R \tag{6.4}$$

This inequality applies for all the other alkalis. On this basis, we expect that the slow center-of-mass dynamics can be treated within an adiabatic approximation. The internal dynamics evolves into the local steady-state and corrections to this steady-state can be systematically produced.

6.1.2 Localization

The center-of-mass motion can be treated classically if the atom is "pointlike" both in position and momentum space:

$$\Delta R \ll \lambda \longrightarrow k_L \Delta R \ll 1 \tag{6.5a}$$

$$\frac{k_L \Delta P}{M} \ll \gamma \tag{6.5b}$$

Taking the product of these inequalities and considering a minimum uncertainty product state, i.e. $\Delta R \Delta P \approx \hbar$, one can see that the necessary condition is

$$\frac{\hbar k_L^2}{M} \ll \gamma \,, \tag{6.6}$$

which expresses exactly the possibility of separating two distinct time scales, as given in Eq. (6.4). Note, however, that a sufficient condition is still missing. Morover, even if at an initial time $t = 0$ both conditions (6.7) are satisfied, at a later time t, for free motion one has

$$\begin{aligned} \Delta P(t) &= \Delta P(0) \,, \\ \Delta R(t) &= \Delta R(0) + \frac{\Delta P(0)}{M} t \,, \end{aligned} \tag{6.7}$$

expressing the spreading of an initial localized wavepacket. Localization on a wavelength scale is maintained during a time t if

$$\frac{k_L \Delta P(0)}{M} t \ll 1 \ . \tag{6.8}$$

That is, if the wavepacket was localized in momentum space, then, from Eq. (6.7b) the position localization is maintained for a time τ_R. For times longer than τ_R many spontaneous emissions occur and the state of the system is described no longer by a wavefunction but by a density matrix.

The spatial coherence at a position difference $\mathbf{d}$ is given by

$$F(\mathbf{d}) = \int d^3\mathbf{R} \ \langle \mathbf{R}| \, \hat{\rho} \, |\mathbf{R}+\mathbf{d}\rangle = \int d^3\mathbf{P} \, e^{i\mathbf{P}\mathbf{d}/\hbar} \, \langle \mathbf{P}| \, \hat{\rho} \, |\mathbf{P}\rangle \ , \tag{6.9}$$

where the second equation results from a simple Fourier transform into the momentum representation. From the normalization of the density matrix $\hat{\rho}$ follows that $F(0) = 1$. The coherence length is the characteristic distance $|\mathbf{d}|$ in which the coherence function decays from 1 down to 0. From the basic properties of Fourier transform pairs follow that the narrower the momentum distribution, the longer is the spatial coherence length. For example, for an atom of mass M being in thermal equilibrium at temperature T, the width of the momentum distribution is related to the temperature by the equipartition theorem

$$k_B T = \frac{\Delta P^2}{M} \ , \tag{6.10}$$

and the coherence length is approximately the thermal de Broglie wavelength $\Delta R = \lambda_T \equiv \sqrt{2\pi\hbar^2/Mk_BT}$.

Let us consider the effect of a single photon scattering event on the spatial coherence function. The initial state of the atomic center-of-mass wavefunction is

$$|\phi\rangle = \int d^3\mathbf{R} \, \phi(\mathbf{R}) \, |\mathbf{R}\rangle = \int d^3\mathbf{K} \, \tilde{\phi}(\mathbf{K}) \, |\mathbf{K}\rangle \ , \tag{6.11}$$

in position and momentum ($\mathbf{K} = \mathbf{P}/\hbar$) representations, respectively. The scattering of a photon of initial wavevector $\mathbf{k_i}$ into one with final wavevector $\mathbf{k_f}$ is

$$|\mathbf{K}\rangle \otimes |\mathbf{k}_i\rangle \rightarrow |\mathbf{K} + \mathbf{k}_i - \mathbf{k}_f\rangle \otimes |\mathbf{k}_f\rangle \ , \tag{6.12}$$

where momentum conservation has been taken into account[1]. This process has an amplitude $S(\mathbf{k}_i, \mathbf{k}_f; \mathbf{K})$, and the corresponding scattering matrix S can be calculated, for example, by second order perturbation theory. The scattering matrix S accounts for the energy conservation. Its dependence on the atomic velocity $\hbar\mathbf{K}/M$ can be attributed to the Doppler effect. Starting from the initial state of the total system,

$$|\Psi_{\rm in}\rangle = |\phi\rangle \otimes |\mathbf{k}_i\rangle = \int d^3\mathbf{K} \, \tilde{\phi}(\mathbf{K}) \otimes |\mathbf{k}_i\rangle \ , \tag{6.13}$$

[1]Note that this condition is not imposed for atoms being trapped in an external potential. As the recoil following the scattering is inhibited, the back-action on the state of the atom is suppressed. There are various consequences of this difference with respect to freely moving scatterers, e.g., the Mössbauer effect.

the final state is

$$|\Psi_{\text{fin}}\rangle = \int d^3\mathbf{k}_f \int d^3\mathbf{K}\, S(\mathbf{k}_i, \mathbf{k}_f; \mathbf{K})\tilde{\phi}(\mathbf{K})\, |\mathbf{K} + \mathbf{k}_i - \mathbf{k}_f\rangle \otimes |\mathbf{k}_f\rangle$$
$$= \int d^3\mathbf{k}_f \int d^3\mathbf{K}\, S(\mathbf{k}_i, \mathbf{k}_f; \mathbf{K}) e^{i(\mathbf{k}_i - \mathbf{k}_f)\mathbf{R}} \tilde{\phi}(\mathbf{K})\, |\mathbf{K}\rangle \otimes |\mathbf{k}_f\rangle \ . \quad (6.14)$$

Let us assume that the scattering amplitude depends only negligibly on the atomic velocity around the mean velocity, $S(\mathbf{k}_i, \mathbf{k}_f; \mathbf{K}) \approx S(\mathbf{k}_i, \mathbf{k}_f; \langle\mathbf{K}\rangle)$. That is, we assume that the Doppler broadening is negligible with respect to the atomic linewidth γ, in accordance with the momentum localization condition Eq. (6.7b). Then the integral over $\mathbf{K}$ can be performed,

$$|\Psi_{\text{fin}}\rangle \approx \int d^3\mathbf{k}_f\, S(\mathbf{k}_i, \mathbf{k}_f; \langle\mathbf{K}\rangle) e^{i(\mathbf{k}_i - \mathbf{k}_f)\mathbf{R}}\, |\phi\rangle \otimes |\mathbf{k_f}\rangle = \int d^3\mathbf{R}\, \phi(\mathbf{R})\, |\mathbf{R}\rangle \otimes |\chi_{\mathbf{R}}\rangle \ , \quad (6.15)$$

where

$$|\chi_{\mathbf{R}}\rangle = \int d^3\mathbf{k}_f\, S(\mathbf{k}_i, \mathbf{k}_f; \langle\mathbf{K}\rangle) e^{i(\mathbf{k}_i - \mathbf{k}_f)\mathbf{R}}\, |\mathbf{k}_f\rangle \ . \quad (6.16)$$

The form of the final state in Eq. (6.15) reflects that photon scattering is a quantum measurement of the position: each component $|\mathbf{R}\rangle$ entangles to the photon state $|\chi_{\mathbf{R}}\rangle$ given above. The probability distribution of the atomic position is not changed immediately after the scattering (the momentum distribution changes, on the other hand). The spatial coherence Eq. (6.9) reduces,

$$F_{\text{fin}}(\mathbf{d}) = \int d^3\mathbf{R}\, \phi(\mathbf{R})\phi^*(\mathbf{R} + \mathbf{d})\, \langle\chi_{\mathbf{R}+\mathbf{d}} \mid \chi_{\mathbf{R}}\rangle = F_{\text{in}}(\mathbf{d})\, \langle\chi_{\mathbf{d}} \mid \chi_0\rangle \ . \quad (6.17)$$

The reduction factor is

$$\langle\chi_{\mathbf{d}} \mid \chi_0\rangle = \int d^3\mathbf{k}_f\, |S(\mathbf{k}_i, \mathbf{k}_f; \langle\mathbf{K}\rangle)|^2 e^{i(\mathbf{k}_i - \mathbf{k}_f)\mathbf{d}} \ , \quad (6.18)$$

being precisely the Fourier transform of the square modulus of the scattering matrix S. The modulus of the final photon momentum is about the initial one, $k_f \approx k_i$, however, its direction spans the whole solid angle according to the dipole pattern. Therefore, in each cartesian direction, the support of the function $|S(\mathbf{k}_i, \mathbf{k}_f; \langle\mathbf{K}\rangle)|^2$ is from $-k_i$ to k_i. The Fourier transform has then the bandwidth of $\pi/k_i = \lambda_i/2$. Spatial positions separated by more than half of the wavelength, $|\mathbf{d}| > \lambda/2$, are resolved in a single photon scattering process. In other words, a single spontaneous photon scattering reduces the coherence length below half of the wavelength. Without proof, we note that repeated photon scatterings further reduce the coherence length well below the optical wavelength. The density matrix becomes closely diagonal, which is equivalent to a classical statistical mixture of narrow wavepackets. Each of these wavepacket can be considered as a classical pointlike particle obeying classical dynamics in accordance with the Ehrenfest theorem.

In momentum representation the density matrix is also closely diagonal. Here the width of the momentum distribution is related to the temperature by the equipartition theorem. This is the definition of the temperature in this theory, and experimental measurements are made exactly on the momentum spread. This can be performed, e.g., by

releasing the atom cloud and measuring the position distribution after a ballistic expansion.

In the following we will introduce a semiclassical model: the interaction of the radiation field with internal degrees of freedom is described by quantum theory, while the center-of-mass motion is treated classically. The position and momentum variables will be classical random variables obeying a Langevin-type equation. Then, these classical variables will be inserted, as parameters, in the quantum problem describing the interaction of the electronic degrees of freedom with the laser and the free electromagnetic field. The validity of this approach can be justified *a posteriori*, by checking the position and momentum localization.

6.2 Langevin-equation

Let us consider the following scalar Langevin-equation:

$$\dot{x} = p/m \ , \tag{6.19a}$$

$$\dot{p} = f - \frac{\beta}{m} p + \xi(t) \ . \tag{6.19b}$$

which includes a deterministic force f, a friction linear in velocity with coefficient β, and a diffusion process represented by the noise term $\xi(t)$. This latter is defined by the moments

$$\langle \xi(t) \rangle = 0 \ , \qquad \langle \xi(t)\xi(t') \rangle = D\delta(t-t') \ . \tag{6.20}$$

Because of the Dirac-δ correlated noise, i.e., its Fourier spectrum contains (infinitely/very) large frequencies, the $\Delta t \longrightarrow 0$ limiting procedure in the differentiation of the momentum requires some care. To avoid ambiguities, the noise is defined in the Ito sense:

$$p(t+\Delta t) = p(t) + \Delta p = p(t) + (f - \frac{\beta}{m} p(t))\Delta t + \Delta\xi(t) \ , \tag{6.21}$$

where

$$\Delta\xi(t) \equiv \int_t^{t+\Delta t} dt' \xi(t') \ . \tag{6.22}$$

Its properties are

$$\langle \Delta\xi \rangle = 0 \ , \tag{6.23a}$$

$$\langle p(t)\Delta\xi \rangle = 0 \ , \tag{6.23b}$$

$$\left\langle \Delta\xi^2 \right\rangle = D\Delta t \ . \tag{6.23c}$$

The equation in the middle follows from the fact that the variable $p(t)$ can contain noise contribution originating from the time before t.

Now, one can check that the discrete time step evolution of the average is well-behaved,

$$\left\langle \frac{p(t+\Delta t) - p(t)}{\Delta t} \right\rangle = f - \frac{\beta}{m} \langle p \rangle \ , \tag{6.24}$$

that is, one can simply take the average of the differential equation. On the other hand, this is not the case with the square of the momentum:

$$\begin{aligned} p^2(t+\Delta t) &= p^2(t) + 2p(t)\Delta p + \Delta p^2 \\ &= p^2(t) + 2p(t)(f - \frac{\beta}{m}p(t))\Delta t + 2p(t)\Delta\xi + \\ &\quad + (f - \frac{\beta}{m}p)^2\Delta t^2 + 2(f - \frac{\beta}{m}p)\Delta t\Delta\xi(t) + \Delta\xi^2 \ , \end{aligned} \tag{6.25}$$

from which, by taking the average,

$$\left\langle \frac{p^2(t+\Delta t) - p^2(t)}{\Delta t} \right\rangle \longrightarrow \left\langle 2p(t)(f - \frac{\beta}{m}p(t)) \right\rangle + D \ . \tag{6.26}$$

As an example, for free motion, $f = 0$, the momentum square is increased by the diffusion D meanwhile it is damped by the friction β. In equilibrium $\langle \Delta p^2/\Delta t\rangle = 0$, which implies

$$k_B T = \left\langle \frac{p^2}{m} \right\rangle = \frac{D}{\beta} \ , \tag{6.27}$$

known as the Einstein relation for dissipation and fluctuation.

6.3 Mean force

Obviously, the quantum mechanical mean of the force operator will be identified with f of Eq. (6.19).

$$\begin{aligned} \langle F_L\rangle &= \hbar\nabla\Omega(\mathbf{R}_A)2u_{\rm st} - \hbar\Omega(\mathbf{R}_A)\nabla\Phi(\mathbf{R}_A))2v_{\rm st} \\ &= -\hbar\frac{\nabla(\Omega(\mathbf{R}_A)^2)\Delta_A}{\Delta_A^2 + \gamma^2 + 2\Omega^2} - \hbar\frac{\Omega(\mathbf{R}_A)^2\nabla(\Phi(\mathbf{R}_A))\gamma}{\Delta_A^2 + \gamma^2 + 2\Omega^2} \end{aligned} \tag{6.28}$$

The first term, which is proportional to the real part of the atomic polarizability, c.f. Eq. (5.19), is called the *dipole force*. As this is intimately related to the process of absorption and stimulated emission into one of the populated modes, this is a dispersive effect. The second term, corresponding to the absorptive part of the polarizability, is called the *radiation pressure*[2] or scattering force.

6.3.1 Radiation pressure

Assume the driving electric field is a propagating plane wave with wave vector $\mathbf{k}_L$

$$\mathbf{E}_L(\mathbf{R}, t) = \epsilon\mathcal{E}_L\cos(\omega_L t - \mathbf{k}_L\mathbf{R}) \ , \tag{6.29}$$

[2]This nomenclature should be used with care and only in connection with atoms. In general, by dipole force one could mean the Lorentz force acting on a dipole, which certainly comprises both the absorptive and dispersive parts. On the other hand, when illuminating a mirror by light, the force resulting from the momentum change of reflected photons is often referred to as radiation pressure. This force, however, is related to coherent redistribution and thus to the dipole force component.

with fixed polarization. Then the Rabi frequency is constant, $\Omega(\mathbf{R}) = \Omega$, hence the dipole force vanishes ($\nabla\Omega(\mathbf{R}) = 0$). The radiation pressure force, on using Eq. (5.16), is

$$F_{\rm rp} = \hbar\mathbf{k}\frac{2\Omega^2\gamma}{\Delta_A^2 + \gamma^2 + 2\Omega^2} = \hbar\mathbf{k}\, 2\gamma \left\langle \sigma^\dagger\sigma \right\rangle \ , \tag{6.30}$$

which offers a clear physical interpretation: The atom spontaneously emits photons into random directions at a rate $2\gamma \left\langle \sigma^\dagger\sigma \right\rangle$, each emission having been preceded by the absorption of a laser photon with the well-defined momentum $\hbar\mathbf{k}$.

6.3.2 Dipole force

Consider now a laser standing wave,

$$\mathbf{E}_L(\mathbf{R}, t) = \epsilon\mathcal{E}_L \cos\left(\mathbf{k}_L\mathbf{R}\right)\cos\left(\omega_L t\right) \ . \tag{6.31}$$

This wave in momentum space represents two peaks at $\pm\hbar\mathbf{k}$. It could be composed of two counter-propagating modes. Photons can be scattered between the two populated modes by stimulated emission. As the process behind the dipole force is a coherent redistribution of photons between lasers modes, the force is conservative and derives from a potential

$$\begin{aligned} F_{\rm dip} &= -\nabla U_{\rm dip} \ , \\ U_{\rm dip}(\mathbf{R}) &= \frac{\hbar\Delta_A}{2}\ln\left(\Delta_A^2 + \gamma^2 + 2\Omega^2(\mathbf{R})\right) = const. + \frac{\hbar\Delta_A}{2}\ln\left(1 + \frac{2\Omega^2(\mathbf{R})}{\Delta_A^2 + \gamma^2}\right) . \end{aligned} \tag{6.32}$$

For low saturation the logarithmic function can be expanded and one gets

$$U_{\rm dip}(\mathbf{R}) = \frac{\hbar\Omega^2(\mathbf{R})\Delta_A}{\Delta_A^2 + \gamma^2} \ , \tag{6.33}$$

It is very important to notice that the potential is substantially dependent on the detuning. On resonance, $\Delta_A = 0$, there is no force at all. For $\Delta_A < 0$, "red detuning", the potential minima coincide with the intensity maxima of the electric field. The atom is "high-field seeker", this makes the possibility of atom trapping. In the opposite case, $\Delta_A > 0$, "blue detuning" the atom is repulsed from the high intensity regions.

There is an interesting limit of the dipole potential, when the detuning is very large. Far-off-resonance dipole traps (FORT) are commonly used for long-time capturing and localization of neutral atoms by laser light fields. The basic idea behind tuning the laser frequency $\omega_{\rm L}$ very far below the atomic resonance $\omega_{\rm A}$ resides in the fact that the depth of the trap potential and the spontaneous photon scattering rate scale differently with the detuning $\Delta_{\rm A} = \omega_{\rm L} - \omega_{\rm A}$. The former is proportional to $\Omega^2/\Delta_{\rm A}$ (see Eq. (6.33) with γ neglected in the denominator), while the latter to $\Omega^2/\Delta_{\rm A}^2$. As a consequence, deep traps can be formed at a reduced level of the recoil noise generated by spontaneous emissions in the large detuning limit. This scheme of almost conservative trapping preserves the coherence of the atomic gross motion.

Optical standing wave in three-dimension can be routinely formed by phase-locked counter-propagating laser fields. This creates a three-dimensional perfectly periodic potential for the atoms. The system of atoms organized by the dipole potential into perfect periodic order is called the "optical lattice".

Chapter 7

Force on a moving atom: Doppler cooling

In this chapter the mean force on a moving atom will be discussed. The analysis will be restricted to the case where the atomic center-of-mass is well localized both in real and in momentum spaces. The position $\mathbf{R}$ and the velocity $\mathbf{V}$ of the atom will be taken into account parametrically in the internal dynamics. The same model is used as in Chapter 5 that introduces the Bloch-equations. The only difference is that the atomic position is not fixed, therefore the Rabi frequency Ω and the local phase Φ vary in time according to the atomic trajectory. The system Hamiltonian is

$$\mathcal{H} = \hbar\omega_A\sigma_z + \hbar\Omega(\mathbf{R}_A(t))\left(\sigma^\dagger e^{-i(\omega_L t+\Phi(\mathbf{R}_A(t)))} + \sigma e^{i(\omega_L t+\Phi(\mathbf{R}_A(t)))}\right) + \mathcal{H}_F + \mathcal{H}_{\text{vac}} \ , \qquad (7.1)$$

Due to the variation of the phase, on keeping the definition Eq. (5.8) of the real u, v, w variables, the Bloch-equations are slightly modified with respect to Eq. (5.9):

$$\dot{u} = -(\Delta_A + \dot{\Phi}(\mathbf{R}_A))v - \gamma u \ , \qquad (7.2a)$$

$$\dot{v} = (\Delta_A + \dot{\Phi}(\mathbf{R}_A))u - \gamma v - 2\Omega(\mathbf{R}_A)w \ , \qquad (7.2b)$$

$$\dot{w} = 2\Omega(\mathbf{R}_A)v - 2\gamma(w + 1/2) \ . \qquad (7.2c)$$

This set of equations can be written in the compact form for the vector $\underline{s} = (u, v, w)$,

$$\dot{\underline{s}} = \underline{\underline{B}}\underline{s} + \underline{\eta} \ , \text{with } \underline{\underline{B}} = \begin{pmatrix} -\gamma & \Delta_A + \dot{\Phi} & 0 \\ -(\Delta_A + \dot{\Phi}) & -\gamma & -2\Omega \\ 0 & 2\Omega & -2\gamma \end{pmatrix} \ , \text{and } \underline{\eta} = \begin{pmatrix} 0 \\ 0 \\ -\gamma \end{pmatrix} \ . \qquad (7.3)$$

7.1 Single propagating plane wave

We will consider first a single laser mode which is a plane wave propagating in the x direction with wave number k. The atomic motion is also restricted to one dimension. From the definition of the electric field given in Eq. (5.2), the parameters of the Bloch-equations follow:

$$\Omega(\mathbf{R}_A) = \Omega \ , \text{independent of time}$$
$$\Phi(\mathbf{R}_A) = -kx \ \Rightarrow \dot{\Phi} = -kv_A$$

and the force is

$$F_{\rm rp} = \hbar k\, \Omega\, 2v_{\rm st} \ . \tag{7.4}$$

The characteristic time scale of the variation of the center-of-mass motion is assumed to be much longer than that of the internal dynamics, therefore the velocity can be considered constant to derive a velocity-dependent force from the steady-state solutions of the Bloch-equations. The solution is formally the same as the one for immobile atom with the replacement $\Delta_A \longrightarrow \Delta_A - kv_A$. This similarity reflects the fact that, for a single plane wave exciting field, the atomic motion with constant velocity can be eliminated by choosing a co-moving reference frame and transforming the field frequency according to the Doppler-effect. More generally, it can be understood that the atomic velocity, although it does not directly appear in the system Hamiltonian, has an influence on the internal dynamics (steady-state solution, etc.) via the Doppler effect. Indirectly, this influence gives rise to a velocity dependence of the mechanical effect on the center-of-mass motion.

The steady-state solution is

$$v_{\rm st} = \frac{\gamma\Omega}{(\Delta_A - kv_A)^2 + \gamma^2 + 2\Omega^2} \ , \tag{7.5}$$

and the force follows:

$$F_{\rm rp} = \hbar k \frac{2\gamma\Omega^2}{(\Delta_A - kv_A)^2 + \gamma^2 + 2\Omega^2} \ , \tag{7.6}$$

which is valid for arbitrary velocity v_A. For low velocities, $kv_A \ll \gamma, \Delta_A, \Omega$, the force can be expanded to linear order so that the linear friction, $F^{(1)} = -\beta v_A$ can be obtained. By using

$$\frac{\partial}{\partial v_A} F_{\rm rp} = -\hbar k \frac{2\gamma\Omega^2}{\left((\Delta_A - kv_A)^2 + \gamma^2 + 2\Omega^2\right)^2} 2(\Delta_A - kv_A)(-k) \ , \tag{7.7}$$

the linear friction force is

$$F^{(1)}_{\rm rp} = \hbar k^2 \, \frac{s}{(1+s)^2} \, \frac{2\gamma\Delta_A}{\Delta_A^2 + \gamma^2} v_A \ , \tag{7.8}$$

where the saturation $s = 2\Omega^2/(\Delta_A^2 + \gamma^2)$. It is very important to realize that the sign of β is determined by the sign of the detuning Δ_A. The so-called red detuning $\omega_L < \omega_A$ leads to friction, i.e., dissipating the motional energy of the atom (cooling). Blue detuning yields heating of the motion.

The factor depending on the saturation s has a maximum at $s = 1$. The factor depending on the detuning also has a maximum. The optimum tuning for maximum friction is $\Delta_A = -\gamma$, then the friction coefficient is $\beta = \hbar k^2/4$. The maximum rate of change for the velocity is determined by the recoil frequency $\omega_{\rm rec} = \hbar k^2/M$, which is much less than the spontaneous emission rate γ. It was thus well justified to consider a constant velocity while letting the Bloch-equations evolve into the steady-state regime.

One would naively expect that a gas of atoms irradiated by light absorbs energy and it should heat up in any circumstances. It is surprising that cooling is possible at all. How is this related to detuning?

Interpretation of Doppler cooling in terms of scattering

Absorbing laser irradiation means scattering, as depicted in Fig. 7.1. The atom is ex-

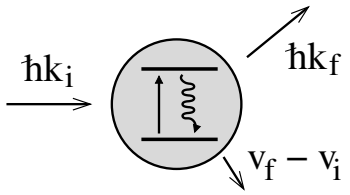

Figure 7.1: Absorption as scattering. The incoming photon carries $\hbar\mathbf{k}_i$ momentum, the scattered photon has $\hbar\mathbf{k}_f$ momentum. The photon scattering imparts a momentum change $M(\mathbf{v}_f - \mathbf{v}_i)$ to the atom.

cited from the ground state by absorbing a photon. Deexcitation back to the ground state happens via spontaneous emission of a photon into a random direction. On a time scale much longer than the lifetime of the excited state (typically 10–100 ns), this is a scattering process in which the incoming photon with $\hbar\mathbf{k}_i$ momentum is transmitted into an outgoing photon with $\hbar\mathbf{k}_f$ momentum. Accompanying the photon scattering, the atom undergoes a recoil. The photon scattering is inelastic: the difference in the energy of the incoming and outgoing photons provides the change of the kinetic energy of the atomic center-of-mass motion. All this can be included in the following energy and momentum balance equations:

$$\begin{aligned} \hbar\omega_i + \frac{1}{2}Mv_i^2 &= \hbar\omega_f + \frac{1}{2}Mv_f^2 \\ \hbar\mathbf{k}_i + M\mathbf{v}_i &= \hbar\mathbf{k}_f + M\mathbf{v}_f\,, \end{aligned} \tag{7.9}$$

where M is the atom mass. Expressing the change of the kinetic energy,

$$\Delta E_{\rm kin} = \frac{\hbar^2(\mathbf{k}_i - \mathbf{k}_f)^2}{2m} + \hbar(\mathbf{k}_i - \mathbf{k}_f)\mathbf{v}_i\,. \tag{7.10}$$

Typically the absorption cycle occurs many times during the observation time, therefore one has to average the above energy balance equation. The first term is always positive, that is, it increases the kinetic energy. This is the recoil term responsible for the naive expectation that light irradiated atoms heat up. The second term, however, can be negative. Any value different from zero corresponds to a correlation between photon scattering and the initial velocity. Such correlation can derive from the Doppler effect, as was discovered by Hänsch and Schawlow in 1975. [**?**].

Let us assume that the atomic velocity fluctuates around zero (a finite mean velocity v_0 can be incorporated into the atomic frequency $\omega_A \to \omega_A + k_i v_0$. An atom moving with velocity $\mathbf{v}_-$ opposite to the direction of the laser experiences the laser frequency Doppler shifted at $\omega_L + k_i v_-$. An atom co-propagating with the laser beam with v_+ velocity the actual laser frequency is shifted to $\omega_L - k_i v_+$. If the laser frequency is detuned below the atomic frequency, ω_A or $\omega_A + k_L v_0$, the atom counter-propagating with the laser beam gets closer to the resonance (see Fig. 7.2) and absorbs more likely photons than the co-propagating atom. In conclusion, the momentum $\mathbf{k}_i$ and the velocity $\mathbf{v}_i$ are

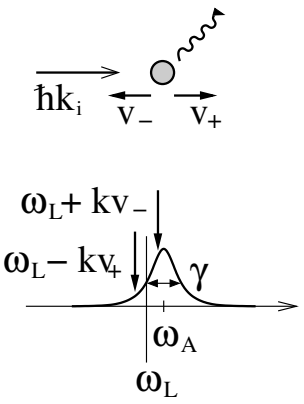

Figure 7.2: Atomic resonance curve at ω_A with width 2γ and Doppler-shifted driving frequencies associated with velocities v_- and v_+, respectively.

not independent in the actual scattering processes, and on average

$$\langle \mathbf{k}_i \mathbf{v}_i \rangle \sim \langle k_i (v_+ - v_-) \rangle < 0 \,. \tag{7.11}$$

The outgoing photon momentum and the initial velocity are not correlated, $\langle \mathbf{k}_f \mathbf{v}_i \rangle = 0$, therefore in Eq. (7.10) the second term is negative. Moreover it can dominate the first, recoil term, which leads to cooling. The kinetic energy reduction implies that the outgoing photon must have a higher frequency than the incoming one.

7.2 Single standing plane wave

Two counter-propagating plane waves, which geometry was invoked above, form a standing wave provided the phases of the two beams are locked. This is not necessary the case and than the forces exerted independently by the propagating plane waves can simply be added. When there is a coherence between the beams, in a standing wave laser field mode, the atom-field interaction is substantially different.

In the compact form given in Eq. (5.2), the standing wave field corresponds to that there is no local phase, $\Phi \equiv 0$, and only the spatially inhomogeneous Rabi-frequency $\Omega(\mathbf{R}_A(t))$ depends on time. The force now originates from the dipole force,

$$\mathbf{F}_{\rm dip} = \hbar \nabla \Omega \, 2u_{\rm st} \ , \tag{7.12}$$

which clearly shows the important difference inasmuch as the dispersive part of the susceptibility $u_{\rm st}$ appears in the force.

By contrast to the propagating plane wave case, here the Bloch matrix $\underline{\underline{B}}$ in Eq. (7.3) depends on time. Although this specific problem can be solved for arbitrary velocity with the continued fraction method, we will resort to a method which applies only to small velocities, however, which is a much more general approach.

As time dependence originates partly from motion, the time derivative is replaced by the hydrodynamic derivative and the solution is expanded into a power series of the velocity,

$$\frac{d}{dt} \to \frac{\partial}{\partial t} + \mathbf{v}\nabla \text{ and } \underline{s} = \underline{s}^{(0)} + \underline{\underline{s}}^{(1)} \mathbf{v} + \dots \ , \tag{7.13}$$

respectively. Note that $\underline{\underline{s}}^{(1)}$ is a tensor mapping from the 3D space into the abstract space of the Bloch vector, since all the spatial components of the velocity $v_{x,y,z}$ can have an effect on all the elements of the vector $\underline{s} = (u, v, w)$. The Bloch-equation becomes

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\nabla\right)\left(\underline{s}^{(0)} + \underline{\underline{s}}^{(1)}\mathbf{v} + \ldots\right) = \underline{\underline{B}}\left(\underline{s}^{(0)} + \underline{\underline{s}}^{(1)}\mathbf{v} + \ldots\right) + \eta \,. \tag{7.14}$$

In steady-state the explicit time derivative vanishes, and one gets the hierarchy of equations to different orders of the velocity v,

$$0 = \underline{\underline{B}}\underline{s}^{(0)} + \eta \,, \tag{7.15a}$$

$$(\mathbf{v}\nabla)\underline{s}^{(0)} = \left(\underline{\underline{B}}\underline{s}^{(1)}\right)\mathbf{v} \,, \tag{7.15b}$$

and so on. The first line yields the steady-state for an atom in fixed position,

$$\underline{s}^{(0)} = -\underline{\underline{B}}^{-1}\underline{\eta} \,. \tag{7.16}$$

This solution is needed to determine the solution in the next order,

$$\underline{s}^{(1)} = \underline{\underline{B}}^{-1}\nabla \circ \underline{s}^{(0)} = -\underline{\underline{B}}^{-1}\nabla \circ \underline{\underline{B}}^{-1}\eta \,. \tag{7.17}$$

In order to avoid the complications imposed by the tensors involved, we will use this approach in a simplified system. We will consider an atom in the low saturation regime, $s \ll 1$, where the w component can be eliminated assuming $\sigma_z = -1/2$ in Eq. (5.7a):

$$\left\langle\dot{\tilde{\sigma}}\right\rangle = (i\Delta_A - \gamma)\left\langle\tilde{\sigma}\right\rangle + i\Omega(R) \,. \tag{7.18}$$

This is a simple linear equation. Physically this is an important limit of the atomic system, because it furnishes a microscopic model for linearly polarizable particles which are ubiquitous in electrodynamics. The commutation relation for the associated quantum operator modifies to

$$\left[\sigma, \sigma^\dagger\right] = -2\sigma_z \approx 1 \,, \tag{7.19}$$

i.e., the atom being close to the ground state behaves as a bosonic system, as if the atom were a harmonic oscillator whose excited states higher than the first one could be completely neglected.

Now the expansion method can be illustrated on Eq. (7.18) which is exempt from the tensorial character due to the Bloch-vector. The steady-state in zeroth and first order read

$$\left\langle\tilde{\sigma}\right\rangle^{(0)} = \frac{-i\Omega(\mathbf{R})}{i\Delta_A - \gamma} \,, \tag{7.20a}$$

$$\left\langle\tilde{\sigma}\right\rangle^{(1)} = \frac{1}{i\Delta_A - \gamma}\nabla\frac{-i\Omega(\mathbf{R})}{i\Delta_A - \gamma} = \nabla\Omega(\mathbf{R})\frac{2\Delta_A\gamma - i(\gamma^2 - \Delta_A^2)}{(\Delta_A^2 + \gamma^2)^2} \,, \tag{7.20b}$$

As $u = \mathrm{Re}\langle\tilde{\sigma}\rangle$ follows from Eq. (5.8), the force to first order in velocity is

$$\mathbf{F}^{(1)}_{\mathrm{dip}} = 2\hbar\nabla\Omega(\mathbf{R})\left(\underline{u}^{(1)}\mathbf{v}\right) = 2\hbar\nabla\Omega(\mathbf{R}) \circ \nabla\Omega(\mathbf{R})\frac{2\Delta_A\gamma}{(\Delta_A^2 + \gamma^2)^2}\,\mathbf{v} \,. \tag{7.21}$$

For a plane wave $\Omega(\mathbf{R}) = \Omega\ \cos(\mathbf{kR})$, in one dimension the friction force is

$$F_{\rm dip}^{(1)} = 2\hbar k^2\ \sin^2 kx \frac{\Omega^2}{\Delta_A^2+\gamma^2}\ \frac{2\Delta_A\gamma}{\Delta_A^2+\gamma^2}\ v\ . \tag{7.22}$$

The friction is maximum at the nodes of the standing wave, where the derivative of the mode function is the maximum. On spatially averaging this inhomogeneous result, one gets back the same linear friction force as the one obtained in a propagating plane wave. However, this equality holds only for the linear polarizability regime.

Chapter 8

Force fluctuations and momentum diffusion

In this chapter we will consider the force terms which have vanishing mean value but give rise to a momentum diffusion process.

8.1 Vacuum field force

The atom, regardless of being laser driven or not, is embedded in the electromagnetic radiation field. The Hamiltonian accounting for the coupling of the atom to the electromagnetic modes is

$$\mathcal{H}_{\rm vac} = -i\hbar \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} \left(\sigma^\dagger a_{\mathbf{k},\lambda} e^{i\mathbf{k}\mathbf{R}_A} - a^\dagger_{\mathbf{k},\lambda} \sigma e^{-i\mathbf{k}\mathbf{R}_A} \right) \ . \tag{8.1}$$

This coupling gives rise to a force exerted by the vacuum field. By definition, the force is

$$\mathbf{F}_{\rm vac} = -\nabla H_{\rm vac} = -\sum_{\mathbf{k},\lambda} \hbar \mathbf{k} g_{\mathbf{k},\lambda} \left(\sigma^\dagger a_{\mathbf{k},\lambda} e^{i\mathbf{k}\mathbf{R}_A} + a^\dagger_{\mathbf{k},\lambda} \sigma e^{-i\mathbf{k}\mathbf{R}_A} \right) \ . \tag{8.2}$$

To evaluate the vacuum force, we use the same separation of the vacuum field into free field and radiated field components as previously in Chapter 3. The Heisenberg equations of motion for the field amplitudes are

$$\dot{a}_{\mathbf{k},\lambda} = -i\omega_k a_{\mathbf{k},\lambda} + g_{\mathbf{k},\lambda} \sigma e^{-i\mathbf{k}\mathbf{R}_A} \ , \tag{8.3}$$

from which the formal solution follows

$$a_{\mathbf{k},\lambda}(t) = a_{\mathbf{k},\lambda}(0) e^{-i\omega_k t} + g_{\mathbf{k},\lambda} \int_0^t dt' \sigma(t') e^{-i\mathbf{k}\mathbf{R}_A} e^{-i\omega_k (t-t')} \ . \tag{8.4}$$

On inserting back this solution into the force, one gets two terms,

$$\begin{aligned} \mathbf{F}_{\rm vac} = &-\sum_{\mathbf{k},\lambda} \hbar \mathbf{k} g_{\mathbf{k},\lambda} \left(\sigma^\dagger(t) a_{\mathbf{k},\lambda}(0) e^{-i\omega_k t} e^{i\mathbf{k}\mathbf{R}_A} + a^\dagger_{\mathbf{k},\lambda}(0) \sigma(t) e^{i\omega_k t} e^{-i\mathbf{k}\mathbf{R}_A} \right) \\ &-\sum_{\mathbf{k},\lambda} \hbar \mathbf{k} g^2_{\mathbf{k},\lambda} \int_0^t dt' \left(\sigma^\dagger(t) \sigma(t') e^{-i\omega_k (t-t')} + \sigma^\dagger(t') \sigma(t) e^{i\omega_k (t-t')} \right) \ . \end{aligned} \tag{8.5}$$

The second term is identically zero since the terms belonging $\pm\mathbf{k}$ annihilate in the sum. Physically, the field radiated by the atom has no force acting back on it. Thus the vacuum field force is

$$\mathbf{F}_{\rm vac} = -\sum_{\mathbf{k},\lambda} \hbar\mathbf{k} g_{\mathbf{k},\lambda} \left(\sigma^\dagger(t) a_{\mathbf{k},\lambda}(0) e^{-i\omega_k t} e^{i\mathbf{k}\mathbf{R}_A} + a^\dagger_{\mathbf{k},\lambda}(0)\sigma(t) e^{i\omega_k t} e^{-i\mathbf{k}\mathbf{R}_A} \right) \tag{8.6}$$

The quantum mechanical mean value of this force is obviously zero. However, it makes a huge difference that the operator is not zero, hence there are non-vanishing higher order moments which we are going to calculate in the following.

8.2 Vacuum field force fluctutations

For later convenience, we assume that there is a dominant carrier frequency ω_L and define the slowly varying atomic operators $\tilde\sigma$ and $\tilde\sigma^\dagger$ in a frame rotating with this frequency. Let us study the second-order correlation of the vacuum field force,

$$\begin{aligned}
\langle \mathbf{F}_{\rm vac}(t_1) \circ \mathbf{F}_{\rm vac}(t_2) \rangle = \hbar^2 \sum_{\mathbf{k}_1,\lambda_1} \sum_{\mathbf{k}_2,\lambda_2} \mathbf{k}_1 \circ \mathbf{k}_2 \, g_{\mathbf{k}_1,\lambda_1} g_{\mathbf{k}_2,\lambda_2} \\
\Bigg(\left\langle \tilde\sigma^\dagger(t_1) a_{\mathbf{k}_1,\lambda_1}(t_0) a^\dagger_{\mathbf{k}_2,\lambda_2}(t_0) \tilde\sigma(t_2) \right\rangle e^{i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{R}_A} e^{-i(\omega_1-\omega_L)t_1} \, e^{i(\omega_2-\omega_L)t_2} \\
+ \left\langle \tilde\sigma^\dagger(t_1) a_{\mathbf{k}_1,\lambda_1}(t_0) \tilde\sigma^\dagger(t_2) a_{\mathbf{k}_2,\lambda_2}(t_0) \right\rangle e^{i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{R}_A} e^{-i(\omega_1-\omega_L)t_1} \, e^{-i(\omega_2-\omega_L)t_2} \\
+ \left\langle a^\dagger_{\mathbf{k}_1,\lambda_1}(t_0) \tilde\sigma(t_1) a^\dagger_{\mathbf{k}_2,\lambda_2}(t_0) \tilde\sigma(t_2) \right\rangle e^{-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{R}_A} e^{i(\omega_1-\omega_L)t_1} \, e^{i(\omega_2-\omega_L)t_2} \\
+ \left\langle a^\dagger_{\mathbf{k}_1,\lambda_1}(t_0) \tilde\sigma(t_1) \tilde\sigma^\dagger(t_2) a_{\mathbf{k}_2,\lambda_2}(t_0) \right\rangle e^{-i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{R}_A} e^{i(\omega_1-\omega_L)t_1} \, e^{-i(\omega_2-\omega_L)t_2} \Bigg) .
\end{aligned} \tag{8.7}$$

In the last three lines, either the operator $a_{\mathbf{k},\lambda}(t_0)$ is on the far most right or $a^\dagger_{\mathbf{k},\lambda}(t_0)$ is on the far most left in the bracket. Therefore all these terms vanish at zero temperature. In the first line, on using the commutation rule $\left[a_{\mathbf{k}_1,\lambda_1}(t_0), a^\dagger_{\mathbf{k}_2,\lambda_2}(t_0) \right] = \delta_{\mathbf{k}_1,\mathbf{k}_2}\delta_{\lambda_1,\lambda_2}$, one gets

$$\begin{aligned}
\langle \mathbf{F}_{\rm vac}(t_1) \circ \mathbf{F}_{\rm vac}(t_2) \rangle = \hbar^2 \sum_{\mathbf{k},\lambda} \mathbf{k} \circ \mathbf{k} \, g^2_{\mathbf{k},\lambda} \left\langle \tilde\sigma^\dagger(t_1) \tilde\sigma(t_2) \right\rangle e^{-i(\omega_k-\omega_L)(t_1-t_2)} \\
+ \hbar^2 \left\langle \tilde\sigma^\dagger(t_1) \mathbf{f}^\dagger(t_2) \circ \mathbf{f}(t_1) \tilde\sigma(t_2) \right\rangle ,
\end{aligned} \tag{8.8}$$

where

$$\mathbf{f}(t) = \sum_{\mathbf{k},\lambda} \mathbf{k} g_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda}(t_0) e^{i\mathbf{k}\mathbf{R}_A} e^{-i(\omega_k-\omega_L)t} = -i\nabla\xi \tag{8.9}$$

As $\mathbf{f}^\dagger(t_2)$ contains only the operators $a^\dagger_{\mathbf{k},\lambda}(t_0)$, its action on the bra state would be zero. Similarly, $\mathbf{f}(t_1)$ is composed of the annihilation operators $a_{\mathbf{k},\lambda}(t_0)$ and it maps the initial ket state to zero. The problem is, however, that the commutation relation with the atomic operators $\tilde\sigma$ and $\tilde\sigma^\dagger$ is unknown. This can be calculated with the trick used once for the calculation of the quantum noise correlations of ξ at the end of Chap. 3. Let

us express the free field operators at $t = t_0$ from the ones at $t = t_2$ by propagating 'backward' in time, i.e., using the formal solution in Eq. (3.4),

$$a_{\mathbf{k},\lambda}(0) = a_{\mathbf{k},\lambda}(t_2)e^{i\omega_k t_2} + g_{\mathbf{k},\lambda}\int_0^{t_2} dt'\tilde{\sigma}(t')e^{-i\mathbf{k}\mathbf{R}_A}e^{i(\omega_k-\omega_L)t'} \ . \tag{8.10}$$

Operators $a_{\mathbf{k},\lambda}(t_2)$ and $\tilde{\sigma}(t_2)$ commute, since they are at equal times, thus

$$\begin{aligned}
[\xi(t_1),\tilde{\sigma}(t_2)] &= -\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}e^{i\mathbf{k}\mathbf{R}_A}e^{-i(\omega_k-\omega_L)t_1}g_{\mathbf{k},\lambda}\int_{t_0}^{t_2} dt' e^{-i\mathbf{k}\mathbf{R}_A}e^{i(\omega_k-\omega_L)t'}\,[\tilde{\sigma}(t'),\tilde{\sigma}(t_1)]\,x \\
&= -\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2\int_{t_0}^{t_2} dt'\,[\tilde{\sigma}(t'),\tilde{\sigma}(t_2)]\,e^{i(\omega_k-\omega_L)(t'-t_1)} \\
&\approx -\theta(t_2-t_1)\,[\tilde{\sigma}(t_1),\tilde{\sigma}(t_2)]\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2\int_{t_0}^{t_2} dt' e^{i(\omega_k-\omega_L)(t'-t_1)} \\
&= -\gamma\theta(t_2-t_1)\,[\tilde{\sigma}(t_1),\tilde{\sigma}(t_2)] \ ,
\end{aligned} \tag{8.11}$$

where we used the Markov-approximation. This expresses the fact that the noise operators at time t_1 commute with the system operators at a prior time $t_2 < t_1$. By contrast, at later times $t_2 > t_1$ the system operator involves the previous noise and then the commutation relation becomes non-trivial.

Concerning the second term of Eq. (8.8), it follows that

$$\left\langle \tilde{\sigma}^\dagger(t_1)\mathbf{f}^\dagger(t_2)\circ\mathbf{f}(t_1)\tilde{\sigma}(t_2)\right\rangle \propto \Theta(t_2-t_1)\,\Theta(t_1-t_2) \ , \tag{8.12}$$

which is zero except for precisely at $t_1 = t_2$. At his single point the commutator is negligibly small with respect to the contribution of the first term of Eq. (8.8).

Finally we arrive at

$$\langle \mathbf{F}_{\rm vac}(t_1)\circ\mathbf{F}_{\rm vac}(t_2)\rangle = \hbar^2\sum_{\mathbf{k},\lambda}\mathbf{k}\circ\mathbf{k}\,g_{\mathbf{k},\lambda}^2\left\langle\tilde{\sigma}^\dagger(t_1)\tilde{\sigma}(t_2)\right\rangle e^{-i(\omega-\omega_L)(t_1-t_2)} \ . \tag{8.13}$$

The summation involves a broadband frequency range, therefore any finite time difference $|t_1-t_2| > 1/\Omega_B$, where Ω_B is the reservoir bandwidth, makes the complex phase factor average out the sum. Again, in the spirit of the Markov approximation,

$$\langle \mathbf{F}_{\rm vac}(t_1)\circ\mathbf{F}_{\rm vac}(t_2)\rangle = \hbar^2 k_A^2\,\gamma\left\langle\sigma^\dagger\sigma\right\rangle\begin{pmatrix} 2/5 & 0 & 0\\ 0 & 2/5 & 0\\ 0 & 0 & 1/5\end{pmatrix}\delta(t_1-t_2) \ . \tag{8.14}$$

This force correlation function with the magnitude $D_{\rm rec}$ can be identified with the diffusion coefficient of a classical stochastic process. The diffusion coefficient expresses that the corresponding Brownian motion has a "stepsize" $\hbar k_A$ with a numerical factor accounting for the projection onto the different cartesian directions, and random steps occur at the rate of the spontaneous emission, $2\gamma\left\langle\sigma^\dagger\sigma\right\rangle$. That is the physical origin is the recoil, accompanying each spontaneous emission event, into a random direction.

8.3 Laser field force fluctuations

One effect of the vacuum field modes was discussed in the previous chapter. There is a diffusion of the center-of-mass motion stemming from the random recoil following a spontaneous emission, and this process is incorporated into the vacuum force term Eq. (6.3b). This is not all: the noise due to coupling to the vacuum field penetrates the system variables and therefore the force originating from the coherent laser field also picks up a fluctuating character. Eq. (6.3a) presents the force due to the laser irradiation, having a linear dependence on the atomic polarization operators σ and $\sigma^\dagger$. Besides the mean value of the laser field force corresponding to the mean polarization, there is an additional diffusion from the quantum fluctuations of the atomic polarization. The fluctuations are of quantum nature originating from the coupling to the electromagnetic radiation field in vacuum state, since the system is considered at zero temperature. The second order autocorrelation function of the force operator involves the correlations such as $\left\langle \delta\sigma(t_1)\delta\sigma^\dagger(t_2)\right\rangle$ that can be calculated by invoking the quantum regression theorem, as it was done to calculate the incoherent spectrum of the dipole radiation in Sec. 5.3.

Here we will adopt a different, more direct approach which reveals some generic properties of noise processes. In a frame rotating at the laser frequency, the Heisenberg equations of motion for the atomic operators read

$$\dot{\tilde{\sigma}} = (i\Delta_A - \gamma)\tilde{\sigma} - i2\sigma_z\Omega e^{-i\Phi} + \mathbf{\Xi}(t) \;, \tag{8.15a}$$

$$\dot{\sigma}_z = -2\gamma(\sigma_z + 1/2) + i\Omega\left(\tilde{\sigma}^\dagger e^{-i\Phi} - \tilde{\sigma}e^{i\Phi}\right) - \mathbf{\Xi}_z(t) \;, \tag{8.15b}$$

$$\text{where} \quad \mathbf{\Xi}(t) = 2\sigma_z(t)\xi(t) \;, \quad \mathbf{\Xi}_z(t) = \tilde{\sigma}^\dagger(t)\xi(t) + \xi^\dagger(t)\tilde{\sigma}(t) \;, \tag{8.15c}$$

$$\text{with} \quad \xi(t) = \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}a_{\mathbf{k},\lambda}(0)e^{i\mathbf{k}\mathbf{R}_A}e^{-i(\omega_k-\omega_L)t} \;. \tag{8.15d}$$

The properties of the noise term are descibed by the second-order correlations derived in Section 3.4.

$$\begin{aligned}\left\langle \xi(t_1)\xi^\dagger(t_2)\right\rangle &= \sum_{\mathbf{k}_1,\lambda_1}\sum_{\mathbf{k}_2,\lambda_2} g_{\mathbf{k}_1,\lambda_1}g_{\mathbf{k}_2,\lambda_2}\left\langle a_{\mathbf{k}_1,\lambda_1}(t_0)a^\dagger_{\mathbf{k}_2,\lambda_2}(t_0)\right\rangle e^{-i(\omega_1-\omega_L)t_1}e^{i(\omega_2-\omega_L)t_2} \\ &= \sum_{\mathbf{k},\lambda} g^2_{\mathbf{k},\lambda}e^{-i(\omega_k-\omega_L)(t_1-t_2)} = \gamma\delta(t_1-t_2)\end{aligned} \tag{8.16a}$$

$$\left\langle \xi(t_1)\xi(t_2)\right\rangle = 0 \;, \quad \left\langle \xi^\dagger(t_1)\xi^\dagger(t_2)\right\rangle = 0 \;, \quad \left\langle \xi^\dagger(t_1)\xi(t_2)\right\rangle = 0 \;. \tag{8.16b}$$

The linear Bloch equations can be integrated including the quantum noise, $\mathbf{\Xi}(t)$ and $\mathbf{\Xi}_z(t)$, which represents an inhomogeneous driving term. Besides the decaying homogeneous part, the general solution is a linear combination of the time integrated noise. The noise, evidently, does not contribute to the mean value, however, it has a non-vanishing second-order moment and thus leads to diffusion.

Let us solve this problem in the weak excitation limit, $\sigma_z \approx -\frac{1}{2}$, where the Bloch-equations decouple. The polarization obeys a simple linear equation which can be

integrated as

$$\sigma = e^{(i\Delta_A-\gamma)t}\sigma(0) + i\Omega e^{-i\Phi}\int_0^t dt' e^{(i\Delta_A-\gamma)(t-t')} - \int_0^t dt' e^{(i\Delta_A-\gamma)(t-t')}\xi(t')$$
$$\to -\frac{i\Omega e^{-i\Phi}}{i\Delta_A-\gamma} - \int_0^t dt' e^{(i\Delta_A-\gamma)(t-t')}\xi(t') \tag{8.17}$$

The quantum correlation of the atomic polarization is

$$\begin{aligned}\left\langle\tilde\sigma(t_1)\tilde\sigma^\dagger(t_2)\right\rangle - \left\langle\tilde\sigma(t_1)\right\rangle\left\langle\tilde\sigma^\dagger(t_2)\right\rangle &= \\ &= \int_0^{t_1}dt'\int_0^{t_2}dt'' e^{(i\Delta_A-\gamma)(t_1-t')}e^{-(i\Delta_A+\gamma)(t_2-t'')}\left\langle\xi(t')\xi^\dagger(t'')\right\rangle \\ &= \int_0^{t_1}dt'\int_0^{t_2}dt'' e^{(i\Delta_A-\gamma)(t_1-t')}e^{-(i\Delta_A+\gamma)(t_2-t'')}\sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2 e^{-i(\omega_k-\omega_L)(t'-t'')} \\ &= \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda}^2 e^{(i\Delta_A-\gamma)t_1}e^{-(i\Delta_A+\gamma)t_2}\int_0^{t_1}dt' e^{[-i(\omega_k-\omega_A)+\gamma]t'}\int_0^{t_2}dt'' e^{[i(\omega_k-\omega_A)+\gamma]t''} \\ &= \sum_{\mathbf{k},\lambda}\frac{g_{\mathbf{k},\lambda}^2}{(\omega_k-\omega_A)^2+\gamma^2}e^{-i(\omega_k-\omega_L)(t_1-t_2)}\ .\end{aligned} \tag{8.18}$$

This result expresses a profound physical effect. Although the quantum noise source is supposed to be broadband, corresponding to the relevant frequency range of the vacuum field mode spectrum, the quantum noise associated with the polarization dynamics is filtered through its Lorentz-type resonance curve. This latter has a width of γ. The argument that the prefactor of the 'fast oscillating' exponential is slowly varying function of the frequency ω_k applies only for a frequency range well within the bandwidth γ. That is, the correlation function is strongly peaked around $t_1 \approx t_2$ only if the time is resolved on a much larger scale than the natural lifetime $1/\gamma$. However, this is still a good resolution for the center-of-mass dynamics which takes place on a time scale of $1/\omega_{\rm rec} \gg 1/\gamma$. As a consequence, the correlation can be considered a Dirac-δ on this time scale,

$$\left\langle\tilde\sigma(t_1)\tilde\sigma^\dagger(t_2)\right\rangle - \left\langle\tilde\sigma(t_1)\right\rangle\left\langle\tilde\sigma^\dagger(t_2)\right\rangle = \frac{\gamma}{\Delta_A^2+\gamma^2}\delta_{1/\gamma}(t_1-t_2)\ , \tag{8.19}$$

where we explicitly indicate the physical 'width' of the Dirac-δ.

8.4 Diffusion from polarization noise

The dipole force correlation function is

$$\begin{aligned}\langle\delta F_{\rm dip}(t_1)\delta F_{\rm dip}(t_2)\rangle &= \hbar^2\nabla\Omega\circ\nabla\Omega \\ &\left\langle\left(\delta\tilde\sigma^\dagger(t_1)e^{-i\Phi(\mathbf{R}_A)} + \delta\tilde\sigma(t_1)e^{i\Phi(\mathbf{R}_A)}\right)\left(\delta\tilde\sigma^\dagger(t_2)e^{-i\Phi(\mathbf{R}_A)} + \delta\tilde\sigma(t_2)e^{i\Phi(\mathbf{R}_A)}\right)\right\rangle = \\ &= \hbar^2\nabla\Omega\circ\nabla\Omega\left\langle\tilde\sigma(t_1)\tilde\sigma^\dagger(t_2)\right\rangle = \hbar^2\nabla\Omega\circ\nabla\Omega\frac{\gamma}{\Delta_A^2+\gamma^2}\delta_{1/\gamma}(t_1-t_2)\ .\end{aligned} \tag{8.20}$$

In a one-dimensional, standing wave laser field, $\Omega(\mathbf{R}_A) = \Omega \cos k_L x$, the diffusion coefficient is

$$D_{\rm dip} = (\hbar k_L)^2 \frac{\gamma \Omega^2}{\Delta_A^2 + \gamma^2} \sin^2 (k_L x) \ . \tag{8.21}$$

This diffusion is responsible for the spread of the momentum square, thus the increase of the kinetic energy occurs in units of the recoil energy $(\hbar k_L)^2/M$ per spontaneous scattering event. This fact justifies again that the characteristic energy scale of the center-of-mass dynamics is determined by the recoil frequency.

Note that the recoil diffusion in such a laser field is

$$D_{\rm rec} = \frac{2}{5} (\hbar k_A)^2 \frac{\gamma \Omega^2}{\Delta_A^2 + \gamma^2} \cos^2 (k_L x) \ , \tag{8.22}$$

being similar in order of magnitude. However, the two types of diffusion process have a maximum shifted in space. With respect to the dipole potential in such a laser field,

$$U = \frac{\hbar \Delta_A \Omega^2}{\Delta_A^2 + \gamma^2} \cos^2 (k_L x) \ , \tag{8.23}$$

the recoil noise is maximum at the antinodes where the excited state population $\langle \sigma^\dagger \sigma \rangle$ is maximum, while the dipole force fluctuations are maximum at the largest slope of the dipole potential.

The radiation pressure force correlation function can be similarly derived,

$$\begin{aligned} \langle \delta F_{\rm rp}(t_1) \delta F_{\rm rp}(t_2) \rangle &= -\hbar^2 \Omega^2 \nabla\Phi \circ \nabla\Phi \\ &\left\langle \left(\delta\tilde{\sigma}^\dagger(t_1) e^{-i\Phi(\mathbf{R}_A)} - \delta\tilde{\sigma}(t_1) e^{i\Phi(\mathbf{R}_A)} \right) \left(\delta\tilde{\sigma}^\dagger(t_2) e^{-i\Phi(\mathbf{R}_A)} - \delta\tilde{\sigma}(t_2) e^{i\Phi(\mathbf{R}_A)} \right) \right\rangle = \\ &= \hbar^2 \nabla\Phi \circ \nabla\Phi \Omega^2 \left\langle \tilde{\sigma}(t_1) \tilde{\sigma}^\dagger(t_2) \right\rangle = \hbar^2 \nabla\Phi \circ \nabla\Phi \frac{\gamma \Omega^2}{\Delta_A^2 + \gamma^2} \delta_{1/\gamma}(t_1 - t_2) \ . \end{aligned} \tag{8.24}$$

In a one-dimensional propagating plane wave $\nabla\Phi = -\mathbf{k}_L$, thus the diffusion reads

$$D_{\rm rp} = (\hbar k_L)^2 \frac{\gamma \Omega^2}{\Delta_A^2 + \gamma^2} \ . \tag{8.25}$$

8.5 Optical molasses, Doppler temperature

For proper setting of the laser field, the atoms undergo a frictional force damping the motional energy. The atoms irradiated from a pair of counter-propagating laser fields from each of the three spatial dimensions form what is called *the optical molasses*. The atoms are not trapped in a potential, but move diffusively under the strong viscous effect of the cooling laser beams. Since the friction is linear in velocity, the larger the mean kinetic energy, the larger amount of heat is dissipated. This cooling process is counteracted by the diffusion originating from the recoil diffusion and the one associated with the polarization fluctuations. The two processes are in balance at a given value of the mean kinetic energy. In this stationary situation, by the equipartition theorem, the kinetic energy is associated with a temperature.

Assume the atoms move in one dimension along a red detuned standing wave laser field. Neglecting the localization around field antinodes, the friction can be approximated by spatially averaging the result Eq. (7.22),

$$\bar{\beta} = \frac{1}{2}\hbar k^2 \frac{2\Omega^2}{\Delta_A^2 + \gamma^2} \frac{2\left|\Delta_A\right|\gamma}{\Delta_A^2 + \gamma^2} \ . \tag{8.26}$$

The diffusion coefficient, also spatially averaged, reads

$$\bar{D} = \frac{1}{2}\left(1 + \frac{2}{5}\right)(\hbar k)^2 \frac{\Omega^2 \gamma}{\Delta_A^2 + \gamma^2} \ , \tag{8.27}$$

from which the temperature, according to Eq. (6.27),

$$k_B T_{\text{Doppler}} \approx \frac{\bar{D}}{\bar{\beta}} = \frac{7}{10}\hbar\gamma \frac{\Delta_A^2 + \gamma^2}{2\left|\Delta_A\right|\gamma} \ . \tag{8.28}$$

The temperature is limited by the atomic linewidth. This is due to the fact that the dissipation channel is spontaneous emission. The velocity-dependence arises from the Doppler effect, finely tuning the resonance of width γ. The optimum detuning to minimize the temperature is $\Delta_A = -\gamma$. With this choice the temperature is about $k_B T_{\text{Doppler}} \approx \hbar\gamma$, the so-called Doppler temperature. Numerically,

$$\begin{array}{ll} 240\mu K & \text{Sodium} \\ 145\mu K & \text{Rubidium} \\ 124\mu K & \text{Cesium} \end{array} \ . \tag{8.29}$$

To a large surprise, the measurements yielded somewhat lower temperatures, moreover, the lowest temperature was obtained at a detuning $\Delta_A = -3\gamma$. These observations indicated that there is a mechanism responisble for cooling other than the Doppler-cooling that we have studied so far. For a better understanding, one needs to consider the multilevel structure of atoms.

Chapter 9

Polarization-gradient cooling

9.1 Radiation field with polarization gradient

Let us consider the field arising from two counterpropagating, monochromatic plane-wave modes having orthogonal linear polarizations. This configuration is called 'lin⊥lin'. The electric field, to be real, has a positive and negative frequency part,

$$\mathbf{E}(z,t) = \mathcal{E}^{(+)}(z)e^{-i\omega_L t} + \mathcal{E}^{(-)}(z)e^{i\omega_L t} \,, \tag{9.1}$$

with the two modes

$$\mathcal{E}^{(+)}(z) = \mathcal{E}_0\epsilon e^{ikz} + \mathcal{E}_0'\epsilon' e^{-ikz} \,. \tag{9.2}$$

Let us shift the origin of the coordiante space to $z \to z + \lambda/8$ for later convenience. The polarizations are $\epsilon = \epsilon_x$ and $\epsilon' = \epsilon_y$. For simplicity, the amplitudes are chosen to be equal, i.e., $\mathcal{E}_0 = \mathcal{E}_0'$. The total amplitude can be expressed in various equivalent forms,

$$\begin{aligned}
\mathcal{E}^{(+)}(z)/\mathcal{E}_0 &= \epsilon_x \frac{1+i}{\sqrt{2}}(\cos kz + i\sin kz) + \epsilon_y \frac{1-i}{\sqrt{2}}(\cos kz - i\sin kz) \\
&= \frac{\epsilon_x+\epsilon_y}{\sqrt{2}}(\cos kz - \sin kz) + i\frac{\epsilon_x-\epsilon_y}{\sqrt{2}}(\cos kz + \sin kz) \qquad (9.3a) \\
&= (1+i)\left(\cos kz \frac{\epsilon_x - i\epsilon_y}{\sqrt{2}} + i\sin kz \frac{\epsilon_x + i\epsilon_y}{\sqrt{2}}\right) \,. \qquad (9.3b)
\end{aligned}$$

The expression in the second line shows that the field is linearly polarized in the positions where $\cos kz = \pm \sin kz$. For $\tan kz = 1$, which occurs with periodicity π, the polarization is $\frac{\epsilon_x+\epsilon_y}{\sqrt{2}}$, while for $\pi/2$ shifted positions it is $\frac{\epsilon_x-\epsilon_y}{\sqrt{2}}$. Both directions make an angle of $\pi/4$ with x and y. In the middle positions, i.e., $kz = (n+1/4)\pi$, the field has a circular polarization alternatively in the $\epsilon_\pm$ directions. These are two basis vectors of the spherical coordinate system, defined as

$$\epsilon_+ = -\frac{1}{\sqrt{2}}(\epsilon_x + i\epsilon_y) \,, \tag{9.4a}$$

$$\epsilon_0 = \epsilon_z \,, \tag{9.4b}$$

$$\epsilon_- = \frac{1}{\sqrt{2}}(\epsilon_x - i\epsilon_y) \,. \tag{9.4c}$$

In summary the field has a spatially dependent polarization. Any transition with a given polarization is driven with spatially varying strength, hence the Rabi frequency has a gradient because of the varying polarization, not because of the varying intensity. At the same time, the atomic internal dynamics cannot be restricted to two levels, since the transitions with different rotational symmetry are excited by the laser field at different positions.

9.2 Atomic multiplet transitions

In the spherical coordinate system defined by the unit ortho-normalized basis vectors ϵ_q, $q = \pm, 0$, the components of a vector can be expressed as,

$$r_+ = -\frac{1}{\sqrt{2}} r \sin\theta e^{i\phi} = \left(\frac{4\pi}{3}\right)^{1/2} r Y_{1,1}(\theta,\phi) \tag{9.5a}$$

$$r_0 = r\cos\theta = \left(\frac{4\pi}{3}\right)^{1/2} \hat{r} Y_{1,0}(\hat{\theta},\hat{\phi}) \ , \tag{9.5b}$$

$$r_- = -\frac{1}{\sqrt{2}} r \sin\theta e^{-i\phi} = \left(\frac{4\pi}{3}\right)^{1/2} r Y_{1,-1}(\theta,\phi) \tag{9.5c}$$

where $Y_{J,M}(\theta,\phi)$ are the spherical harmonics. Thus the position vector is

$$\mathbf{r} = \left(\frac{4\pi}{3}\right)^{1/2} r \sum_{q=-1,0,1} \epsilon_q Y_{1,q}(\theta,\phi) \ . \tag{9.6}$$

The matrix elements of the dipole operator can be conveniently calculated in this basis

$$\begin{aligned}\langle J_e M_e |\, e\hat{\mathbf{r}} \,| J_g M_g\rangle &= \langle J_e |\, er \,| J_g\rangle \sum_q \epsilon_q \left(\frac{4\pi}{3}\right)^{1/2} \int d\Omega Y^*_{J_e,M_e}(\theta,\phi) Y_{1,q}(\theta,\phi) Y_{J_g,M_g}(\theta,\phi) \\ &= d_{eg}\sqrt{\frac{2J_g+1}{2J_e+1}} \langle J_g 100 \mid J_e 0\rangle \sum_q \epsilon_q \langle J_g 1 M_g q \mid J_e M_e\rangle \ , \end{aligned} \tag{9.7}$$

where we used the relation

$$\begin{aligned}\int d\Omega Y^*_{J_e,M_e}(\theta,\phi) Y_{1,q}(\theta,\phi) Y_{J_g,M_g}(\theta,\phi) &= (-1)^{M_e} \int d\Omega Y_{J_g,M_g} Y_{1,q} Y_{J_e,-M_e} \\ &= \left((-1)^{M_e}\right)^2 \left(\frac{(2J_g+1)\,3}{4\pi(2J_e+1)}\right)^{1/2} \langle J_g 100 \mid J_e 0\rangle \langle J_g 1 M_g q \mid J_e M_e\rangle \ , \end{aligned} \tag{9.8}$$

and the definition

$$d_{eg} = \langle J_e |\, er \,| J_g\rangle = \int dr r^3 R^*_{e,J_e} R_{g,J_g} \ . \tag{9.9}$$

Note that the radial functions depend on the multiplicity J in general (the Coulomb problem is an exception).

Thus the dipole operator for an atomic transition between multiplets can be written as

$$\hat{\mathbf{d}} = d_{eg}\sqrt{\frac{2J_g+1}{2J_e+1}} \langle J_g 100 \mid J_e 0\rangle \sum_{q=0,\pm1} \left(\epsilon_q \sigma_q + \epsilon_q^* \sigma_q^\dagger\right) \ , \tag{9.10}$$

where the generalized polarization operators are defined as

$$\sigma_q = \sum_{M_g} \langle J_g 1 M_g q \mid J_e, M_g + q \rangle \, |J_g M_g\rangle \, \langle J_e, M_g + q| \ . \tag{9.11}$$

A given polarization q may induce several transitions, however, the corresponding weights, referred to as the "Clebsch-Gordon" coefficients are different. In most cases of interest $J_e = J_g + 1$, then

$$\langle J_g 100 \mid J_e 0 \rangle = \sqrt{\frac{J_e}{2J_g + 1}} \ , \quad \text{for} \quad J_e = J_g + 1 \ . \tag{9.12}$$

Let us consider the special case of a $J_g = 0 \longleftrightarrow J_e = 1$ transition and relate it to the two-level approximation of atoms.

$$\hat{\mathbf{d}} = \frac{d_{eg}}{\sqrt{3}} \sum_{q=-1}^{1} \epsilon_q \, |00\rangle \, \langle 1q| + h.c. \ , \tag{9.13}$$

where we used $\langle 010q \mid 1q \rangle = 1$. Each transition corresponds to one given polarization. Note that $d_{eg}/\sqrt{3}$ corresponds to what we have defined d_{eg} in the two-level atom approximation. Since the dipole moment is the same in each directions (also in the x,y,z cartesian basis), the absolute square of the dipole moment vector is $3(d_{eg}/\sqrt{3})^2 = d_{eg}^2$, i.e., the one we used for the two-level atom.

9.3 $J_g = \frac{1}{2} \leftrightarrow J_e = \frac{3}{2}$ transition in lin $\perp$ lin configuration

The Clebsch-Gordon coefficients are summarized in Fig. 9.1.

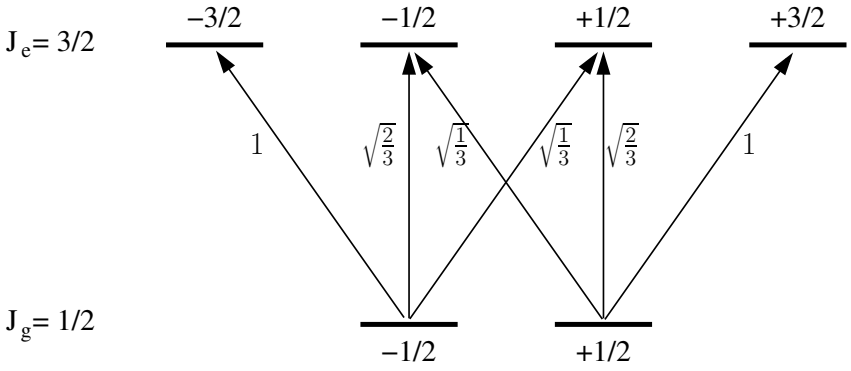

Figure 9.1: The Clebsch-Gordon coefficients for $1/2 \leftrightarrow 3/2$ transition.

The atom-laser coupling in the dipole and rotating-wave approximations is described by the Hamiltonian

$$H_{AL} = -\mathbf{dE}(\mathbf{R}_A, t) = -\sqrt{\frac{3}{8}} d_{eg} \sum_{q=0,\pm 1} \epsilon_q^* \sigma_q^\dagger \mathcal{E}(z) e^{-i\omega_L t} + H.c \tag{9.14}$$

In a frame rotating at the laser frequency

$$H = -\hbar\Delta_A \sum_{M_e} |J_e, M_e\rangle \langle J_e, M_e| - \sqrt{\frac{3}{8}} d_{eg}\sqrt{2}\mathcal{E}_0 \sum_{q=0,\pm1} \frac{1+i}{\sqrt{2}} \epsilon_q^* \sigma_q^\dagger (\epsilon_- \cos kz - i\epsilon_+ \sin kz) + H.c$$
$$= -\hbar\Delta_A \hat{P}_e - \hbar\Omega \cos kz \left(|e_{-3/2}\rangle \langle g_{-1/2}| + \frac{1}{\sqrt{3}} |e_{-1/2}\rangle \langle g_{1/2}| + H.c \right) -$$
$$- i\hbar\Omega \sin kz \left(\frac{1}{\sqrt{3}} |e_{1/2}\rangle \langle g_{-1/2}| + |e_{3/2}\rangle \langle g_{1/2}| - H.c \right) \quad (9.15)$$

where Ω is the Rabi frequency. The equations of motion for the mean values are readily obtained. Denoting the means $\rho(a_i, b_j) = \langle |a_i\rangle \langle b_j| \rangle$, where $a, b = e, g$ and i, j are the Zeeman-sublevel indices, the polarizations evolve as

$$\dot{\rho}(g_{1/2}, e_{3/2}) = (i\Delta_A - \gamma)\rho(g_{1/2}, e_{3/2}) - \Omega \sin kz \left(\rho(g_{1/2}, g_{1/2}) - \rho(e_{3/2}, e_{3/2})\right)$$
$$- i\Omega/\sqrt{3} \cos kz \rho(e_{-1/2}, e_{3/2}) \,,$$

$$\dot{\rho}(g_{1/2}, e_{-1/2}) = (i\Delta_A - \gamma)\rho(g_{1/2}, e_{-1/2}) + i\Omega/\sqrt{3} \cos kz \left(\rho(g_{1/2}, g_{1/2}) - \rho(e_{-1/2}, e_{-1/2})\right)$$
$$+ \Omega \sin kz \rho(e_{3/2}, e_{-1/2}) \,,$$

$$\dot{\rho}(g_{-1/2}, e_{1/2}) = (i\Delta_A - \gamma)\rho(g_{-1/2}, e_{1/2}) - \Omega/\sqrt{3} \sin kz \left(\rho(g_{-1/2}, g_{-1/2}) - \rho(e_{1/2}, e_{1/2})\right)$$
$$- i\Omega \cos kz \rho(e_{-3/2}, e_{1/2}) \,,$$

$$\dot{\rho}(g_{-1/2}, e_{-3/2}) = (i\Delta_A - \gamma)\rho(g_{-1/2}, e_{-3/2}) + i\Omega \cos kz \left(\rho(g_{-1/2}, g_{-1/2}) - \rho(e_{-3/2}, e_{-3/2})\right) +$$
$$\Omega/\sqrt{3} \sin kz \rho(e_{1/2}, e_{-3/2}) \,.$$

The excited state populations evolve as

$$\dot{\rho}(e_{3/2}, e_{3/2}) = -2\gamma\rho(e_{3/2}, e_{3/2}) - \Omega \sin kz \left(\rho(e_{3/2}, g_{1/2}) + \rho(g_{1/2}, e_{3/2})\right) \,,$$
$$\dot{\rho}(e_{1/2}, e_{1/2}) = -2\gamma\rho(e_{1/2}, e_{1/2}) - \frac{\Omega}{\sqrt{3}} \sin kz \left(\rho(e_{1/2}, g_{-1/2}) + \rho(g_{-1/2}, e_{1/2})\right) \,,$$
$$\dot{\rho}(e_{-1/2}, e_{-1/2}) = -2\gamma\rho(e_{-1/2}, e_{-1/2}) + \frac{i\Omega}{\sqrt{3}} \cos kz \left(\rho(e_{-1/2}, g_{1/2}) - \rho(g_{1/2}, e_{-1/2})\right) \,,$$
$$\dot{\rho}(e_{-3/2}, e_{-3/2}) = -2\gamma\rho(e_{-3/2}, e_{-3/2}) + i\Omega \cos kz \left(\rho(e_{-3/2}, g_{-1/2}) - \rho(g_{-1/2}, e_{-3/2})\right) \,.$$

Let us consider the weak driving limit realized by a Rabi frequency Ω much smaller than the detuning Δ_A, or the linewidth γ. There is a small saturation $s = \frac{\Omega^2}{\Delta_A^2+\gamma^2} \ll 1$, correspondingly, the population is dominantly in the ground states, i.e., $\rho(g_{\pm1/2}, g_{\pm1/2}) = \mathcal{O}(1)$. The polarization associated with each transition is of first order in Ω, while the populations in the excited states is of second order in Ω. One can systematically derive the leading order solution of the total system of equations by

considering the steady-state polarizations approximated by

$$\rho(g_{1/2}, e_{3/2}) \approx -\frac{\Omega}{-i\Delta_A + \gamma} \sin kz \, \Pi_{1/2} \ , \tag{9.16a}$$

$$\rho(g_{1/2}, e_{-1/2}) \approx \frac{i}{\sqrt{3}} \frac{\Omega}{-i\Delta_A + \gamma} \cos kz \, \Pi_{1/2} \ , \tag{9.16b}$$

$$\rho(g_{-1/2}, e_{1/2}) \approx -\frac{1}{\sqrt{3}} \frac{\Omega}{-i\Delta_A + \gamma} \sin kz \, \Pi_{-1/2} \ , \tag{9.16c}$$

$$\rho(g_{-1/2}, e_{-3/2}) \approx i \frac{\Omega}{-i\Delta_A + \gamma} \cos kz \, \Pi_{-1/2} \ , \tag{9.16d}$$

where we have introduced the notation $\Pi_{\pm 1/2} \equiv \rho(g_{\pm 1/2}, g_{\pm 1/2}$ for the ground state populations. Similarly, the excited state populations are given in leading order by

$$\rho(e_{3/2}, e_{3/2}) \approx \frac{\Omega^2}{\Delta_A^2 + \gamma^2} \sin^2 kz \, \Pi_{1/2} \ , \tag{9.17a}$$

$$\rho(e_{1/2}, e_{1/2}) \approx \frac{1}{3} \frac{\Omega^2}{\Delta_A^2 + \gamma^2} \sin^2 kz \, \Pi_{-1/2} \ , \tag{9.17b}$$

$$\rho(e_{-1/2}, e_{-1/2}) \approx \frac{1}{3} \frac{\Omega^2}{\Delta_A^2 + \gamma^2} \cos^2 kz \, \Pi_{1/2} \ , \tag{9.17c}$$

$$\rho(e_{-3/2}, e_{-3/2}) \approx \frac{\Omega^2}{\Delta_A^2 + \gamma^2} \cos^2 kz \, \Pi_{-1/2} \ , \tag{9.17d}$$

$$\tag{9.17e}$$

The adiabatic dynamics of the ground state populations

The polarizations and the excited state populations evolve fast, the dynamical timescale is being given by Δ_A and γ, therefore these variables of the system can be "slaved" to the slowly varying ground state populations by the relations Eq. (9.16) and Eq. (9.17). An adiabatic Hamiltonian can be constructed from Eq. (9.15) by using the adiabatic solution for the polarizations with the populations retained as operators,

$$H_{\rm ad} = \hbar \Delta_A \, s \, \frac{1}{3} \left[(1 + 2\cos^2 kz) \left| g_{-1/2} \right\rangle \left\langle g_{-1/2} \right| + (1 + 2\sin^2 kz) \left| g_{1/2} \right\rangle \left\langle g_{1/2} \right| \right] \ . \tag{9.18}$$

This Hamiltonian is diagonal in the ground states $\left|g_{-1/2}\right\rangle$ and $\left|g_{1/2}\right\rangle$, which remain thus eigenstates of the interacting system in the low saturation limit. Therefore there are no oscillations in the dynamics, only the corresponding eigenenergies are redefined, remarkably, the energies pick up a spatially dependent character. This simple structure of the Hamiltonian originates from the lack of coherent two-photon coupling between the two ground states by the two laser fields. The adiabatic population redistribution between the ground states arises solely from decay processes via the virtually excited $\left|e_{\pm 1/2}\right\rangle$ states. The slow evolution of the master variables can be obtained from the

original Bloch-equations by using the adiabatic expressions for the slaved variables,

$$\begin{aligned}\dot{\Pi}_{-1/2} &= i\Omega\cos kz\left(\rho(g_{-1/2},e_{-3/2})-\text{c.c.}\right)+\frac{\Omega}{\sqrt{3}}\sin kz\left(\rho(g_{-1/2},e_{1/2})+\text{c.c.}\right)\\ &+2\gamma\left(\rho(e_{-3/2},e_{-3/2})+\frac{2}{3}\rho(e_{-1/2},e_{-1/2})+\frac{1}{3}\rho(e_{1/2},e_{1/2})\right)\\ &=-2\gamma\, s\,\cos^2 kz\Pi_{-1/2}-\frac{1}{3}2\gamma\, s\,\sin^2 kz\Pi_{-1/2}\\ &+2\gamma\, s\left(\cos^2 kz\Pi_{-1/2}+\frac{2}{3}\frac{1}{3}\cos^2 kz\Pi_{1/2}+\frac{1}{3}\frac{1}{3}\sin^2 kz\Pi_{-1/2}\right)\\ &=-2\gamma\, s\left(\frac{2}{9}\sin^2 kz\Pi_{-1/2}-\frac{2}{9}\cos^2 kz\Pi_{1/2}\right)\approx-\frac{4\gamma\, s}{9}\left(\Pi_{-1/2}-\cos^2 kz\right)\ , \quad (9.19a)\end{aligned}$$

where in the last step we used $\Pi_{-1/2}+\Pi_{1/2}=1-\mathcal{O}(s)$. For the other ground state $|1/2\rangle$, the derivation follows analogously and leads to

$$\dot{\Pi}_{+1/2}=-\frac{4\gamma\, s}{9}\left(\Pi_{1/2}-\sin^2 kz\right)\ . \quad (9.19b)$$

The stationary solution reads

$$\Pi^{\text{st}}_{\pm 1/2}=\begin{cases}\sin^2 kz\\ \cos^2 kz\end{cases}+\mathcal{O}(s)\ . \quad (9.20)$$

This result reflects the effect of *optical pumping*: the population is irreversibly transfered into the state $\left|g_{-1/2}\right\rangle$ under the effect of a field with ϵ_- polarization and, reversely, it is transfered into $\left|g_{+1/2}\right\rangle$ in a ϵ_+ polarized driving field. The reason is that the system is trapped, when the field is ϵ_- polarized, in the $\left|g_{-1/2}\right\rangle \leftrightarrow \left|e_{-3/2}\right\rangle$ transition. Meanwhile, the system leaks out from the state $\left|g_{+1/2}\right\rangle$ via the state $\left|e_{-1/2}\right\rangle$, this latter spontaneously decaying into $\left|g_{-1/2}\right\rangle$. This happens in the positions $kz=0$, and the reverse optical pumping process takes place in the positions $kz=\pi/2$.

It follows from the differential equations (9.19) that the time scale of this optical pumping is about $(s_0\gamma)^{-1}$, much longer than the decay time of the excited states and that of the polarizations (γ^{-1}). As we learned from the mechanism of Doppler cooling, some non-adiabatic evolution of the internal degrees of freedom is needed to produce velocity dependent forces. For a two-level atom the only time scale characteristic of the internal dynamics was γ^{-1}, and velocities as small as $kv\ll\gamma$ can induce closely adiabatic variation of the σ operators. By contrast, here we found that the adiabatic limit is reached at much slower velocities, $kv\ll s\gamma$. As a consequence, the cooling mechanism, which we will refer to as *polarization gradient cooling*, remains efficient for much lower velocities.

9.4 The Sisyphus-cooling effect

For an atom at rest, the populations reach the local values $\cos^2 kz$ and $\sin^2 kz$ in the state $\left|g_{-1/2}\right\rangle$ and $\left|g_{1/2}\right\rangle$, respectively. Note that the larger population can be found in the state having lower energy. Optical pumping in this scheme transfers thus the

population from the higher- to the lower-lying ground state. For a moving atom, the spatially modulated ground state energy appears as a potential. One can imagine the atomic motion as an adiabatic following of the $\cos^2 kz$ potential, randomly interrupted by quantum jumps into the other ground state. These jumps can represent the optical pumping. Therefore, if an atom changes its position it is likely that it climbs up the potential hill and then will be optically pumped to the lower-lying state, then the opposite process. On average, the atom loses kinetic energy, i.e., it is cooled. This is the Sisyphus-type interpretation of the cooling mechanism.

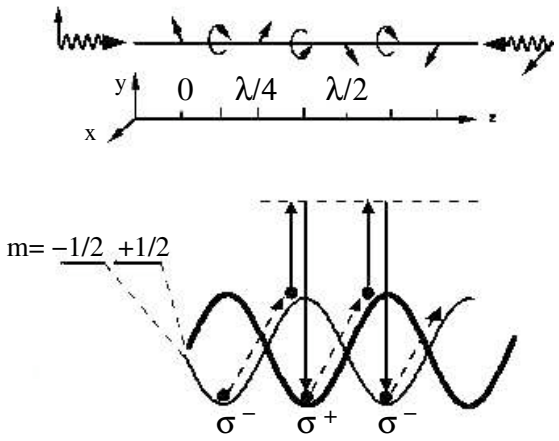

Figure 9.2: Combination of light shifts and optical pumping induced by the field with polarization gradient. The cooling interpreted in terms of the Sysiphus mechanism.

The force can be directly accessed as it is the gradient of the Hamiltonian Eq. (9.14),

$$\begin{aligned} F &= -\hbar k\Omega \sin kz \left(\rho(g_{-1/2}, e_{-3/2}) + \frac{1}{\sqrt{3}}\rho(g_{1/2}, e_{-1/2}) + \text{c.c.} \right) \\ &\quad - \hbar k\Omega \cos kz\, i \left(\frac{1}{\sqrt{3}}\rho(g_{-1/2}, e_{1/2}) + \rho(g_{1/2}, e_{3/2}) - \text{c.c.} \right) \\ &= -\hbar k\Omega \sin kz \left(\frac{-2\Delta_A\Omega}{\Delta_A^2+\gamma^2} \cos kz\, \Pi_{-1/2} + \frac{1}{3}\, \frac{-2\Delta_A\Omega}{\Delta_A^2+\gamma^2} \cos kz\, \Pi_{1/2} \right) \\ &\quad + \hbar k\Omega \cos kz \left(-\frac{1}{3}\, \frac{2\Delta_A\Omega}{\Delta_A^2+\gamma^2} \sin kz\, \Pi_{-1/2} - \frac{2\Delta_A\Omega}{\Delta_A^2+\gamma^2} \sin kz\, \Pi_{1/2} \right) \\ &= \frac{2}{3}\, \hbar k\, \Delta_A\, s\, \left(\Pi_{-1/2} - \Pi_{1/2} \right) \sin 2kz \end{aligned} \tag{9.21}$$

Let us calculate the response of the force to displacement. Assume that the atom moves with a constant velocity v, and insert $z = vt$ into the differential equation (9.19):

$$\dot{\Pi}_i(t) = -\frac{1}{\tau_p} \left(\Pi_i(t) - \Pi_i^{st}(vt) \right) \ , \tag{9.22}$$

where $i = \pm 1/2$, and $1/\tau_p = 4s\gamma/9$. This equation can be solved for arbitrary velocity v,

$$\Pi_i(t) = e^{-t/\tau_p}\Pi_i(0) + \frac{1}{\tau_p}\int_0^t e^{\frac{t'-t}{\tau_p}} \Pi_i^{st}(vt')\mathrm{d}t' \approx e^{-t/\tau_p} \int_{-\infty}^{t/\tau_p} e^x \Pi_i^{st}(v\tau_p x)\mathrm{d}x \ , \tag{9.23}$$

where the initial transient is removed. From the integral

$$\int \mathrm{d}x\, e^x \cos ax = \frac{e^x(\cos ax + a \sin ax)}{1+a^2} \,, \tag{9.24}$$

on identifying $a = 2kv\tau_p$, one arrives at

$$\Pi_\pm = \frac{1}{2} \mp \frac{1}{2} \frac{\cos 2kvt + 2kv\tau_p \sin 2kvt}{1 + (2kv\tau_p)^2} \,. \tag{9.25}$$

By using the force in Eq. (9.21), the velocity dependence is obtained,

$$F(v) = \frac{2}{3} \hbar k \, \Delta_A \, s \, \frac{\sin 4kvt + 4kv\tau_p \sin^2 2kvt}{1 + (2kv\tau_p)^2} \,. \tag{9.26}$$

Assuming that the atom passes through several wavelength during the time τ_p, this instantaneous force can be averaged over the position, which yields

$$\bar{F}(v) = \frac{2}{3} \hbar k^2 \, \Delta_A \, s \, \tau_p \frac{v}{1 + \left(\frac{v}{v_c}\right)^2} \,, \tag{9.27}$$

where $v_c = \frac{1}{2k\tau_p}$ is a characteristic velocity corresponding to the maximum of the force and it also defines the velocity capture range. The velocity dependent force amounts to friction if the detuning is negative, i.e., $\Delta_A < 0$.

The maximum friction coefficient exceeds that of the Doppler cooling scheme by a factor of $1/s$, however, the velocity capture range is smaller by a factor of s. Thus this efficient cooling mechanism operates at low velocities. The friction force depends only weakly on s (in higher order powers of v), which shows that the friction cooling ceases to work when the atom gets trapped in one of the potential wells given by the internal energy expression Eq. (9.18). The momentum uncertainty arises from the randomness of the direction of the last scattered photon. The limiting temperature thus is the recoil temperature $k_B T_{\mathrm{rec}} = \hbar^2 k^2 / 2M$.

Chapter 10

Basic methods in laser cooling and trapping

In this chapter we review the basic principles of the most common techniques used nowadays in the laboratories. The magneto-optical trapping (MOT) is the standard method to produce cold atomic sample with high density and large atom numbers. This trap has a mechanism which simultaneously confines in space and cools the atoms. The sideband cooling method can be applied to trapped atoms, eventually in a quantized center-of-mass motional state, and results in very low temperatures well below the recoil limit.

10.1 Magneto-optical trapping

The interaction of atoms with a magnetic field via the magnetic moment of atoms has not been previously included in the theory which was based on the electric dipole approximation. This higher order interaction can be taken into account by the Hamiltonian term

$$H = -\mu \mathbf{B} \ . \tag{10.1}$$

The atomic magnetic moment is

$$\mu = g_F \mu_B \mathbf{F} \ , \tag{10.2}$$

i.e., the product of the Bohr-magneton $\mu_B = e\hbar/2m_e = 9.3 \times 10^{-24} J/T$, the Landé-factor g_F, and the quantum operator $\mathbf{F}$ associated with the total angular momentum of the atom. Let us assume that the atom moves very slowly on the length scale characterizing the magnetic field variation. In that case the moving atom adiabatically follows an eigenstate of the z component of the angular momentum where the orientation of the quantization axis is alway defined parallel with the direction of the local magnetic field. Therefore the scalar product can be replaced and the force acting on an atom in an inhomogeneous static magnetic field is

$$F = g_F \mu_B \, M \, \nabla |\mathbf{B}(\mathbf{R})| \ , \tag{10.3}$$

where M is the angular momentum projection on the direction of the local magnetic field. The atomic states are characterized by the total electron spin S, the total orbital

momentum of the electron cloud L, the total angular momentum of the electrons J, and the nucleus spin I. The Landé-factor is

$$g_F = g_j \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)} \tag{10.4}$$

$$g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \tag{10.5}$$

The quantum number M takes on the values $M = -F, -F+1, \ldots F-1, F$, altogether $2F+1$ states. As the modulus of the magnetic field can have a local minimum in three dimension, atoms can be confined in space. With static magnetic fields one can trap only the "low-field seekers" which are the positive or negative M states, depending on the sign of g_F.

The Helmholtz configuration of coils, i.e., in two circular wires sharing the same axis the currents flow in opposite directions, produces a quadrupole trap. The magnetic field close to the center is approximately

$$|B(\mathbf{R})| = A\sqrt{\rho^2 + 4z^2}\,, \tag{10.6}$$

in cylindrical coordinates. Because of the anisotropy the angular momentum of the center-of-mass motion is not conserved. The main problem with this very simple configuration is that the magnetic field vanishes in the trap center, $|\mathbf{B}(0,0,0)| = 0$, which results in non-adiabatic transition between the states M, the so-called Majorana spin flips. A transition from a low-field seeking state into a high field seeking one leads to the loss of the atom from the trap. This problem can be avoided by adding a homogeneous offset magnetic field, which is provided for example in the Ioffe-Pritchard configuration.

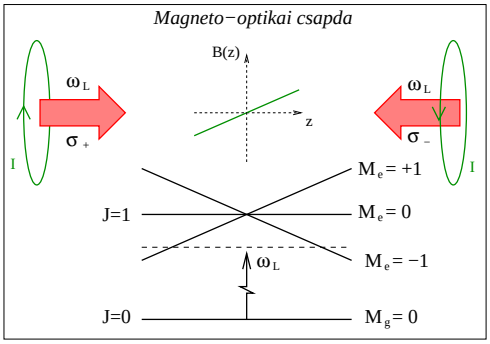

Figure 10.1: Basic scheme of magneto-optical trapping. The spatially inhomogeneous magnetic field induced Zeeman shift tunes the optical resonance with respect to the pump lasers.

Underlying the principle of magneto-optical trapping, there is the effect of the Zeeman-shift on the optical properties of atoms. So it is not directly the mechanical force exerted by the inhomogeneous magnetic field, according to Eq. (10.3), that is considered but that the transition frequencies in the atom spatially vary. This can induce a spatially dependent radiation pressure force, for example,

$$\mathbf{F} = \hbar\mathbf{k}\gamma \frac{2\Omega^2}{(\Delta_A - \mathbf{kv} - \mu' B(\mathbf{R})/\hbar)^2 + \gamma^2 + 2\Omega^2}\,, \tag{10.7}$$

where $\mu' = (g_e M_e - g_g M_g)\mu_B$, using the adiabatic shift of the energies originating from the Hamiltonian Eq. (10.1). For small Zeeman shift and small Doppler shift, the linearization yields

$$\mathbf{F} = -\beta v - \kappa z \ , \tag{10.8}$$

with

$$\kappa = \frac{\mu' A}{\hbar k}\beta = \mu' A\, k\, \frac{s}{(1+s)^2}\frac{2\gamma\Delta_A}{\Delta_A^2+\gamma^2} \ . \tag{10.9}$$

The magnetic field gradient along the axis is denoted by A. The magneto-optical force, benefiting from the resonant character of the transition, is a factor of kz larger than the bare magnetic gradient force $\sim \mu A$.

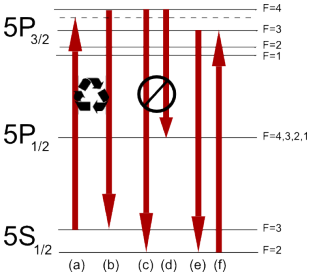

Figure 10.2: Levels scheme: Cooling on the $F_g = I + S \leftrightarrow F_e = F_g + 1$ transition (for Rb85, I=5/2, S=1/2, so $F_g = 3 \leftrightarrow F_e = 4$). However, there is a small probability of exciting $F'_e = 3$ from which state the atom can decay into $F'_g = I - S = 2$. By applying a resonant driving on the $F'_g = 2 \leftrightarrow F'_e = 3$ transition, the so-called *repumper*, the atom can get back into the cooling cycle.

10.2 Sideband cooling

We will consider the motion of a two-level atom of mass m in a harmonic potential in one-dimension along the axis z. The atom is illuminated by a single propagating laser field from a direction making an angle θ with the z axis. The Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\nu^2 z^2 + \hbar\omega_A\sigma_z + \hbar\Omega\left(\sigma^\dagger e^{-i(\omega_L t + k_z z)} + \sigma e^{i(\omega_L t + k_z z)}\right) \ . \tag{10.10}$$

Let us introduce the bosonic creation and annihilation operators, $b^\dagger$ and b, of vibrational quanta. The harmonic oscillator energy becomes $\hbar\nu b^\dagger b$. The position operator can be expressed as $z = \sqrt{\frac{\hbar}{2m\nu}}(b + b^\dagger)$. The prefactor expresses the width of the ground state wavefunction in the harmonic trap. This is usually small compared to the wavelength, therefore the *the Lamb-Dicke parameter*, $\eta = \sqrt{\frac{\hbar k^2}{2m\nu}}$ is a small one. The exponential function can be expanded into power series,

$$e^{-i\eta(b+b^\dagger)} = 1 - i\eta(b+b^\dagger) - \frac{\eta^2}{2}(b+b^\dagger)^2 + i\frac{\eta^3}{6}(b+b^\dagger)^3 + \dots \ . \tag{10.11}$$

In the Lamb-Dicke regime only the first non-trivial term is retained. Higher order terms lead to intriguing nonlinear effects which are subject to research in other fields

of quantum optics. The Hamiltonian in interaction picture reads

$$H_{\text{int}} = -i\hbar\,\Omega\,\eta\,\left[\left(\sigma^\dagger e^{-i\Delta_A t} - \sigma e^{i\Delta_A t}\right)\left(b e^{-i\nu t} + b^\dagger e^{i\nu t}\right)\right]\,. \tag{10.12}$$

For the most efficient sideband cooling, the laser has to be tuned one vibrational quantum below the atomic resonance, i.e., $\omega_L = \omega_A - \nu$. In the interaction picture Hamiltonian some of the terms become time independent (or slowly oscillating in case of near resonance, $\Delta_A \approx -\nu$), the remaining ones rotate at least with an angular frequency of 2ν. When the vibrational frequency is much larger than any other frequency in the dynamical system, that is, the effective Rabi frequency $\eta\Omega$ and the spontaneous decay rate γ, the system is in *the resolved sideband limit*, and the rotating terms can be neglected (secular approximation). The effective Hamiltonian simplifies to

$$H_{\text{int}} = -i\hbar\,\Omega\,(\sigma^\dagger b + b^\dagger\sigma)\,. \tag{10.13}$$

The vibrational motion of the atom in the trap can be dissipated via the spontaneous emission channel. This process will be described in the low saturation limit, when the atom is hardly excited and σ_z can be replaced by the c-number $-\frac{1}{2}$. The operators σ and $\sigma^\dagger$ formally are considered bosonic operators. One gets a simple set of coupled linear differential equations

$$\dot{b} = -\eta\Omega\sigma\,, \tag{10.14a}$$

$$\dot{\sigma} = -\gamma\sigma + \eta\Omega b + \xi\,, \tag{10.14b}$$

where ξ is the quantum noise associated with the decay process. The eigenfrequencies of the linear system are

$$\lambda_\pm = -\frac{\gamma}{2} \pm \sqrt{\left(\frac{\gamma}{2}\right)^2 - (\eta\Omega)^2} \approx -\frac{\gamma}{2} \pm \frac{\gamma}{2} \mp \frac{(\eta\Omega)^2}{\gamma} + \gamma\mathcal{O}\left(\frac{(\eta\Omega)}{\gamma}\right)^4\,, \tag{10.15}$$

where, in the approximation, we considered the overdamped limit, $\frac{\eta\Omega}{\gamma} \ll 1$. The vibrational mode is damped with a characteristic rate $\frac{(\eta\Omega)^2}{\gamma}$.