

# Chapter 4

## The quantum theory of light

In this chapter we study the quantum theory of interactions between light and matter. Historically the understanding how light is created and absorbed by atoms was central for development of quantum theory, starting with Planck's revolutionary idea of *energy quanta* in the description of black body radiation. Today a more complete description is given by the theory of *quantum electrodynamics* (QED), which is a part of a more general relativistic quantum field theory (the standard model) that describe the physics of the elementary particles. Even so the non-relativistic theory of photons and atoms has continued to be important, and has been developed further, in directions that are referred to as *quantum optics*. We will study here the basics of the non-relativistic description of interactions between photons and atoms, in particular with respect to the processes of spontaneous and stimulated emission. As a particular application we study a simple model of a laser as a source of *coherent light*.

### 4.1 Classical electromagnetism

The Maxwell theory of electromagnetism is the basis for the classical as well as the quantum description of radiation. With some modifications due to *gauge invariance* and to the fact that this is a *field theory* (with an infinite number of degrees of freedom) the quantum theory can be derived from classical theory by the standard route of *canonical quantization*. In this approach the natural choice of generalized coordinates correspond to the *field amplitudes*.

In this section we make a summary of the classical theory and show how a Lagrangian and Hamiltonian formulation of electromagnetic fields interacting with point charges can be given. At the next step this forms the basis for the quantum description of interacting fields and charges.

#### 4.1.1 Maxwell's equations

Maxwell's equations (in Heaviside-Lorentz units) are

$$\nabla \cdot \mathbf{E} = \rho$$

$$\begin{aligned}
\nabla \times \mathbf{B} - \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} &= \frac{1}{c} \mathbf{j} \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} &= 0
\end{aligned} \tag{4.1}$$

with  $\mathbf{E}$  and  $\mathbf{B}$  as the electric and magnetic field strengths and  $\rho$  and  $\mathbf{j}$  as the charge density and current density. The equations are invariant under the relativistic Lorentz transformations, and this symmetry is manifest in a covariant formulation of the equations. In the covariant formulation the electric and magnetic fields are combined in the *electromagnetic field tensor*  $F^{\mu\nu}$ , where the indices  $\mu$  and  $\nu$  run from 0 to 3, with  $\mu = 0$  representing the time component and  $\mu = 1, 2, 3$  the space components of the space-time variables<sup>1</sup>. Written as a matrix the field tensor takes the form (when the first line and row correspond to the 0th component),

$$F = \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & B_z & -B_y \\ -E_y & -B_z & 0 & B_x \\ -E_z & B_y & -B_x & 0 \end{pmatrix} \tag{4.2}$$

The *dual field tensor* is defined by  $\tilde{F}^{\mu\nu} = (1/2)\epsilon^{\mu\nu\rho\sigma}F_{\rho\sigma}$ , where  $\epsilon^{\mu\nu\rho\sigma}$  is the four-dimensional Levi-Civita symbol, which is anti-symmetric in permutation of all pairs of indices, and with the non-vanishing elements determined by the condition  $\epsilon^{0123} = +1$ . Note that in this and other relativistic expressions we apply *Einstein's summation convention* with summation over repeated (upper and lower) indices. In matrix form the dual tensor is

$$\tilde{F} = \begin{pmatrix} 0 & B_x & B_y & B_z \\ -B_x & 0 & -E_z & E_y \\ -B_y & E_z & 0 & -E_x \\ -B_z & -E_y & E_x & 0 \end{pmatrix} \tag{4.3}$$

When written in terms of the field tensors and the 4-vector current density  $j^\mu = (c\rho, \mathbf{j})$  Maxwell's equations get the following compact form

$$\begin{aligned}
\partial_\nu F^{\mu\nu} &= \frac{1}{c} j^\mu \\
\partial_\nu \tilde{F}^{\mu\nu} &= 0
\end{aligned} \tag{4.4}$$

The Maxwell equations are, except for the presence of source terms, symmetric under the *duality transformation*  $F^{\mu\nu} \rightarrow \tilde{F}^{\mu\nu}$ , which corresponds to the following interchange of electric and magnetic fields

$$\mathbf{E} \rightarrow \mathbf{B}, \quad \mathbf{B} \rightarrow -\mathbf{E} \tag{4.5}$$

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<sup>1</sup>We use here the form of the metric tensor with diagonal matrix elements  $g_{00} = -1, g_{ii} = +1, i = 1, 2, 3$ . This means that there is a sign change when raising or lowering the time-index but not a space index, in particular  $x^\mu = (ct, \mathbf{r})$  and  $x_\mu = (-ct, \mathbf{r})$ . We also use the short hand notations for differentiation,  $\partial_\mu = \frac{\partial}{\partial x^\mu}$ , and when convenient  $\partial_\mu \phi = \phi_{,\mu}$  and  $\partial_\nu A_\mu = A_{\mu,\nu}$ .

In fact, the equations for the free fields are invariant under a continuous *electric-magnetic transformation*, which is an extension of the discrete duality transformation,

$$\begin{aligned}\mathbf{E} &\rightarrow \cos \theta \mathbf{E} + \sin \theta \mathbf{B} \\ \mathbf{B} &\rightarrow -\sin \theta \mathbf{E} + \cos \theta \mathbf{B}\end{aligned}\quad (4.6)$$

This symmetry is broken by the source terms of the Maxwell equation.

Formally the symmetry can be restored by introducing *magnetic charge* and *magnetic current* in addition to electric charge and current. In such an extended theory there would be two kinds of sources for electromagnetic fields, electric charge and magnetic charge, and in the classical theory such an extension would be unproblematic. However for the corresponding quantum theory, some complications would arise, since the standard theory is based on the use of *electromagnetic potentials*, which depend on the “magnetic equations” being source free.

A consistent quantum theory can however be formulated with magnetic charges, provided both electric and magnetic charges are associated with point particles and provided they satisfy a *quantization condition*.<sup>2</sup> This is interesting, since such a consistence requirement would give a fundamental explanation for the observed quantization of electric charge. Theoretical considerations like this have, over the years, lead to extensive searches for magnetic charges (or *magnetic monopoles*), but at this stage there is no evidence for the existence of magnetic charges in nature.

We will here follow the standard approach and assume the Maxwell equations (4.1) without magnetic sources to be correct. This admits the introduction of electromagnetic potentials

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}, \quad \mathbf{B} = \nabla \times \mathbf{A} \quad (4.7)$$

In covariant form this is written as

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu \equiv A^{\nu,\mu} - A^{\mu,\nu} \quad (4.8)$$

where  $A^\mu$  are the components of the four potential,  $A = (\phi, \mathbf{A})$ . When the fields  $\mathbf{E}$  and  $\mathbf{B}$  are expressed in terms of the potentials, the source free Maxwell equations are automatically fulfilled and the inhomogeneous equations get the covariant form

$$\partial_\nu \partial^\nu A^\mu - \partial^\mu \partial_\nu A^\nu = -\frac{1}{c}j^\mu \quad (4.9)$$

Separated in time and space components the equations are

$$\begin{aligned}\nabla^2\phi + \frac{\partial}{\partial t}\nabla \cdot \mathbf{A} &= -\rho \\ \nabla^2\mathbf{A} - \nabla(\nabla \cdot \mathbf{A}) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{A} - \frac{1}{c}\frac{\partial}{\partial t}\nabla\phi &= -\frac{1}{c}\mathbf{j}\end{aligned}\quad (4.10)$$

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<sup>2</sup>*Dirac's quantization condition* relates the strength of the fundamental electric charge  $e$  to the fundamental magnetic charge  $g$  in the following way,  $eg/(4\pi\hbar c) = 1/2$ . Since the (electric) fine structure constant is small,  $\alpha_e = e^2/(4\pi\hbar c) \approx 1/137$ , the quantization condition gives a correspondingly *large* value to the magnetic fine structure constant,  $\alpha_g = g^2/(4\pi\hbar c) = (eg/(4\pi\hbar c))^2 \times [e^2/(4\pi\hbar c)]^{-1} \approx 137/4$ .

### 4.1.2 Field energy and field momentum

Maxwell's equations describe how moving charges give rise to electromagnetic fields. The fields on the other hand act back on the charges, through the *Lorentz force*, which for a pointlike charge  $q$  has the form

$$\mathbf{F} = q(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}) \quad (4.11)$$

When the field is acting with a force on a charged particle this implies that energy and momentum is transferred between the field and the particle. Thus, the electromagnetic field carries energy and momentum, and the form of the energy and momentum density can be determined from Maxwell's equation and the form of the Lorentz force, by assuming *conservation of energy* and *conservation of momentum*.

To demonstrate this we consider a single pointlike particle is affected by the field, and the charge and momentum density therefore can be expressed as

$$\begin{aligned} \rho(\mathbf{r}, t) &= q \delta(\mathbf{r} - \mathbf{r}(t)) \\ \mathbf{j}(\mathbf{r}, t) &= q \mathbf{v}(t) \delta(\mathbf{r} - \mathbf{r}(t)) \end{aligned} \quad (4.12)$$

where  $\mathbf{r}(t)$  and  $\mathbf{v}(t)$  describe the position and velocity of the particle as functions of time. The time derivative of the field energy  $\mathcal{E}$  will (up to a sign change) equal the effect of the work performed on the particle

$$\frac{d}{dt} \mathcal{E} = -\mathbf{F} \cdot \mathbf{v} = -q \mathbf{v} \cdot \mathbf{E} \quad (4.13)$$

For a (large) volume  $V$  with surface  $S$  we rewrite this relation by use of the field equations,

$$\begin{aligned} \frac{d}{dt} \mathcal{E} &= - \int_V d^3r \mathbf{j} \cdot \mathbf{E} \\ &= - \int_V d^3r \left[ c \mathbf{E} \cdot (\nabla \times \mathbf{B}) - \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t} \right] \\ &= \int_V d^3r \left[ \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t} + \mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial t} - c \nabla \cdot (\mathbf{E} \times \mathbf{B}) \right] \\ &= \frac{d}{dt} \frac{1}{2} \int_V d^3r \left[ E^2 + B^2 \right] - c \int_S (\mathbf{E} \times \mathbf{B}) \cdot d\mathbf{S} \end{aligned} \quad (4.14)$$

where in the last step surface terms a part of the volume integral has been rewritten as a surface integral by use of Gauss' theorem. The two terms have a direct physical interpretation, with the first term corresponding to the time derivative of the field energy within the volume  $V$ , and the second term corresponding to the energy current through the surface  $S$ . This gives the standard expressions for the energy density

$$u = \frac{1}{2} [E^2 + B^2] \quad (4.15)$$

and the energy current density

$$\mathbf{S} = c\mathbf{E} \times \mathbf{B} \quad (4.16)$$

which is also called *Pointing's vector*.

In a similar way we consider the change in the field momentum  $\mathcal{P}$ ,

$$\frac{d}{dt}\mathcal{P} = -\mathbf{F} = -q\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right) \quad (4.17)$$

This we re-write as

$$\begin{aligned} \frac{d}{dt}\mathcal{P} &= -\int d^3r \left[ \rho\mathbf{E} + \frac{1}{c}\mathbf{j} \times \mathbf{B} \right] \\ &= -\int d^3r \left[ \mathbf{E}(\nabla \cdot \mathbf{E}) + (\nabla \times \mathbf{B} - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{E}) \times \mathbf{B} \right] \\ &= -\int d^3r \left[ -(\nabla \times \mathbf{E}) \times \mathbf{E} + (\nabla \times \mathbf{B} - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{E}) \times \mathbf{B} \right] \\ &= \int d^3r \left[ -\frac{1}{c}\frac{\partial}{\partial t}\mathbf{B} \times \mathbf{E} + \frac{1}{c}\frac{\partial}{\partial t}\mathbf{E} \times \mathbf{B} \right] \\ &= \frac{d}{dt} \int d^3r \frac{1}{c}\mathbf{E} \times \mathbf{B} \end{aligned} \quad (4.18)$$

where we here have taken the infinite volume limit,  $V \rightarrow \infty$ , and have assumed that in this limit all surface contributions vanish. The expression for the field momentum density is then

$$\mathbf{g} = \frac{1}{c}\mathbf{E} \times \mathbf{B} \quad (4.19)$$

which up to a factor  $1/c^2$  is identical to the energy current density. In the relativistic formulation the energy density and the momentum density are combined in the symmetric *energy-momentum tensor*,

$$T^{\mu\nu} = -(F^{\mu\rho}F^\nu{}_\rho + \frac{1}{4}g^{\mu\nu}F_{\rho\sigma}F^{\rho\sigma}) \quad (4.20)$$

The energy density corresponds to the component  $T^{00}$  and Pointing's vector to  $(c \text{ times})$  the components  $T^{0i}$ ,  $i = 1, 2, 3$ .

### 4.1.3 Lagrange and Hamilton formulations of the classical Maxwell theory

#### *The Lagrangian density*

Maxwell' equation can be derived from a variational principle, similar to Hamilton's principle for a mechanical system. Since the variable is a *field*, i.e., a function of both  $\mathbf{r}$  and  $t$ , the action is an integral over space and time, of the form

$$S[A^\mu(\mathbf{r}, t)] = \int_{\Omega} d^4x \mathcal{L}(A^\mu, A^{\mu,\nu}) \quad (4.21)$$

where  $\mathcal{L}$  is the *Lagrangian density* and  $\Omega$  is the chosen space-time region. The Lagrangian density is a *local* function of the field variable  $A^\mu$  and its derivatives,

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{c}A^\mu j_\mu \quad (4.22)$$

where  $F^{\mu\nu} = A^{\nu,\mu} - A^{\mu,\nu}$  should be treated as a derivative of the field variable.

A dynamical field, *i.e.*, a solution of Maxwell's equations with given boundary conditions (on the boundary of  $\Omega$ ), corresponds to a solution of the variational equation,

$$\delta S = 0 \quad (4.23)$$

where this condition should be fulfilled for *arbitrary* variations in the field variables, with fixed values on the boundary of  $\Omega$ . The equivalence between this variational equation and the differential (Maxwell) equations is shown in the same way as for the equation of motion of a mechanical system, with a discrete set of coordinates.

The variation in  $S$  is, to first order in the variation of the field variable  $A^\mu$ , given by

$$\delta S = \int_{\Omega} d^4x \left[ \frac{\partial \mathcal{L}}{\partial A^\mu} - \partial_\nu \left( \frac{\partial \mathcal{L}}{\partial A^{\mu,\nu}} \right) \right] \delta A^\mu \quad (4.24)$$

where in this expression we have made a partial integration and used the fact that  $\delta A^\mu$  vanishes on the boundary of  $\Omega$ . Since the variation should otherwise be free, the variational equation (4.23) is satisfied only if the field satisfies the Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial A^\mu} - \partial_\nu \left( \frac{\partial \mathcal{L}}{\partial A^{\mu,\nu}} \right) = 0 \quad \mu = 0, 1, 2, 3. \quad (4.25)$$

With  $\mathcal{L}$  given by (4.22) it is straight forward to check that the Euler-Lagrange equation reproduces the inhomogeneous Maxwell equations.

### *The canonical field momentum*

The Lagrange and Hamilton formulations give equivalent descriptions of the dynamics of a mechanical system. Also in the case of field theories, a Hamiltonian can be derived from the Lagrangian density, but with electromagnetism there are some complications to be dealt with. We first note that the Lagrangian formulation is well suited to fit the relativistic invariance of the theory, since it makes no difference in the treatment of the space and time coordinates. That is not so for the Hamiltonian formulation, which *does* distinguish the time direction. This carries over to the (standard) quantum description, where time is distinguished in the Schrödinger equation. This does not mean that relativistic invariance cannot be incorporated in the Hamiltonian description, but it is not as explicit as in the Lagrange formulation.

To define the Hamiltonian we first need to identify a set of independent variables and their corresponding canonical momenta. As field variables we tentatively use the potential  $A^\mu(\mathbf{r})$ , where  $\mathbf{r}$  can be viewed as a continuous and  $\mu$  as a discrete index for the field coordinate. (For a mechanical system  $\mathbf{r}$  and  $\mu$  correspond to the discrete index  $k$  which labels the independent

generalized coordinates  $q_k$ .) Like the field variable, the canonical momentum now is a *field*,  $\Pi^\mu = \Pi^\mu(\mathbf{r})$ . It is defined by

$$\Pi^\mu = \frac{\partial \mathcal{L}}{\partial \dot{A}_\mu} = \frac{1}{c} \frac{\partial \mathcal{L}}{\partial A_{\mu,0}} \quad (4.26)$$

We note here the different treatment of the time and space coordinate.

The Lagrangian density (4.22) gives the following expression for the canonical field momentum

$$\begin{aligned} \Pi^\mu &= \frac{1}{c} \frac{\partial}{\partial A_{\mu,0}} \left[ -\frac{1}{2} (A_{\mu,\nu} A^{\mu,\nu} - A_{\mu,\nu} A^{\nu,\mu}) - \frac{1}{c} A^\mu j_\mu \right] \\ &= \frac{1}{c} F^{\mu 0} \end{aligned} \quad (4.27)$$

The space part ( $\mu = 1, 2, 3$ ) is proportional to the electric field, but note that the time component vanishes,  $\Pi^0 = 0$ . Also note that the *canonical* momentum defined by the Lagrangian is this way is not directly related to the *physical* momentum density carried by the electromagnetic field, as earlier has been found from momentum conservation.

The fact that there is no canonical momentum corresponding to the field component  $A^0$  indicates that the choice we have made for the generalized coordinates of the electromagnetic field is not completely satisfactory. The field amplitudes  $A^\mu$  cannot all be seen as describing independent degrees of freedom. This has to do with the gauge invariance of the theory, and we proceed to discuss how this problem can be handled.

### *Gauge invariance and gauge fixing*

We consider the following transformation of the electromagnetic potentials

$$\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla \chi, \quad \phi \rightarrow \phi' = \phi + \frac{1}{c} \frac{\partial}{\partial t} \chi \quad (4.28)$$

where  $\chi$  is a (scalar) function of space and time. In covariant form it is

$$A^\mu \rightarrow A'^\mu = A^\mu + \partial^\mu \chi \quad (4.29)$$

This is a *gauge transformation* of the potentials, and it is straight forward to show that such a transformation leaves the field strengths  $\mathbf{E}$  and  $\mathbf{B}$  invariant. The usual way to view the invariance of the fields under this transformation is that it reflects the presence of *non-physical degrees of freedom* in the potentials. Thus, the potentials define an overcomplete set of variables for the electromagnetic field. For the Hamiltonian formulation to work it is necessary to identify the independent, physical degrees of freedom.

There are two different constraints, or gauge conditions, that are often used to remove the unphysical degrees of freedom associated with gauge invariance. The Coulomb (or radiation) gauge condition is

$$\nabla \cdot \mathbf{A} = 0 \quad (4.30)$$

and the Lorentz (or covariant) gauge condition is

$$\partial_\mu A^\mu = 0 \quad (4.31)$$

The first one is often used when the interaction between radiation and atoms is considered, since the electrons then move non-relativistically and therefore there is no need for a covariant form of the gauge condition. This is the condition we will use here. The Lorentz gauge condition is often used in the description of interactions between radiation and relativistic electrons and other charged particles. The relativistic form of the field equations then are not explicitly broken by the gauge condition, but the prize to pay is that in the quantum description one has to include unphysical photon states.

### *Hamiltonian in the Coulomb gauge*

In the Coulomb gauge Maxwell's (inhomogeneous) equations reduce to the following form

$$\nabla^2 \phi = -\rho \quad (4.32)$$

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2\right) \mathbf{A} = \frac{1}{c} \mathbf{j}_T \quad (4.33)$$

Where

$$\mathbf{j}_T = \mathbf{j} - \frac{\partial}{\partial t} \nabla \phi \quad (4.34)$$

is the *transverse* component of the current density.<sup>3</sup> It satisfies the transversality condition as a consequence of the continuity equation for charge,

$$\begin{aligned} \nabla \cdot \mathbf{j}_T &= \nabla \cdot \mathbf{j} - \frac{\partial}{\partial t} \nabla^2 \phi \\ &= \nabla \cdot \mathbf{j} + \frac{\partial}{\partial t} \rho \\ &= 0 \end{aligned} \quad (4.35)$$

We note that the equation for the scalar field  $\phi$  contains no time derivatives, and can be solved in terms of the charge distribution,

$$\phi(\mathbf{r}, t) = \int d^3 r' \frac{\rho(\mathbf{r}', t)}{4\pi |\mathbf{r} - \mathbf{r}'|} \quad (4.36)$$

This is the same as the electrostatic (Coulomb) potential of a *stationary* charge distribution which coincides with the true charge distribution  $\rho(\mathbf{r}, t)$  at time  $t$ . Thus, the scalar field does not include the relativistic retardation effects associated with the motion of charges, and these relativistic effects have therefore to be accounted for by the vector potential  $\mathbf{A}$ .

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<sup>3</sup>Any vector field  $\mathbf{j}(\mathbf{r})$  can be written as  $\mathbf{j} = \mathbf{j}_T + \mathbf{j}_L$ , where  $\nabla \cdot \mathbf{j}_T = 0$  and  $\nabla \times \mathbf{j}_L = 0$ .  $\mathbf{j}_T$  is referred to as the *transverse* or *solenoidal* part of the field and  $\mathbf{j}_L$  as the *longitudinal* or *irrotational* part of the field. In the present case, with  $\mathbf{j}_L = -\nabla \phi$  the irrotational form of  $\mathbf{j}_L$  follows directly, while the transversality of  $\mathbf{j}_T$  follows from charge conservation.



The  $\phi$ -field carries no independent degrees of freedom of the electromagnetic field, it is fully determined by the position of the charges. The dynamics of the Maxwell field is then carried solely by the vector potential  $\mathbf{A}$ . In the quantum description the photons are therefore associated only with the field amplitude  $\mathbf{A}$  and not with  $\phi$ .<sup>4</sup>

Expressed in terms of the dynamical  $\mathbf{A}$  field the Lagrangian density gets the form

$$\begin{aligned}\mathcal{L} &= -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{c}j_\mu A^\mu \\ &= \frac{1}{2c^2}\dot{\mathbf{A}}^2 + \frac{1}{c}\dot{\mathbf{A}} \cdot \nabla\phi + \frac{1}{2}(\nabla\phi)^2 - \frac{1}{2}(\nabla \times \mathbf{A})^2 + \frac{1}{c}\mathbf{j} \cdot \mathbf{A} - \rho\phi\end{aligned}\quad (4.37)$$

Two of the terms we re-write as

$$\begin{aligned}\frac{1}{c}\dot{\mathbf{A}} \cdot \nabla\phi &= \frac{1}{c}\nabla \cdot (\dot{\mathbf{A}}\phi) - \frac{1}{c}\phi\nabla \cdot \dot{\mathbf{A}} \\ &= \frac{1}{c}\nabla \cdot (\dot{\mathbf{A}}\phi)\end{aligned}\quad (4.38)$$

and

$$\begin{aligned}\frac{1}{2}(\nabla\phi)^2 &= \frac{1}{2}\nabla \cdot (\phi\nabla\phi) - \frac{1}{2}(\phi\nabla^2\phi) \\ &= \frac{1}{2}\nabla \cdot (\phi\nabla\phi) + \frac{1}{2}\rho\phi\end{aligned}\quad (4.39)$$

where the Coulomb gauge condition has been used in the first equation. We note that the divergences in these expressions give unessential contributions to the Lagrangian and can be deleted. This is so since divergences only give rise to surface terms in the action integral and therefore do not affect the field equations.

With the divergence terms neglected the Lagrangian density gets the form<sup>5</sup>

$$\mathcal{L} = \frac{1}{2c^2}\dot{\mathbf{A}}^2 - \frac{1}{2}(\nabla \times \mathbf{A})^2 + \frac{1}{c}\mathbf{j} \cdot \mathbf{A} - \frac{1}{2}\rho\phi\quad (4.40)$$

The field degrees of freedom are now carried by the components of the vector field, which still have to satisfy the constraint equation  $\nabla \cdot \mathbf{A} = 0$ . The conjugate momentum is

$$\mathbf{\Pi} = \frac{1}{c^2} \cdot \dot{\mathbf{A}} \equiv -\frac{1}{c}\mathbf{E}_T\quad (4.41)$$

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<sup>4</sup>A curious consequence is that whereas for a stationary charge there are no photons present, only the non-dynamical Coulomb field, for a uniformly moving charge there will be a “cloud” of photons present to give the field the right Lorentz transformed form. This is so even if there is no radiation from the charge. We may see this as a consequence of the Coulomb gauge condition and our separation of the system into field degrees of freedom (photons) and particle degrees of freedom. In reality, for the interacting system of charges and fields this separation is not so clear, since on one hand the Coulomb field is non-dynamically coupled to the charges, and on the other hand is dynamically coupled to the radiation field.

<sup>5</sup>In this expression we have used the freedom to replace the transverse current  $\mathbf{j}_T$  with the full current  $\mathbf{j}$ , which is possible since the difference gives rise to an irrelevant derivative term. Note, however, that when the full current is used, the transversality condition  $\nabla \cdot \mathbf{A} = 0$  has to be imposed as a constraint to derive the correct field equations from the Lagrangian. When the  $\mathbf{A}$ -field is coupled to the transverse current, that is not needed.

where  $\mathbf{E}_T$  denotes the transverse part of the electric field, the part where  $-\nabla\phi$  is not included.

So far we have not worried about the degrees of freedom associated with the charges. We will now include them in the description by assuming the charges to be carried by point particles. This means that we express the charge density and current as

$$\begin{aligned}\rho(\mathbf{r}, t) &= \sum_i e_i \delta(\mathbf{r} - \mathbf{r}_i(t)) \\ \mathbf{j}(\mathbf{r}, t) &= \sum_i e_i \mathbf{v}_i(t) \delta(\mathbf{r} - \mathbf{r}_i(t))\end{aligned}\quad (4.42)$$

where the sum is over all the particles with  $\mathbf{r}_i(t)$  and  $\mathbf{v}_i(t)$  as the position and velocity of particle  $i$  as functions of time. The action integral of the full interacting system we write as

$$S = \int dt L = \int dt (L_{field} + L_{int} + L_{part}) \quad (4.43)$$

where  $L_{field} + L_{int}$  is defined as the space integral of the Lagrangian density (4.40) and  $L_{part}$  is identical to the non-relativistic kinetic energy of the particles. By performing the space integral over the charge density and current, we find the following expression for the Lagrangian  $L$ ,<sup>6</sup>

$$\begin{aligned}L &= \int d^3r \left[ \frac{1}{2c^2} \dot{\mathbf{A}}^2 - \frac{1}{2} (\nabla \times \mathbf{A})^2 \right] + \sum_i \frac{e_i}{c} \mathbf{v}_i \cdot \mathbf{A}(\mathbf{r}_i) \\ &\quad - \frac{1}{2} \sum_{i \neq j} \frac{e_i e_j}{4\pi |\mathbf{r}_i - \mathbf{r}_j|} + \sum_i \frac{1}{2} m_i \mathbf{v}_i^2\end{aligned}\quad (4.44)$$

The corresponding Hamiltonian is found by performing a (Legendre) transformation of the Lagrangian in the standard way

$$\begin{aligned}H &= \int d^3r \, \Pi \cdot \dot{\mathbf{A}} + \sum_i \mathbf{p}_i \cdot \mathbf{v}_i - L \\ &= \int d^3r \, \frac{1}{2} (\mathbf{E}_T^2 + \mathbf{B}^2) + \sum_{i < j} \frac{e_i e_j}{4\pi |\mathbf{r}_i - \mathbf{r}_j|} + \sum_i \frac{1}{2m_i} \left( \mathbf{p}_i - \frac{e_i}{c} \mathbf{A}(\mathbf{r}_i) \right)^2\end{aligned}\quad (4.45)$$

This expression for the Hamiltonian is derived for the classical system of interacting fields and particles, but it has the same form as the Hamiltonian *operator* that is used to describe the quantum system of non-relativistic electrons interacting with the electromagnetic field. However, to include correctly the effect of the intrinsic *magnetic dipole moment* of the charged particles, a spin contribution has to be added to the Hamiltonian. It has the standard form of a magnetic dipole term,

$$H_{spin} = - \sum_i \frac{g_i e_i}{2m_i c} \mathbf{S}_i \cdot \mathbf{B}(\mathbf{r}_i) \quad (4.46)$$

where  $g_i$  is the g-factor of particle  $i$ , which is close to 2 for electrons. Often the spin term is small corresponding to the other interaction terms and can be neglected.

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<sup>6</sup>For point charges an ill-defined *self energy contribution* may seem to appear from the Coulomb interaction term. It is here viewed as irrelevant since it gives no contribution to the *interaction* between the particles and is therefore not included. In a more complete field theoretic treatment of the interaction of charges and fields such problems will reappear and have to be handled within the framework of *renormalization theory*.

## 4.2 Photons – the quanta of light

With the degrees of freedom of the electromagnetic field and of the electrons disentangled, we may consider the space of states of the full quantum system as the product space of a *field*-state space and a *particle*-state space,

$$\mathcal{H} = \mathcal{H}_{field} \otimes \mathcal{H}_{particle} \quad (4.47)$$

In this section we focus on the quantum description of the *free* electromagnetic field, which defines the space  $\mathcal{H}_{field}$  and the operators (observables) acting there. The energy eigenstates of the free field are the *photon states*. When we as a next step include interactions, these will introduce processes where photons are emitted and absorbed.

### 4.2.1 Constructing Fock space

Since the field amplitude  $\mathbf{A}$  is constrained by the transversality condition  $\nabla \cdot \mathbf{A} = 0$  it is convenient to make a Fourier transform to plane wave amplitudes. In a standard way we introduce a periodicity condition on the components of the space coordinate  $\mathbf{r}$ , so that the components of the Fourier variable  $\mathbf{k}$  take discrete values,  $k_i = 2\pi n_i/L$ , with  $L$  as a (large) periodic length and  $n_i$  as a set of integers for the components  $i = 1, 2, 3$ . The field amplitude then can be written as a discrete Fourier sum

$$\mathbf{A}(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \sum_{a=1}^2 A_{\mathbf{k}a}(t) \boldsymbol{\epsilon}_{\mathbf{k}a} e^{i\mathbf{k} \cdot \mathbf{r}} \quad (4.48)$$

where the  $V = L^3$  is the normalization volume and the vectors  $\boldsymbol{\epsilon}_{\mathbf{k}a}$  are unit vectors which satisfy  $\mathbf{k} \cdot \boldsymbol{\epsilon}_{\mathbf{k}a} = 0$  as a consequence of the transversality condition  $\nabla \cdot \mathbf{A} = 0$ . With the constraint on the field taken care of in this way, amplitudes  $A_{\mathbf{k}a}$  can be taken to represent the independent degrees of freedom of the field. Note, however that the amplitudes for opposite wave vectors  $\mathbf{k}$  and  $-\mathbf{k}$  are not independent, as we shall discuss below.

The *normal modes* of the field are the plane wave solutions of the field equations,

$$A_{\mathbf{k}a}(t) = A_{\mathbf{k}a}^0 e^{\pm i\omega_k t}, \quad \omega_k = ck \quad (k = |\mathbf{k}|) \quad (4.49)$$

They represent plane waves of *monochromatic, polarized light*. The two vectors  $\boldsymbol{\epsilon}_{\mathbf{k}a}$  are the *polarization vectors*, which may be taken to be two orthonormal vectors in the sense,

$$\boldsymbol{\epsilon}_{\mathbf{k}a}^* \cdot \boldsymbol{\epsilon}_{\mathbf{k}'a'} = \delta_{kk'} \delta_{aa'} \quad (4.50)$$

Both vectors are perpendicular to  $\mathbf{k}$ . The polarization vectors can be taken to be real, in which case the normal modes correspond to plane polarized light or they may be complex, in which case they correspond to circularly or more generally to elliptically polarized light.

The fact that the field  $\mathbf{A}(\mathbf{r}, t)$  is a real field gives the following relation between the field amplitudes at wave vectors  $\mathbf{k}$  and  $-\mathbf{k}$ ,

$$\sum_a A_{-\mathbf{k}a} \boldsymbol{\epsilon}_{-\mathbf{k}a} = \sum_a A_{\mathbf{k}a}^* \boldsymbol{\epsilon}_{\mathbf{k}a}^* \quad (4.51)$$

The polarization vectors can be chosen so that

$$\epsilon_{-\mathbf{k}a} = \epsilon_{\mathbf{k}\bar{a}}^* \quad (4.52)$$

with  $\bar{a}$  is determined from  $a$  by interchanging the two polarization directions 1 and 2. (This change is done to keep the set of orthogonal vectors as a right-handed set.) For the field amplitude this give the relation

$$A_{\mathbf{k}a}^* = A_{-\mathbf{k}\bar{a}} \quad (4.53)$$

The Lagrangian of the free electromagnetic field expressed in terms of the Fourier amplitudes is

$$L = \frac{1}{2} \sum_{\mathbf{k}a} \left[ \frac{1}{c^2} \dot{A}_{\mathbf{k}a}^* \dot{A}_{\mathbf{k}a} - k^2 A_{\mathbf{k}a}^* A_{\mathbf{k}a} \right] \quad (4.54)$$

We note that there is no coupling between the different Fourier components, and for each component the Lagrangian has the same form as for a harmonic oscillator of frequency  $\omega = ck$ . The variables are however complex rather than real, since reality of the field is represented by the relation (4.53) with each Fourier component being complex. Thus, the variables in (4.54), for each  $\mathbf{k}$  and  $a$ , correspond to the complex coordinate  $z$  of the harmonic oscillator rather than the real  $x$ . A rewriting of the Lagrangian in terms of real variables is straight forward, but it is more convenient to continue to work with the complex variables.

The conjugate momentum to the variable  $A_{\mathbf{k}a}$  is

$$\Pi_{\mathbf{k}a} = \frac{1}{c^2} \dot{A}_{\mathbf{k}a}^* = -\frac{1}{c} E_{\mathbf{k}a}^* \quad (4.55)$$

where  $E_{\mathbf{k}a}$  is the Fourier component of the electric field. From this the form of the free field Hamiltonian is found

$$\begin{aligned} H &= \sum_{\mathbf{k}a} \Pi_{\mathbf{k}a} \dot{A}_{\mathbf{k}a} - L \\ &= \sum_{\mathbf{k}a} \frac{1}{2} (E_{\mathbf{k}a}^* E_{\mathbf{k}a} + k^2 A_{\mathbf{k}a}^* A_{\mathbf{k}a}) \end{aligned} \quad (4.56)$$

which is consistent with the earlier expression found for the Hamiltonian of the electromagnetic field, represented by the first term of (4.45) written in Fourier transformed field components.

Quantization of the theory means that the classical field amplitude  $\mathbf{A}$  and field strength  $\mathbf{E}$  are now replaced by operators  $\hat{\mathbf{A}}$  and  $\hat{\mathbf{E}}$ , while the complex conjugate fields are replaced by hermitian conjugate operators. The conjugate field variables satisfy the canonical commutation relations in the form

$$[\hat{E}_{\mathbf{k}a}^\dagger, \hat{A}_{\mathbf{k}'b}] = -\frac{1}{c} [\hat{\dot{A}}_{\mathbf{k}a}^\dagger, \hat{A}_{\mathbf{k}'b}] = i\hbar c \delta_{\mathbf{k}\mathbf{k}'} \delta_{ab} \quad (4.57)$$

It is convenient to change to new variables,

$$\begin{aligned}\hat{A}_{\mathbf{k}a} &= c\sqrt{\frac{\hbar}{2\omega_k}}(\hat{a}_{\mathbf{k}a} + \hat{a}_{-\mathbf{k}\bar{a}}^\dagger) \\ \hat{E}_{\mathbf{k}a} &= i\sqrt{\frac{\hbar\omega_k}{2}}(\hat{a}_{\mathbf{k}a} - \hat{a}_{-\mathbf{k}\bar{a}}^\dagger)\end{aligned}\quad (4.58)$$

where the reality condition (4.51) has been made explicit. In terms of the new variables the Hamiltonian takes the form

$$\hat{H} = \sum_{\mathbf{k}a} \frac{1}{2} \hbar \omega_k (\hat{a}_{\mathbf{k}a} \hat{a}_{\mathbf{k}a}^\dagger + \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}) \quad (4.59)$$

and the canonical commutation relations are

$$\begin{aligned}[\hat{a}_{\mathbf{k}a}, \hat{a}_{\mathbf{k}'b}^\dagger] &= \delta_{\mathbf{k}\mathbf{k}'} \delta_{ab} \\ [\hat{a}_{\mathbf{k}a}, \hat{a}_{\mathbf{k}'b}] &= 0\end{aligned}\quad (4.60)$$

Expressed in this way the Hamiltonian has exactly the form of a collection of independent quantum oscillators, one for each field mode, with  $\hat{a}_{\mathbf{k}a}$  as lowering operator and  $\hat{a}_{\mathbf{k}a}^\dagger$  as raising operator in the energy spectrum of the oscillator labeled by  $(\mathbf{k}a)$ .

It is convenient to work, in the following, in the Heisenberg picture, where the observables are time dependent. In this picture the vector potential and electric field strength now are *field operators*,

$$\begin{aligned}\hat{\mathbf{A}}(\mathbf{r}, t) &= \sum_{\mathbf{k}a} c\sqrt{\frac{\hbar}{2V\omega_k}} \left[ \hat{a}_{\mathbf{k}a} \boldsymbol{\epsilon}_{\mathbf{k}a} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)} + \hat{a}_{\mathbf{k}a}^\dagger \boldsymbol{\epsilon}_{\mathbf{k}a}^* e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)} \right] \\ \hat{\mathbf{E}}(\mathbf{r}, t) &= i \sum_{\mathbf{k}a} \sqrt{\frac{\hbar\omega_k}{2V}} \left[ \hat{a}_{\mathbf{k}a} \boldsymbol{\epsilon}_{\mathbf{k}a} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)} - \hat{a}_{\mathbf{k}a}^\dagger \boldsymbol{\epsilon}_{\mathbf{k}a}^* e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)} \right]\end{aligned}\quad (4.61)$$

The state space of the free electromagnetic field then can be viewed as a product space of harmonic oscillator spaces, one for each normal mode of the field. The vacuum state is defined as the ground state of the Hamiltonian (4.59), which means that it is the state where all oscillators are unexcited,

$$\hat{a}_{\mathbf{k}a}|0\rangle = 0 \quad \text{for all } (\mathbf{k}, a) \quad (4.62)$$

The operator  $\hat{a}_{\mathbf{k}a}^\dagger$ , which excites one of the oscillators, is interpreted as a *creation operator* which creates one *photon* from the vacuum,

$$\hat{a}_{\mathbf{k}a}^\dagger |0\rangle = |1_{\mathbf{k}a}\rangle \quad (4.63)$$

An arbitrary number of photons can be created in the same state  $(\mathbf{k}a)$ ,

$$(\hat{a}_{\mathbf{k}a}^\dagger)^{n_{\mathbf{k}a}} |0\rangle = \sqrt{n_{\mathbf{k}a}!} |n_{\mathbf{k}a}\rangle \quad (4.64)$$

and this shows that the photons are *bosons*. The operator  $\hat{a}_{\mathbf{k}a}$  is an *annihilation operator* which reduces the number of photons in the mode  $(\mathbf{k}a)$ ,

$$\hat{a}_{\mathbf{k}a} |n_{\mathbf{k}a}\rangle = \sqrt{n_{\mathbf{k}a}} |n_{\mathbf{k}a} - 1\rangle \quad (4.65)$$

The photon number operator is

$$\hat{N}_{\mathbf{k}a} = \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a} \quad (4.66)$$

It counts the number of photons present in the state  $(\mathbf{k}a)$ ,

$$\hat{N}_{\mathbf{k}a} |n_{\mathbf{k}a}\rangle = n_{\mathbf{k}a} |n_{\mathbf{k}a}\rangle \quad (4.67)$$

The general photon state, often referred to as a *Fock state*, is a product state with a well-defined number of photons for each set of quantum numbers  $(\mathbf{k}a)$ . It is specified by a set of occupation numbers  $\{n_{\mathbf{k}a}\}$  for the single-photon states. The set of Fock states  $|\{n_{\mathbf{k}a}\}\rangle$  form a basis of orthonormal states that span the state space, the *Fock space*, of the quantized field. Thus a general quantum state of the free electromagnetic field is a linear superposition of Fock states,

$$|\psi\rangle = \sum_{\{n_{\mathbf{k}a}\}} c(\{n_{\mathbf{k}a}\}) |\{n_{\mathbf{k}a}\}\rangle \quad (4.68)$$

with  $c(\{n_{\mathbf{k}a}\})$  are the expansion coefficients in this basis.

The energy operator, which is identical to the Hamiltonian, has the same form as the classical field energy. It is diagonal in the Fock basis and can be expressed in terms of the photon number operator

$$\begin{aligned} \hat{H} &= \int d^3r \frac{1}{2} (\hat{E}^2 + \hat{B}^2) \\ &= \sum_{\mathbf{k}a} \frac{1}{2} \hbar \omega_k (\hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a} + \hat{a}_{\mathbf{k}a} \hat{a}_{\mathbf{k}a}^\dagger) \\ &= \sum_{\mathbf{k}a} \hbar \omega_k (\hat{N}_{\mathbf{k}a} + \frac{1}{2}) \end{aligned} \quad (4.69)$$

One should note that the vacuum energy is formally infinite, since the sum over the ground state energy  $\frac{1}{2}\omega_k$  for all the oscillators diverges. However, since this is an additive constant which is common for all states it can be regarded as unphysical and simply be subtracted. The vacuum energy is on the other hand related to *vacuum fluctuations* of the quantized fields and in this way it is connected to properties of the quantum theory that correspond to real, physical effects.

In a similar way the classical field momentum is replaced by an operator of the same form,

$$\begin{aligned} \hat{\mathcal{P}} &= \int d^3r \frac{1}{c} (\hat{\mathbf{E}} \times \hat{\mathbf{B}}) \\ &= \sum_{\mathbf{k}a} \frac{1}{2} \hbar \mathbf{k} (\hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a} + \hat{a}_{\mathbf{k}a} \hat{a}_{\mathbf{k}a}^\dagger) \\ &= \sum_{\mathbf{k}a} \hbar \mathbf{k} \hat{N}_{\mathbf{k}a} \end{aligned} \quad (4.70)$$

The expressions (4.69) and (4.70) show that a single photon in the mode  $(\mathbf{k}a)$  has energy  $E = \hbar\omega_{\mathbf{k}}$  and momentum  $p = \hbar\mathbf{k}$ , in accordance with the de Broglie relations. Furthermore, the relation  $\omega_{\mathbf{k}} = c\mathbf{k}$ , generally valid for electromagnetic waves, means that the energy-momentum relation is  $E = cp$ , which is the correct one for a *massless* relativistic particle. This supports the idea of the photon as a massless *particle*, not simply as an energy quantum of an electromagnetic mode. In addition, the degree of freedom associated with the two possible polarizations is readily re-interpreted as due to the intrinsic spin of the photon. Thus, the photon carries one unit of spin, and the existence of only two spin states, rather than three, is related to the fact that the photon is massless. A natural choice for two orthogonal spin states are the *helicity* states, corresponding to spin either in the direction of the momentum or in the direction opposite to the momentum. In the language of polarization these two possibilities correspond to circular polarization, which may either be right-handed or left-handed.

### 4.2.2 Coherent and incoherent photon states

In a similar way as for the quantum description of particles, we may view the expectation values of the electromagnetic field operators to represent classical variables within the quantum theory. For example, the expectation value of the electric field operator takes the usual form of a classical electric field. Expanded in plane wave components it is

$$\langle \hat{\mathbf{E}}(\mathbf{r}, t) \rangle = i \sum_{\mathbf{k}a} \sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2V}} \left[ \alpha_{\mathbf{k}a} \boldsymbol{\epsilon}_{\mathbf{k}a} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} - \alpha_{\mathbf{k}a}^* \boldsymbol{\epsilon}_{\mathbf{k}a}^* e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} \right] \quad (4.71)$$

where the complex expansion coefficients  $\alpha_{\mathbf{k}a}$  and  $\alpha_{\mathbf{k}a}^*$  are the expectation values of the annihilation and creation operators.

$$\alpha_{\mathbf{k}a} = \langle \hat{a}_{\mathbf{k}a} \rangle, \quad \alpha_{\mathbf{k}a}^* = \langle \hat{a}_{\mathbf{k}a}^\dagger \rangle \quad (4.72)$$

The quantum field in addition has (quantum) fluctuations around the classical configuration.

We note, from the above expression, the curious fact that for Fock states, with a sharply defined set of photon numbers, the expectation value of the electric (as well as the magnetic) field vanishes. Such a state which may be highly excited in energy, but still have vanishing expectation values for the fields, we may regard as being highly *non-classical states*. In these states the field variables, in a sense, are dominated by the quantum fluctuations. Classical fields, on the other hand, may be represented by states where the expectation values dominate the quantum fluctuations. For a single harmonic oscillator we have already discussed such "classical" states in the form of *coherent states*, states with minimum uncertainty in their phase space positions  $\hat{x}$  and  $\hat{p}$ . For the electromagnetic field the corresponding variables are  $\hat{\mathbf{A}}(\mathbf{r}, t)$  and  $\hat{\mathbf{E}}(\mathbf{r}, t)$ , and since each field mode can be regarded as a harmonic oscillator, the definition of oscillator coherent states can be directly applied to define coherent states of the electromagnetic field. Such states correspond to a particular form of superpositions of Fock states.

For a single electromagnetic field mode ( $\mathbf{k}a$ ), the coherent state has the same form as discussed in Sect. 1.3.3 for the harmonic oscillator,

$$|\alpha_{\mathbf{k}a}\rangle = \sum_{n_{\mathbf{k}a}} e^{-\frac{1}{2}|\alpha_{\mathbf{k}a}|^2} \frac{(\alpha_{\mathbf{k}a})^{n_{\mathbf{k}a}}}{\sqrt{n_{\mathbf{k}a}!}} |n_{\mathbf{k}a}\rangle \quad (4.73)$$

where  $\alpha_{\mathbf{k}a}$  is related to the expectation values of  $\hat{a}_{\mathbf{k}a}$  and  $\hat{a}_{\mathbf{k}a}^\dagger$  as in (4.72). The full coherent state of the electromagnetic field is then a product state of the form

$$|\psi\rangle = \prod_{\mathbf{k}a} |\{\alpha_{\mathbf{k}a}\}\rangle \quad (4.74)$$

and the corresponding expectation value of the electric field is given by (4.71).

The vacuum state is a special case of a coherent state, and in the same way as for a single harmonic oscillator, the quantum fluctuations of this state are the same as for any other coherent state. This follows since the coherent state can be considered as obtained from the vacuum state by shifting the field operators by a classical field contribution<sup>7</sup>. The quantum fluctuations of the fields in a given, sharply defined point in space, are ill defined. The two-point correlation functions, however, give finite expressions for the fluctuations. We examine here the following vacuum correlation function

$$\begin{aligned} C_{ij}(\mathbf{r} - \mathbf{r}') &\equiv \langle E_i(\mathbf{r}) E_j(\mathbf{r}') \rangle - \langle E_i(\mathbf{r}) \rangle \langle E_j(\mathbf{r}') \rangle \\ &= \sum_{\mathbf{k}} \frac{\hbar \omega_{\mathbf{k}}}{2V} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \left( \delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2} \right) \\ &\rightarrow \frac{c\hbar}{2(2\pi)^3} \int d^3k k e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \left( \delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2} \right) \end{aligned} \quad (4.75)$$

where in the last step we have taken the infinite volume limit. For large  $k$  this integral has an undamped oscillatory behavior, but the integral can be made well defined by introducing a damping factor  $e^{-\epsilon k}$  and taking  $\epsilon$  to 0. We note that the correlation function only depend on the relative coordinates of the two points and therefore simply put  $\mathbf{r}' = 0$ , so that  $\mathbf{r}$  represents the relative coordinate of the two points. The correlation function can be re-expressed in the following way

$$C_{ij}(\mathbf{r}) = \frac{c\hbar}{2(2\pi)^3} \left( \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} - \delta_{ij} \sum_k \frac{\partial}{\partial x_k} \frac{\partial}{\partial x_k} \right) \int d^3k \frac{1}{k} e^{i\mathbf{k} \cdot \mathbf{r}} e^{-\epsilon k} \quad (4.76)$$

with the integral evaluated as

$$\begin{aligned} \int d^3k \frac{1}{k} e^{i\mathbf{k} \cdot \mathbf{r}} e^{-\epsilon k} &= 2\pi \int_0^\infty dk k \int_0^\pi d\theta \sin \theta e^{ikr \cos \theta} e^{-\epsilon k} \\ &= 2\pi \int_0^\infty dk k e^{-\epsilon k} \int_{-1}^1 du e^{ikru} \\ &= \frac{4\pi}{r} \int_0^\infty dk \sin kr e^{-\epsilon k} \\ &= \frac{4\pi}{r^2} \end{aligned} \quad (4.77)$$

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<sup>7</sup>*i.e.*, by a contribution proportional to the identity operator



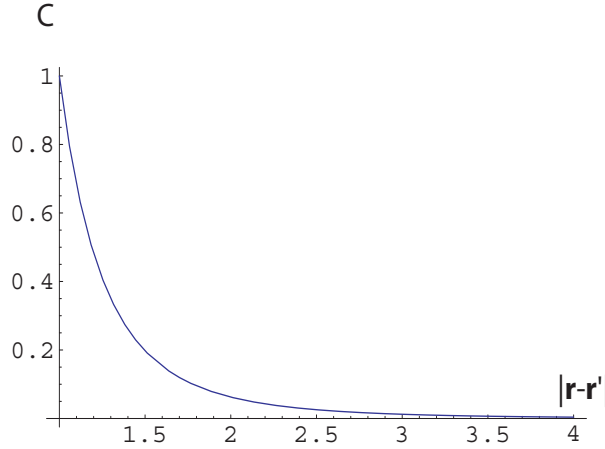


Figure 4.1: The correlation function for the electric field in a coherent state,  $C_{ij}(\mathbf{r} - \mathbf{r}') \equiv \langle E_i(\mathbf{r})E_j(\mathbf{r}') \rangle - \langle E_i(\mathbf{r}) \rangle \langle E_j(\mathbf{r}') \rangle$ . The form of the non-vanishing elements,  $i = j$ , is shown as the function of distance  $\mathbf{r} - \mathbf{r}'$  between two points in space.

where in the last step we have taken the limit  $\epsilon \rightarrow 0^+$ . This gives

$$\begin{aligned}
 C_{ij}(\mathbf{r}) &= \frac{c\hbar}{2(2\pi)^3} \left( \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} - \delta_{ij} \sum_k \frac{\partial}{\partial x_k} \frac{\partial}{\partial x_k} \right) \frac{4\pi}{r^2} \\
 &= \frac{c\hbar}{\pi^2 r^4} \left( 2 \frac{x_i x_j}{r^2} - \delta_{ij} \right) \\
 &= -\frac{c\hbar}{\pi^2 r^4} \left( \delta_{ij} - 2 \frac{x_i x_j}{r^2} \right)
 \end{aligned} \tag{4.78}$$

We note the fall-off of the correlation with increased separation between the two points and also notes that the function diverges as  $r \rightarrow 0$ . This divergence is typical for field theories, and reflects the fact that the *physical* fields cannot be defined with infinite resolution. A way to avoid such infinities is to define the physical fields by averaging over a small volume. This introduces effectively a momentum cut-off in the Fourier transformation of the field.

A similar calculation for the magnetic field shows that the correlation function is the same as for the electric field. This is typical for the coherent state which is symmetric in its dependence of the field variable and its conjugate momentum. Since  $\mathbf{A}$  and  $\mathbf{E}$  are conjugate variables, the electric and magnetic fields do not commute as operator fields. Formally the commutator is

$$[B_i(\mathbf{r}), E_j(\mathbf{r}')] = \delta_{ij} \nabla \times \delta(\mathbf{r} - \mathbf{r}') \tag{4.79}$$

where one should express it in terms of the Fourier transformed fields in order to give the commutator a more precise meaning. There are states where the fluctuations in the  $\mathbf{E}$ -field are suppressed relative to that of the vacuum state, but due to the non-vanishing of the commutator with  $\mathbf{B}$ , the fluctuations in the  $\mathbf{B}$ -field will then be larger than that of the vacuum. States with reduced fluctuations in one of the fields, and which still satisfy the condition of minimum (Heisenberg) uncertainty for conjugate variables, are often referred to as *squeezed states*.

Radio waves, produced by oscillating currents in an antenna, can clearly be regarded as classical electromagnetic waves and are well described as coherent states of the electromagnetic field within the quantum theory of radiation. The mean value of the fields at the receiver antenna induces the secondary current that creates the electric signal to the receiver. Also for shorter wavelengths in the microwave and the optical regimes coherent states of the electromagnetic can be created, but not by oscillating macroscopic currents. In masers and lasers the intrinsic tendency of atoms to correlate their behavior in a strong electromagnetic field is used to create a monochromatic beam with a high degree of coherence. Ordinary light, on the other hand, as emitted by a hot source is highly incoherent, since the emission from different atoms only to a low degree is correlated. The expectation value for the field values at any point in space vanishes, and in this sense the light from a hot source is non-classical. However, this light does not corresponding to a *pure* quantum state, like the Fock state, but instead to a *mixed* state, with a probability distribution over Fock states.

We examine the quantum state of radiation from a hot source, which we assume to have the form of *black body radiation*, with a thermal *Boltzmann distribution* over energy eigenstates. The density operator of this state is

$$\hat{\rho} = \mathcal{N} e^{-\beta \hat{H}}, \quad \mathcal{N} = (\text{Tr } e^{-\beta \hat{H}})^{-1}, \quad \beta = (k_B T)^{-1} \quad (4.80)$$

where  $\hat{H}$  is the Hamiltonian of the free electromagnetic field,  $k_B$  is Boltzmann's constant and  $T$  is the temperature of the radiation. We first calculate the expectation value of the photon numbers

$$\begin{aligned} n_{\mathbf{k}a} &\equiv \langle \hat{N}_{\mathbf{k}a} \rangle \\ &= \mathcal{N} \text{Tr} (e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}) \\ &= \mathcal{N} \text{Tr} (e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} \hat{a}_{\mathbf{k}a}^\dagger e^{\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} \hat{a}_{\mathbf{k}a}) \\ &= \mathcal{N} \text{Tr} (e^{-\beta \hbar \omega_k} \hat{a}_{\mathbf{k}a}^\dagger e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} \hat{a}_{\mathbf{k}a}) \\ &= e^{-\beta \hbar \omega_k} \mathcal{N} \text{Tr} (e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} \hat{a}_{\mathbf{k}a} \hat{a}_{\mathbf{k}a}^\dagger) \\ &= e^{-\beta \hbar \omega_k} \mathcal{N} \text{Tr} (e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} (\hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a} + 1)) \\ &= e^{-\beta \hbar \omega_k} (n_{\mathbf{k}a} + 1) \end{aligned} \quad (4.81)$$

which gives

$$n_{\mathbf{k}a} = \frac{1}{e^{\beta \hbar \omega_k} - 1} \quad (4.82)$$

with  $\omega_k = ck$ . This is the well-known *Bose-Einstein distribution* for photons in thermal equilibrium with a heat bath. From this distribution the *Planck spectrum* of the black body radiation can be determined. The total radiation energy is

$$\begin{aligned} \mathcal{E} &= \sum_{\mathbf{k}a} \hbar \omega_k n_{\mathbf{k}a} \\ &\rightarrow 2 \frac{V}{(2\pi)^3} \int d^3k \frac{\hbar \omega_k}{e^{\beta \hbar \omega_k} - 1} \\ &= \frac{V \hbar}{\pi^2 c^3} \int d\omega \frac{\omega^3}{e^{\beta \hbar \omega} - 1} \end{aligned} \quad (4.83)$$

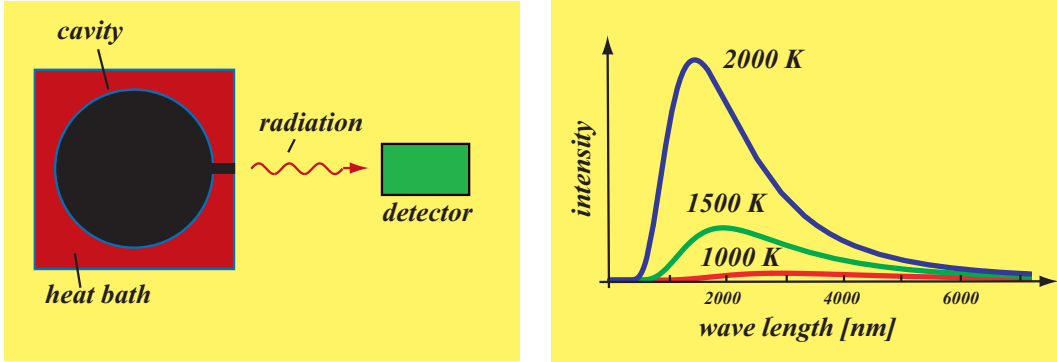


Figure 4.2: The Planck spectrum. A schematic experimental set up is shown where thermal light is created in a cavity surrounded by a heat bath (an oven). The radiation escapes through a narrow hole and can be analyzed in a detector. The right part of the figure shows the intensity (energy density) of the radiation as a function of wave length for three different temperatures.

This corresponds to the following energy density per frequency unit to be

$$u(\omega) = \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{e^{\beta \hbar \omega} - 1} \quad (4.84)$$

which displays the form of the Planck spectrum.

We next consider the expectation values of the photon annihilation and creation operators. A similar calculation as for the number operator gives

$$\begin{aligned} \langle \hat{a}_{\mathbf{k}a}^\dagger \rangle &= \mathcal{N} \text{Tr}(e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} \hat{a}_{\mathbf{k}a}^\dagger) \\ &= \mathcal{N} \text{Tr}(e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} \hat{a}_{\mathbf{k}a}^\dagger e^{\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}}) \\ &= \mathcal{N} \text{Tr}(e^{-\beta \hbar \omega_k} \hat{a}_{\mathbf{k}a}^\dagger e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}}) \\ &= e^{-\beta \hbar \omega_k} \mathcal{N} \text{Tr}(e^{-\beta \hbar \omega_k \hat{a}_{\mathbf{k}a}^\dagger \hat{a}_{\mathbf{k}a}} \hat{a}_{\mathbf{k}a}^\dagger) \\ &= e^{-\beta \hbar \omega_k} \langle \hat{a}_{\mathbf{k}a}^\dagger \rangle \end{aligned} \quad (4.85)$$

This shows that the expectation value of the creation operator vanishes. A similar reasoning applies to the annihilation operator, so that

$$\langle \hat{a}_{\mathbf{k}a}^\dagger \rangle = \langle \hat{a}_{\mathbf{k}a} \rangle = 0 \quad (4.86)$$

As a consequence the expectation value of the electric and magnetic field vanish identically,

$$\langle \mathbf{E}(\mathbf{r}, t) \rangle = \langle \mathbf{B}(\mathbf{r}, t) \rangle = 0 \quad (4.87)$$

There are several ways to interpret this result, that the expectation values of the electromagnetic fields vanishes. We have represented the quantum state of the black body radiation as a

statistical distribution over Fock states, and this indicates that the light from a hot source should be viewed as non-classical in the same sense as the pure Fock states. However, the vanishing of the expectation values of the fields only reflects rotational invariance, or the fact that black body radiation is *unpolarized*. This can be obtained also with statistical distributions over classical field configurations. In fact, the mixed quantum state of black body radiation can be expressed as statistical distributions over two completely different ensembles of pure states. One is the ensemble of Fock states, that we have already discussed. The other is an ensemble of coherent states. Thus, if we write the density operator (4.80) as a product over modes,

$$\hat{\rho} = \prod_{\mathbf{k}a} \hat{\rho}_{\mathbf{k}a} \quad (4.88)$$

the density operator of each mode has a thermal form with the two equivalent expansions

$$\hat{\rho}_{\mathbf{k}a} = \mathcal{N} \sum_n \exp(-\beta \hbar \omega n) |n\rangle \langle n| = \mathcal{N}' \int d^2\alpha \exp(-(e^{\beta \hbar \omega} - 1)|\alpha|^2) |\alpha\rangle \langle \alpha| \quad (4.89)$$

In this expression  $\omega$  is the frequency of the mode,  $\alpha$  is a coherent-state variable and  $\mathcal{N}$  and  $\mathcal{N}'$  are normalization factors. The identity between the two expansions is readily verified by using the expansion of coherent states in energy eigenstates.

This situation, that the density operator of a mixed state can be viewed as statistical distributions over completely different ensembles of pure quantum states, is something we have noticed already in the introductory discussion of pure and mixed states in Sect. 2.1.1. In the present case this means that it is our subjective choice to see the quantum state of the radiation either as a probability distribution over states with well defined photon numbers (the particle representation) or as a probability distribution over coherent states (the wave representation). Thus, the distinction between "classical light" and "non-classical light" is not so obvious for mixed quantum states as it is for pure states of the electromagnetic field.

Let us finally consider the question of how these different views of light are related to the classical demonstrations of the wave nature of light, in particular as shown in Young's interference experiments. These demonstrations may seem to favor the wave representation rather than the particle representation of light. However, even if this type of experiments demonstrate the wave nature of light, one should remember that interference is a direct consequence of *quantum superpositions* and is *not* depending of coherent behavior of many photons. We may compare this with the double slit experiment for electrons where interference can be seen as a single particle effect. Many electrons are needed to build up the interference pattern, but no coherent effect between the states of *different* electrons is needed. The interference can be seen as a single-electron effect, but the geometry of the experiment introduces a correlation in space between the pattern associated with each particle so that a macroscopic pattern can be built. In the same way we may interpret interference in incoherent light to be a single-photon effect. Each photon interferes with itself, without any coherent behavior with other photons. But they all see the same geometrical structure of the slits and this creates a correlated interference pattern.

### 4.2.3 Photon emission and photon absorption

We shall in the following consider processes where only a single electron is involved. To be more specific we may consider transitions in a hydrogen atom, or a hydrogen-like atom, where a single atomic electron can either absorb or emit a photon. The full Hamiltonian has the form

$$\hat{H} = \hat{H}_0^{field} + \hat{H}_0^{atom} + \hat{H}_{int} \quad (4.90)$$

where

$$\hat{H}_0^{atom} = \frac{\hat{p}^2}{2m} + V(\hat{\mathbf{r}}) \quad (4.91)$$

is the unperturbed Hamiltonian of the electron, which moves in the electrostatic potential  $V$  set up by the charges of the rest of the atom (*i.e.*, the nucleus and possibly other, more tightly bound electrons). The transitions are induced by the interaction part of the Hamiltonian of the electron and electromagnetic field,

$$\hat{H}_{int} = -\frac{e}{mc} \hat{\mathbf{A}}(\hat{\mathbf{r}}) \cdot \hat{\mathbf{p}} + \frac{e^2}{2mc^2} \hat{\mathbf{A}}(\hat{\mathbf{r}})^2 - \frac{e}{mc} \hat{\mathbf{S}} \cdot \hat{\mathbf{B}}(\hat{\mathbf{r}}) \quad (4.92)$$

where  $\hat{\mathbf{r}}$  is the electron coordinate and  $\hat{\mathbf{p}}$  is the (conjugate) momentum operator. The  $g$ -factor of the electron has here been set to 2.

The two first terms in  $\hat{H}_{int}$  are *charge interaction terms* which describe interactions between the charge of the electron and the electromagnetic field. The third term is the *spin interaction term*, which describes interactions between the magnetic dipole moment of the electron and the magnetic field. We note that to lowest order in perturbation expansion, the the first and third term of the interaction Hamiltonian (4.92) describe processes where a single photon is either absorbed or emitted. The second term describe scattering processes for a single photon and *two-photon* emission and absorption processes. This term is generally smaller than the first term and in a perturbative treatment it is natural to collect first order contributions from the second term with second order contributions from the first term. This means that we treat the perturbation series as an expansion in powers of the charge  $e$  (or rather the dimensionless fine-structure constant) instead of as an expansion in the interaction  $\hat{H}_{int}$ .

The spin interaction term is also generally smaller than the first (charge interaction) term. However there are different selection rules for the transitions induced by these two terms, and when the direct contribution from the first term is forbidden the spin term may give an important contribution to the transition. Here we shall in the following restrict the discussion to transitions where the contribution from the first term is dominant and we therefore can neglect the two other terms. For simplicity we use the same notation  $\hat{H}_{int}$  when only the first term is included.

The interaction Hamiltonian we may now separated in a creation (emission) part and an annihilation (absorption) part

$$\hat{H}_{int} = \hat{H}_{emis} + \hat{H}_{abs} \quad (4.93)$$

Separately they are non-hermitian with  $\hat{H}_{emis}^\dagger = \hat{H}_{abs}$ . Expressed in terms of photon creation and annihilation operators they are

$$\begin{aligned}\hat{H}_{emis} &= -\frac{e}{m} \sum_{\mathbf{k}a} \sqrt{\frac{\hbar}{2V\omega_k}} \hat{\mathbf{p}} \cdot \boldsymbol{\epsilon}_{\mathbf{k}a}^* \hat{a}_{\mathbf{k}a}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)} \\ \hat{H}_{abs} &= -\frac{e}{m} \sum_{\mathbf{k}a} \sqrt{\frac{\hbar}{2V\omega_k}} \hat{\mathbf{p}} \cdot \boldsymbol{\epsilon}_{\mathbf{k}a} \hat{a}_{\mathbf{k}a} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\end{aligned}\quad (4.94)$$

Note that when written in this way the operators are expressed in the *interaction picture* where the time evolution is determined by the free (non-interacting) theory. The time evolution of the state vectors are in this picture determined by the interaction Hamiltonian only, not by the free (unperturbed) Hamiltonian. This picture is most conveniently used in perturbative expansions, as previously discussed in Sect. 1.2.1.

From the above expressions we can find the interaction matrix elements corresponding to emission and absorption of a single photon. We note that to first order the photon number only of one mode ( $\mathbf{k}, a$ ) is changed and we write the photon number only of this mode explicitly. We write the initial and final states as

$$\begin{aligned}|i\rangle &= |A, n_{\mathbf{k}a}\rangle \\ |f\rangle &= |B, n_{\mathbf{k}a} \pm 1\rangle\end{aligned}\quad (4.95)$$

where  $|A\rangle$  is the (unspecified) initial state of the atom (*i.e.*, the electron state),  $|B\rangle$  is the final state of the atom, and  $n_{\mathbf{k}a}$  is the photon number of the initial state. This means that we consider transitions between Fock states of the electromagnetic field.

For absorption the matrix element is

$$\begin{aligned}\langle B, n_{\mathbf{k}a} - 1 | \hat{H}_{abs} | A, n_{\mathbf{k}a} \rangle &= -\frac{e}{m} \sqrt{\frac{\hbar}{2V\omega_k}} \langle B, n_{\mathbf{k}a} - 1 | \hat{\mathbf{p}} \cdot \boldsymbol{\epsilon}_{\mathbf{k}a} \hat{a}_{\mathbf{k}a} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)} | A, n_{\mathbf{k}a} \rangle \\ &= -\frac{e}{m} \sqrt{\frac{\hbar n_{\mathbf{k}a}}{2V\omega_k}} \boldsymbol{\epsilon}_{\mathbf{k}a} \cdot \langle B | \hat{\mathbf{p}} e^{i\mathbf{k}\cdot\mathbf{r}} | A \rangle e^{-i\omega_k t}\end{aligned}\quad (4.96)$$

and the corresponding expression for photon emission is

$$\begin{aligned}\langle B, n_{\mathbf{k}a} + 1 | \hat{H}_{emis} | A, n_{\mathbf{k}a} \rangle &= -\frac{e}{m} \sqrt{\frac{\hbar}{2V\omega_k}} \langle B, n_{\mathbf{k}a} + 1 | \hat{\mathbf{p}} \cdot \boldsymbol{\epsilon}_{\mathbf{k}a}^* \hat{a}_{\mathbf{k}a}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)} | A, n_{\mathbf{k}a} \rangle \\ &= -\frac{e}{m} \sqrt{\frac{\hbar(n_{\mathbf{k}a} + 1)}{2V\omega_k}} \boldsymbol{\epsilon}_{\mathbf{k}a}^* \cdot \langle B | \hat{\mathbf{p}} e^{-i\mathbf{k}\cdot\mathbf{r}} | A \rangle e^{i\omega_k t}\end{aligned}\quad (4.97)$$

In the final expressions of both (4.96) and (4.157) note that only the matrix elements for the electron operator between the initial and final states  $A$  and  $B$  remain, while the effect of the photon operators is absorbed in the prefactor, which now depends on the photon number of the initial state.

It is of interest to note that the electron matrix elements found for the interactions with a *quantized* electromagnetic field is quite analogous to those found for interaction with a classical *time-dependent* electromagnetic field of the form

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)} + \mathbf{A}_0^* e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\quad (4.98)$$

where the positive frequency part of the field (*i.e.*, the term proportional to  $e^{-i\omega_k t}$ ) corresponds to the absorption part of the matrix element and the negative frequency part (proportional to  $e^{i\omega_k t}$ ) corresponds to the emission part. The use of this expression for the  $\mathbf{A}$ -field gives a *semi-classical* approach to radiation theory, which in many cases is completely satisfactory. It works well for effects like *stimulated emission* where the classical field corresponds to a large value of the photon number in the initial state and where the relation between the amplitude of the oscillating field and the photon number is given by (4.96) and (4.157). However, for small photon numbers one notes the difference in amplitude for emission and absorption. This difference is not reflected in the classical amplitude (4.98). In the case of *spontaneous emission*, with  $n_{\mathbf{k}a} = 0$  in the initial state, the quantum theory correctly describes the transition of the electron from an excited state by emission of a photon, whereas a semiclassical description does not, since electronic transitions in this approach depends on the presence of an oscillating electromagnetic field.

#### 4.2.4 Dipole approximation and selection rules

For radiation from an atom, the wave length of the radiation field is typically much larger than the dimension of the atom. This difference is exemplified by the wave length of blue light and the Bohr radius of the hydrogen atom

$$\lambda_{blue} \approx 400\text{nm}, \quad a_0 = 4\pi \frac{\hbar^2}{me^2} \approx 0.05\text{nm} \quad (4.99)$$

This means that the effect of spacial variations in the electromagnetic field over the dimensions of an atom are small, and therefore the *time-variations* rather than the space variations of the field are important. In the expression for the transition matrix elements (4.96) and (4.157) this justifies an expansion of the phase factors in powers of  $\mathbf{k} \cdot \mathbf{r}$ ,

$$e^{\pm i\mathbf{k} \cdot \mathbf{r}} = 1 \pm i\mathbf{k} \cdot \mathbf{r} - \frac{1}{2}(\mathbf{k} \cdot \mathbf{r})^2 + \dots \quad (4.100)$$

where the first term is dominant. The approximation where only this term is kept is referred to as the *dipole approximation*. The other terms give rise to higher *multipole* contributions. These may give important contributions to atomic transitions only when the contribution from the first term vanishes due to a selection rule. However the transitions dominated by higher multipole terms are normally much slower than the ones dominated by the dipole contribution.

When the dipole approximation is valid, the matrix elements of the interaction Hamiltonian simplify to

$$\begin{aligned} \langle B, n_{\mathbf{k}a} - 1 | \hat{H}_{abs} | A, n_{\mathbf{k}a} \rangle &= -\frac{e}{m} \sqrt{\frac{\hbar n_{\mathbf{k}a}}{2V\omega_k}} \boldsymbol{\epsilon}_{\mathbf{k}a} \cdot \mathbf{p}_{BA} e^{-i\omega_k t} \\ \langle B, n_{\mathbf{k}a} + 1 | \hat{H}_{emis} | A, n_{\mathbf{k}a} \rangle &= -\frac{e}{m} \sqrt{\frac{\hbar(n_{\mathbf{k}a} + 1)}{2V\omega_k}} \boldsymbol{\epsilon}_{\mathbf{k}a}^* \cdot \mathbf{p}_{BA} e^{i\omega_k t} \end{aligned} \quad (4.101)$$

where  $\mathbf{p}_{BA}$  is the matrix element of the operator  $\hat{\mathbf{p}}$  between the states  $|A\rangle$  and  $|B\rangle$ . It is convenient to re-express it in terms of the matrix elements of the position operator  $\hat{\mathbf{r}}$ , which can be done by

use of the form of the (unperturbed) electron Hamiltonian,

$$\hat{H}_0^{atom} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}) \quad (4.102)$$

where  $V(\hat{\mathbf{r}})$  is the (Coulomb) potential felt by the electron. This gives

$$[\hat{H}_0^{atom}, \hat{\mathbf{r}}] = -i\frac{\hbar}{m}\hat{\mathbf{p}} \quad (4.103)$$

With the initial state  $|A\rangle$  and the final state  $|B\rangle$  as eigenstates of  $\hat{H}_0^{atom}$ , with eigenvalues  $E_A$  and  $E_B$ , we find for the matrix element of the momentum operator between the two states

$$\mathbf{p}_{BA} = i\frac{m}{\hbar}(E_B - E_A)\mathbf{r}_{BA} = im\omega_{BA}\mathbf{r}_{BA} \quad (4.104)$$

where we have introduced  $\omega_{AB} = (E_A - E_B)/\hbar$ . Note that in the expression for the interaction, the change from  $\mathbf{p}_{BA}$  to  $\mathbf{r}_{BA}$  corresponds to the transformation

$$-\frac{e}{mc}\mathbf{A} \cdot \mathbf{p} \rightarrow \frac{e}{c}\mathbf{r} \cdot \dot{\mathbf{A}} = -e\mathbf{r} \cdot \mathbf{E} \quad (4.105)$$

where the last term is identified as the electric dipole energy of the electron. This form justifies the name *electric dipole transitions* for transitions induced by this operator.

By use of the identity (4.104) the interaction matrix elements are finally written as

$$\begin{aligned} \langle B, n_{\mathbf{k}a} - 1 | \hat{H}_{abs} | A, n_{\mathbf{k}a} \rangle &= -ie\sqrt{\frac{\hbar n_{\mathbf{k}a} \omega_{BA}^2}{2V\omega_k}} \boldsymbol{\epsilon}_{\mathbf{k}a} \cdot \mathbf{r}_{BA} e^{-i\omega_k t} \\ \langle B, n_{\mathbf{k}a} + 1 | \hat{H}_{emis} | A, n_{\mathbf{k}a} \rangle &= ie\sqrt{\frac{\hbar(n_{\mathbf{k}a} + 1)\omega_{AB}^2}{2V\omega_k}} \boldsymbol{\epsilon}_{\mathbf{k}a}^* \cdot \mathbf{r}_{BA} e^{i\omega_k t} \end{aligned} \quad (4.106)$$

As we shall later see these expressions may in most cases be simplified by use of *energy conservation*, in the form  $\omega_k = \omega_{BA}$  for photon absorption and  $\omega_k = \omega_{AB}$  for photon emission.

### Selection rules

The matrix elements

$$\mathbf{r}_{BA} = \langle B | \hat{\mathbf{r}} | A \rangle \quad (4.107)$$

are subject to certain *selection rules* which follow from conservation of spin and parity. Thus, the operator  $\hat{\mathbf{r}}$  transforms as a *vector* under rotation and changes sign under space inversion. Since a vector is a *spin 1* quantity, the operator can change the spin of the state  $|A\rangle$  by maximally one unit of spin. Physically we interpret this as due to the spin carried by the photon. The change in sign under space inversion corresponds to the parity of the photon being  $-1$ . This change implies that the parity of the final state is opposite that of the initial state.



Let us specifically consider (orbital) angular momentum states of the atomic electron, characterized by the quantum numbers  $l$  and  $m$  (total angular momentum and angular momentum in the  $z$ -direction). The initial atomic state  $A$  is then characterized by quantum numbers  $l_A$  and  $m_A$ , while the parity is  $P_A = (-1)^{l_A}$ . The corresponding quantum numbers for the state  $B$  are  $l_B, m_B$  and  $P_B = (-1)^{l_B}$ . We note that the change in parity forces the angular momentum to change by one unit ( $l_A \neq l_B$ ) and the formula for spin addition gives  $l_B = l_A \pm 1$ . The selection rules for the electric dipole transitions (referred to as  $E1$  transitions) are therefore

$$\begin{aligned}\Delta l &= \pm 1 \quad (l_A \neq 0), \quad \Delta l \equiv l_B - l_A \\ \Delta l &= +1 \quad (l_A = 0) \\ \Delta m &= 0, \pm 1, \quad \Delta m \equiv m_B - m_A\end{aligned}\tag{4.108}$$

The transitions that do not satisfy these rules are “forbidden” in the sense that the interaction matrix element vanishes in the dipole approximation. Nevertheless such transitions may take place, but at a much slower rate than the  $E1$  transitions. They may be induced by higher multipole terms in the expansion (4.100), or by higher order terms in  $\mathbf{A}$  which give rise to multi-photon processes. The multipole terms include higher powers in the components of the position operator, and these terms transform differently under rotation and space inversion than the vector  $\mathbf{r}$ . As a consequence they are restricted by other selection rules. Physically we may consider the higher multipole transitions as corresponding to non-central photon emission and absorption, where the total spin transferred is not only due to the intrinsic photon spin but also orbital angular momentum of the photon.

## 4.3 Photon emission from excited atom

In this section we examine the photon emission process for an excited atom in some more detail. We make the assumption that the atom at a given instant  $t = t_i$  is in an excited state  $|A\rangle$  and consider the amplitude for making a transition to a state  $|B\rangle$  at a later time  $t = t_f$  by emission of a single photon. The amplitude is determined to first order in the interaction, and the transition probability per unit time and unit solid angle for emission of the photon in a certain direction is evaluated and expressed in terms of the dipole matrix element. We subsequently discuss the effect of decay of the initial atomic state and its relation to the formation of a *line width* for the photon emission line.

### 4.3.1 First order transition and Fermi's golden rule

The perturbation expansion of the time evolution operator in the interaction picture is (see Sect. 1.2.1)

$$\hat{U}_{int}(t_f, t_i) = \mathbf{1} - \frac{i}{\hbar} \int_{t_i}^{t_f} dt \hat{H}_{int}(t) + \frac{1}{2} \left(-\frac{i}{\hbar}\right)^2 \int_{t_i}^{t_f} dt \int_{t_i}^t dt' \hat{H}_{int}(t) \hat{H}_{int}(t') + \dots\tag{4.109}$$

where the time evolution of the interaction Hamiltonian is

$$\hat{H}_{int}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t} \hat{H}_{int} e^{-\frac{i}{\hbar}\hat{H}_0 t} \quad (4.110)$$

with  $\hat{H}_0$  as the unperturbed Hamiltonian. The transition matrix element between an initial state  $|i\rangle$  at time  $t_i$  and final state  $|f\rangle$  at time  $t_f$  is

$$\begin{aligned} \langle f|\hat{U}_{int}(t_f, t_i)|i\rangle &= \langle f|i\rangle - \frac{i}{\hbar} \langle f|\hat{H}_{int}|i\rangle \int_{t_i}^{t_f} dt e^{\frac{i}{\hbar}(E_f - E_i)t} \\ &+ \frac{1}{2} \left(-\frac{i}{\hbar}\right)^2 \sum_m \langle f|\hat{H}_{int}|m\rangle \langle m|\hat{H}_{int}|i\rangle \int_{t_i}^{t_f} dt \int_{t_i}^t dt' e^{\frac{i}{\hbar}(E_f - E_m)t} e^{\frac{i}{\hbar}(E_m - E_i)t'} + \dots \end{aligned} \quad (4.111)$$

In this expressions we have assumed that the initial state  $|i\rangle$  and the final state  $|f\rangle$  as well as a complete set of intermediate states  $|m\rangle$  are eigenstates of the unperturbed Hamiltonian  $\hat{H}_0$ . The corresponding eigenvalues are  $E_i$ ,  $E_f$  and  $E_m$ . We perform the time integrals, and in order to simplify expressions we introduce the notation  $\omega_{fi} = (E_f - E_i)/\hbar$ ,  $T = t_f - t_i$  and  $\bar{t} = (t_i + t_f)/2$ . To second order in the interaction the transition matrix element is

$$\begin{aligned} \langle f|\hat{U}_{int}(t_f, t_i)|i\rangle &= \langle f|i\rangle \\ &- 2i \frac{\sin[\frac{1}{2}\omega_{fi}T]}{\hbar\omega_{fi}} e^{i\omega_{fi}\bar{t}} \left[ \langle f|\hat{H}_{int}|i\rangle - \sum_m \frac{\langle f|\hat{H}_{int}|m\rangle \langle m|\hat{H}_{int}|i\rangle}{\hbar\omega_{mi}} + \dots \right] \\ &- 2ie^{i\omega_{fi}\bar{t}} \sum_m \sin[\frac{1}{2}\omega_{fm}T] e^{i\omega_{mi}T} \frac{\langle f|\hat{H}_{int}|m\rangle \langle m|\hat{H}_{int}|i\rangle}{\hbar^2\omega_{fm}\omega_{mi}} + \dots \end{aligned} \quad (4.112)$$

where we assume the *diagonal* matrix elements of  $\hat{H}_{int}$  to vanish in order to avoid ill-defined terms in the expansion. The factor depending on  $\bar{t}$  is unimportant and can be absorbed in a redefinition of the time coordinate so, that  $\bar{t} = 0$ . (The interesting time dependence lies in the relative coordinate  $T = t_f - t_i$ .) The last term in (4.133) does not contribute (at average) to low order due to rapid oscillations. Without this term the result simplifies to

$$\langle f|\hat{U}_{int}(t_f, t_i)|i\rangle = \langle f|i\rangle - 2i \frac{\sin[\frac{1}{2}\omega_{fi}T]}{\hbar\omega_{fi}} e^{i\omega_{fi}\bar{t}} \mathcal{T}_{fi} \quad (4.113)$$

where  $\mathcal{T}_{fi}$  is the *T-matrix* element

$$\mathcal{T}_{fi} = \left[ \langle f|\hat{H}_{int}|i\rangle - \sum_m \frac{\langle f|\hat{H}_{int}|m\rangle \langle m|\hat{H}_{int}|i\rangle}{\hbar\omega_{mi}} + \dots \right] \quad (4.114)$$

The transition probability for  $f \neq i$  is

$$W_{fi} = \left( \frac{2 \sin[\frac{1}{2}\omega_{fi}T]}{\hbar\omega_{fi}} \right)^2 |\mathcal{T}_{fi}|^2 \quad (4.115)$$

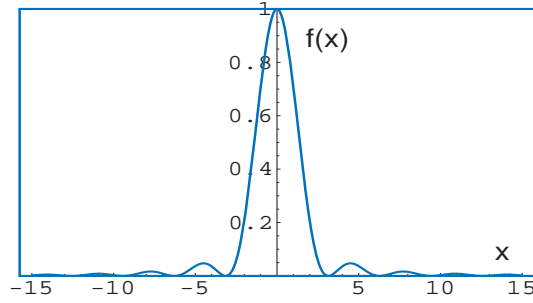


Figure 4.3: Frequency dependence of the transition probability. For finite transition time  $T$  the function has a non-vanishing width. In the limit  $T \rightarrow \infty$  the function tends to a delta-function.

Also this is an oscillating function, but for large  $T$  it gives a contribution proportional to  $T$ . To see this we consider the function

$$f(x) = \left( \frac{\sin x}{x} \right)^2 \quad (4.116)$$

The function is shown in fig.(4.3). It is localized around  $x = 0$  with oscillations that are damped like  $1/x^2$  for large  $x$ . The integral of the function is

$$\int_{-\infty}^{\infty} f(x) dx = \pi \quad (4.117)$$

The prefactor of (4.115) can be expressed in terms of the function  $f(x)$  as

$$\left( \frac{2 \sin[\frac{1}{2} \omega_{fi} T]}{\hbar \omega_{fi}} \right)^2 = \frac{T^2}{\hbar^2} f\left(\frac{1}{2} \omega_{fi} T\right) \quad (4.118)$$

When regarded as a function of  $\omega_{fi}$  this function gets increasingly localized around  $\omega_{fi} = 0$  as  $T$  increases, and in the limit  $T \rightarrow \infty$  it approaches a delta function, with the strength of the delta function being determined by the (normalization) integral (4.117),

$$\left( \frac{2 \sin[\frac{1}{2} \omega_{fi} T]}{\hbar \omega_{fi}} \right)^2 \rightarrow \frac{2\pi}{\hbar} T \delta(\hbar \omega_{fi}) \quad (4.119)$$

This gives a constant transition rate between the initial and final states,

$$w_{fi} = \frac{W_{fi}}{T} = \frac{2\pi}{\hbar} |\mathcal{T}_{fi}|^2 \delta(E_f - E_i) \quad (4.120)$$

where  $\mathcal{T}_{fi}$  to lowest order in the interaction is simply the interaction matrix element. When applied to transitions in atoms, the expression (4.120) for the constant transition rate is often referred to as *Fermi's golden rule*. The delta function expresses energy conservation in the

process. Note, however, that only in the limit  $T \rightarrow \infty$  the energy dependent function is really a delta function. For finite time intervals there is a certain width of the function which means that  $E_f$  can deviate slightly from  $E_i$ . This apparent breaking of energy conservation for finite times may happen since  $E_f$  and  $E_i$  are eigenvalues of the *unperturbed* Hamiltonian rather than the *full* Hamiltonian.

In reality the time  $T$  cannot be taken to infinity for an atomic emission process, since any excited state will have a *finite life time*. The width of the energy-function then has a physical interpretation in terms of a *line width* for the emission line. At this point we neglect this effect of *level broadening*, but we shall return to a description of this effect a coming section.

### 4.3.2 Emission rate

We consider now the case where initially the atom is in an excited state  $A$  and finally in a state  $B$  with one photon being emitted. The initial and final states of the full quantum system are

$$|i\rangle = |A, 0\rangle, \quad |f\rangle = |B, 1_{\mathbf{k}a}\rangle \quad (4.121)$$

where 0 in the initial state indicates the photon vacuum, while  $1_{\mathbf{k}a}$  indicates one photon with quantum numbers  $\mathbf{k}a$ . We will be interested in finding an expression for the *differential* transition rate, *i.e.*, the transition probability per unit time and unit solid angle, as well as the *total* transition rate.

We write the transition rate summed over all final states of the photon as

$$\begin{aligned} w_{BA} &= \sum_{\mathbf{k}a} \frac{2\pi}{\hbar} |\langle B, 1_{\mathbf{k}a} | \hat{H}_{emis} | A, 0 \rangle|^2 \delta(E_A - E_B - \hbar\omega_k) \\ &\rightarrow \frac{V}{(2\pi)^3} \int d^3k \sum_a \frac{2\pi}{\hbar} |\langle B, 1_{\mathbf{k}a} | \hat{H}_{emis} | A, 0 \rangle|^2 \delta(E_A - E_B - \hbar\omega_k) \\ &= \frac{V}{(2\pi)^2 \hbar} \int d\Omega \int_0^\infty dk k^2 \sum_a |\langle B, 1_{\mathbf{k}a} | \hat{H}_{emis} | A, 0 \rangle|^2 \delta(E_A - E_B - \hbar\omega_k) \\ &= \frac{V \omega_{BA}^2}{(2\pi)^2 c^3 \hbar^2} \int d\Omega \sum_a |\langle B, 1_{\mathbf{k}a} | \hat{H}_{emis} | A, 0 \rangle|^2 \end{aligned} \quad (4.122)$$

where the infinite volume limit has been taken in the change from a diskrete momentum sum to a momentum integral. The subsequent integration of  $k = \omega_k/c$  over the delta function then fixes the frequency of the emitted photon to match the atomic frequency,  $\omega_k = \omega_{AB} = (E_A - E_B)/\hbar$ . By use of the expression for the dipole transmission matrix element (4.106), we find the following expression for differential emission rate,

$$\frac{dw_{BA}}{d\Omega} = \frac{e^2 \omega_{AB}^3}{8\pi^2 \hbar c^3} |\mathbf{r}_{BA} \cdot \boldsymbol{\epsilon}_{\mathbf{k}a}^*|^2 \quad (4.123)$$

where  $\boldsymbol{\epsilon}_{\mathbf{k}a}$  is the polarization vector of the emitted photon.

Summed over photon states we have

$$\sum_a |\mathbf{r}_{BA} \cdot \boldsymbol{\epsilon}_{\mathbf{k}a}^*|^2 = |\mathbf{r}_{BA}|^2 - \frac{|\mathbf{r}_{BA} \cdot \mathbf{k}|^2}{k^2} \quad (4.124)$$

From this we find the total transition rate into all final states of the photon,

$$\begin{aligned} w_{BA} &= \frac{e^2 \omega_{AB}^3}{8\pi^2 \hbar c^3} \int d\Omega \left[ |\mathbf{r}_{BA}|^2 - \frac{|\mathbf{r}_{BA} \cdot \mathbf{k}|^2}{k^2} \right] \\ &= \frac{e^2 \omega_{AB}^3}{4\pi \hbar c^3} |\mathbf{r}_{BA}|^2 \int_0^\pi d\theta \sin \theta (1 - \cos^2 \theta) \\ &= \frac{e^2 \omega_{AB}^3}{4\pi \hbar c^3} |\mathbf{r}_{BA}|^2 \int_{-1}^{+1} du (1 - u^2) \\ &= \frac{e^2 \omega_{AB}^3}{3\pi \hbar c^3} |\mathbf{r}_{BA}|^2 \\ &= \frac{4\alpha}{3c^2} \omega_{AB}^3 |\mathbf{r}_{BA}|^2 \end{aligned} \quad (4.125)$$

where  $\alpha$  is the fine structure constant. This expression shows how the transition rate depends on the dipole matrix element  $|\mathbf{r}_{BA}|^2$  and on the energy  $\hbar\omega_{AB}$  released in the transition.<sup>8</sup>

The formalism employed here for the case of spontaneous emission can also be used to describe photon *absorption* processes and *scattering* of photons on atoms. In the latter case the amplitude should be calculated to second order in the electric charge, and that would involve the  $\mathbf{A} \cdot \mathbf{A}$ -term as well as the  $\mathbf{A} \cdot \mathbf{p}$ -term of the interaction. We note from the expression (4.125) that the emission rate increases strongly with the energy of the emitted photon. To a part that can be seen as a *density of states* effect, since for high energy photons many more states are available (within a fixed energy interval) than for low energy photons. This is demonstrated explicitly by (4.122) which shows that a factor  $\omega_{BA}^2$  can be ascribed to the frequency dependence of the density of states. A similar effect takes place when light scattering is considered. This gives a qualitative explanation for why blue light is more readily scattered than red light, and thereby why the sky is blue and the sunset is red.

### 4.3.3 Life time and line width

Fermi's golden rule, which gives a constant transition rate from the excited to the lower energy level of the atom, can be correct only in an approximate sense. Thus, the corresponding expression for the integrated transition probability,

$$W_{BA}(t) = tw_{BA} \quad (4.126)$$

which shows that  $W_{BA}$  increases linearly with time, can obviously be correct only for a sufficiently short time interval  $t < w_{BA}^{-1}$ . One way to view this problem is that the expression (4.115)

<sup>8</sup>Note that in the evaluation we have treated  $\mathbf{r}_{BA}$  as a real vector. In reality  $\mathbf{r}_{BA}$  may be complex, but this does not change the result, one only has to repeat the evaluation for the real and imaginary parts separately.

does not take into account the fact that the probability of state  $A$  to be occupied is reduced during the transition. This motivates the following modification of the expression for the transition rate,

$$\frac{d}{dt}W_{BA} = w_{BA}P_A(t) \quad (4.127)$$

where  $w_{BA}$  is the time independent rate determined from the golden rule and  $P_A(t)$  is the probability for level  $A$  to be occupied after time  $t$ . This probability is on the other hand related to the sum of transition rates over all final states  $B$ ,

$$P_A(t) = 1 - \sum_B W_{BA}(t) \quad (4.128)$$

and taking the time derivative and making use of (4.115), we find

$$\begin{aligned} \frac{d}{dt}P_A &= - \sum_B \frac{d}{dt}W_{BA} \\ &= - \sum_B w_{BA}P_A \\ &\equiv -P_A/\tau_A \end{aligned} \quad (4.129)$$

where  $\tau_A = (\sum_B w_{BA})^{-1}$ . This can be integrated to give

$$P_A(t) = e^{-t/\tau_A} \quad (4.130)$$

which shows an exponential decay of the excited state  $A$ , with  $\tau_A$  as the *life time* of the state. From this follows that the corrected transition rate is

$$\frac{d}{dt}W_{BA} = w_{BA}e^{-t/\tau_A} \quad (4.131)$$

which integrates to

$$W_{BA} = w_{BA} \tau_A (1 - e^{-t/\tau_A}) \quad (4.132)$$

The original expression (4.115) for the transition probability corresponds to (4.132) expanded to first order in  $t/\tau_A$ , and is clearly a good approximation to the full expression only when  $t \ll \tau_A$ .

The decay of the initial state can be built into the expressions for the the transitions to lower energy states in a simple way by including a damping factor  $\exp(-t/2\tau_A)$  as a normalization factor in the amplitude. For the transition amplitude this gives a modified expression

$$\begin{aligned} \langle f|\hat{U}_{int}(t_f, t_i)|i\rangle &= -\frac{i}{\hbar}\langle f|\hat{H}_{int}|i\rangle \int_{t_i}^{t_f} dt e^{\frac{i}{\hbar}(E_f - E_i)t} e^{-\frac{(t-t_i)}{2\tau_A}} + \dots \\ &= -\frac{i}{\hbar}\langle f|\hat{H}_{int}|i\rangle e^{t_i/\tau_A} \int_{t_i}^{t_f} dt e^{\frac{i}{\hbar}(E_f - E_i + \frac{i}{2}\Gamma_A)t} + \dots \end{aligned}$$

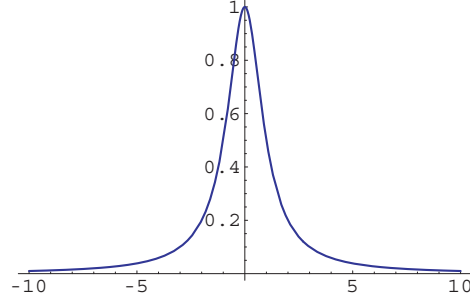


Figure 4.4: Level broadening. The emission probability given by  $W_{fi} = |\langle f | \hat{H}_{int} | i \rangle|^2 / [(\hbar\omega_{fi})^2 + \frac{1}{4}\Gamma_A^2]$  is shown as a function of  $\omega_{fi}$ .

$$\begin{aligned}
 &= -\frac{\langle f | \hat{H}_{int} | i \rangle}{E_f - E_i + \frac{i}{2}\Gamma_A} \left( e^{\frac{i}{\hbar}(E_f - E_i)t_f} e^{-\frac{1}{2\hbar}\Gamma_A(t_f - t_i)} - e^{\frac{i}{\hbar}(E_f - E_i)t_i} \right) + \dots \\
 &\rightarrow \frac{\langle f | \hat{H}_{int} | i \rangle}{E_f - E_i + \frac{i}{2}\Gamma_A} e^{\frac{i}{\hbar}(E_f - E_i)t_i} + \dots
 \end{aligned} \tag{4.133}$$

where we have introduced  $\Gamma_A = \hbar/\tau_A$  and at the last step assumed  $t_f - t_i \gg \tau_A$ . With the initial energy  $E_i = E_A$  and the final energy  $E_f = E_B + \hbar\omega_k$ , the expression shows that the correction due to a finite life time of the atomic level  $A$  can be viewed as represented by an imaginary contribution to the energy of this level,  $E_A \rightarrow E_A - (i/2)\Gamma_A$ .

The transition probability is then, for  $t_f - t_i \gg \tau_A$ , given by

$$W_{fi} = \frac{|\langle f | \hat{H}_{int} | i \rangle|^2}{(E_A - E_B - \hbar\omega_k)^2 + \frac{1}{4}\Gamma_A^2} + \dots \tag{4.134}$$

Viewed as a function of  $\omega_k$ , the transition probability is no longer proportional to a delta function in the difference  $\omega_k - \omega_{AB}$ . The delta function is instead replaced by a *Lorentzian* (Fig.4.4), which is strongly peaked around  $\omega_{fi} = 0$ , but which has a finite width proportional to  $\Gamma_A$ . For the emitted photon this is translated to a finite *line width* for the emission line corresponding to the transition  $A \rightarrow B$ .

If we compare the two figures 4.3 and 4.4 we note that a finite cut-off in the time integral (*i.e.*, a finite value of  $T = t_f - t_i$ ) gives essentially the same frequency dependence for the emitted photon as the one obtained by an exponential damping due to the finite life time of the initial atomic state. We finally note that since  $\Gamma_A$  depends on the transition probabilities, to include it in the lowest order transition amplitude means that we effectively have included higher order contributions. This means that the perturbative expansion is no longer an order by order expansion in the interaction Hamiltonian.

## 4.4 Stimulated photon emission and the principle of lasers

As we have already noticed, the rate for *stimulated* emission of a photon by an atomic transition is larger than the corresponding *spontaneous* emission. Thus, to lowest order in the interaction, the transition probability by photon emission into a given mode is enhanced by a factor  $n$  equal to the number of photons already present in the mode. This means that if an atom in an excited state emits a photon with equal probability in all directions, the same atom, when placed in a strong field which resonates with the atomic transition, will preferably emit the photon into the mode that is already occupied. However, in free space, since a continuum of modes is available, the probability for emission into the preferred mode may still be small.

A laser is based on the principle of stimulated emission, but the probability for emission into the preferred mode is enhanced by use of a reflecting cavity. The boundary conditions imposed by the reflecting mirrors of the cavity reduce the number of available electromagnetic modes to a discrete set, and the trapping of the photons makes it possible to build a large population of photons in one of the modes.

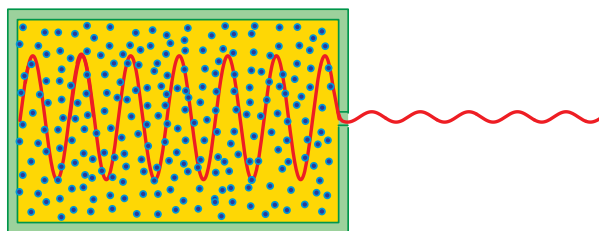


Figure 4.5: Schematic representation of a laser. A gas of atoms is trapped inside a *Fabry-Perot* cavity with reflecting walls. The atoms are *pumped* to an excited state that subsequently make transitions to a lower energy mode. The emitted photons resonate with a longitudinal mode of the cavity and build up a strong field in this mode. Some of the light from this mode escapes through a semi-reflective mirror in one end of the cavity to form a monochromatic laser beam.

A schematic picture of a laser is shown in fig.(4.5) where a elongated cavity is filled with gas of (Rubidium) atoms. These are continuously excited (pumped) from the ground state to a higher energy state. The excited atoms subsequently make transitions to a lower energy state and emit photons with energy that matches one of the modes selected by the distance between the mirrors in the longitudinal direction. The emission tends to increase the excitation of the preferred mode to a high level. Some of the light that builds up inside the cavity escapes through a small hole in one of the mirrors in the form of a monochromatic laser beam.

The laser light is a beam of *coherent* or *classical* light in the sense previously discussed. The reason for this coherence is that the photons emitted by the atoms in the cavity tend to act coherently with the light already trapped in the cavity. However, even if the light to a high degree is coherent, there will be some incoherent admixture due to spontaneous emission. In the following we shall discuss the mechanism of the laser in some more detail.



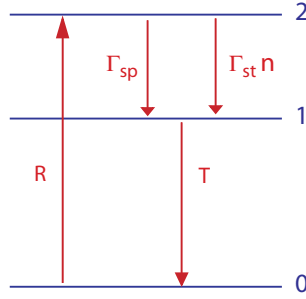


Figure 4.6: Transitions between three atomic levels in a laser.  $R$  is the pumping rate from the ground state 0 to an excited state 2. The transition from level 2 to an intermediate level 1 can go either by spontaneous emission ( $\Gamma_{sp}$ ), or by stimulated emission ( $\Gamma_{st} n$ ) to the laser mode.  $n$  is the photon number of the laser mode. A fast transition  $T$  brings the atoms back to the ground state. The direct transition rate  $2 \rightarrow 0$  is assumed to be negligible.

#### 4.4.1 Three-level model of a laser

We consider a simple model of a laser where a single mode is populated by stimulated emission. A three-level model is used for the atom, where most atoms are in the ground state  $|0\rangle$ , but where there is a continuous rate of “pumping” of atoms to a higher energy level  $|2\rangle$ , by a light source or some other way of excitation. The atoms in the upper level next make transitions to an intermediate level  $|1\rangle$  by emission of a photon. This may be by stimulated emission of a photon to the field mode that is already strongly populated, or by spontaneous emission to one of the other photon states in the emission line that are allowed by the boundary conditions of the cavity. From the state  $|1\rangle$  there is a fast transition back to the ground state due to a strong coupling between the levels  $|1\rangle$  and  $|0\rangle$ .

Due to the assumed strength of the transitions we have

$$N_0 \gg N_2 \gg N_1 \quad (4.135)$$

This means that the number of atoms in the ground state  $N_0$  is essentially identical to the total number of atoms  $N$ . When we consider the two levels 1 and 2, which are relevant for populating the laser mode, the inequality means that there is *population inversion*, since the upper level is more strongly populated than the lower mode. Population inversion is a condition for the atoms to be able to “feed” the preferred photon mode, since the probability of reabsorbing a photon from the preferred mode by the inverse transition  $|1\rangle \rightarrow |2\rangle$  is much smaller than emission of a photon by the process  $|2\rangle \rightarrow |1\rangle$ .

When the atoms are pumped to a higher energy level, this creates initially a situation where the photon modes within the line width of the transition  $2 \rightarrow 1$  begins to get populated, but where no single mode is preferred. If the pumping rate  $R$  is sufficiently large, this is an unstable situation, due to the effect of stimulated emission to preferably populate a mode which already is excited. As a result one of the modes will spontaneously tend to grow at the expense of the others. We will consider the situation after one of the modes has been preferred in this way.

The transition from state 2 to 1 may now go in two ways, either by spontaneous emission to one of the modes that have not been populated or by stimulated emission to the preferred (laser) mode. We denote the transition rate by spontaneous emission  $\Gamma_{sp}$  and by stimulated emission  $\Gamma_{st}n$ , where  $n$  is the photon number of the laser mode. The difference between  $\Gamma_{sp}$  and  $\Gamma_{st}$  is due to the large number available for spontaneous emission compared to the single mode available for stimulated emission. Typical values are

$$\Gamma_{sp} \approx 10^7 s^{-1}, \quad \Gamma_{st} \approx 1 s^{-1} \quad (4.136)$$

The smallness of  $\Gamma_{st}$  is compensated by the factor  $n$  and when a stationary situation is reached the photon number  $n$  in the laser mode will be so large so that the probabilities of the two types of transitions are comparable. The ratio

$$n_s = \frac{\Gamma_{sp}}{\Gamma_{st}} \quad (4.137)$$

is referred to as the *saturation photon number*.

The quantum state of the laser mode should be described by a (mixed state) density matrix  $\rho_{nn'}$  rather than a (pure state) wave function. This is so since we cannot regard the electromagnetic field as a closed (isolated) system. It is a part of a larger system consisting of both atoms and field, but even that is not a closed system due to coupling of the atoms to the pumping field and due to the leak from the laser mode to the escaping laser beam and to the surroundings.

We will not approach the general problem of describing the time evolution of the density matrix  $\rho_{nn'}$ , but rather show that the steady state form of the photon probability distribution  $p_n = \rho_{nn}$  can be found with some simplifying assumptions<sup>9</sup>. We first note that for the steady state there is a balance between transitions to and from atomic level 2,

$$N_0 R = N_2 (\Gamma_{sp} + \Gamma_{st}n) \quad (4.138)$$

where  $R$  is the transition rate, per atom atom, from the ground state to the excited state 2. We assume at this point that the photon number  $n$  in this equation is identical to the expectation value  $\langle n \rangle$ . This means that we neglect the (quantum and statistical) fluctuations in the photon number, which we regard as small compared to its mean value.

We next consider the photon probability distribution  $p_n$ . If this distribution is stationary this means that for any photon number  $n$  there is balance between the processes that tend to increase the photon number and to decrease the photon number. We write this as a balance equation

$$N_2 \Gamma_{st} (np_{(n-1)} - (n+1)p_n) - \Gamma_{cav} (np_n - (n+1)p_{(n+1)}) = 0 \quad (4.139)$$

where we have introduced the *cavity loss rate per photon*,  $\Gamma_{cav}$ . With  $|\mathcal{T}|^2$  as the transmission probability to the outside for each reflection and  $L$  as the length of the cavity, it is given by  $\Gamma_{cav} =$

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<sup>9</sup>The discussion here mainly follows the approach of Rodney Loudon, *The Quantum Theory of Light*, Oxford Science Publications, 2000.

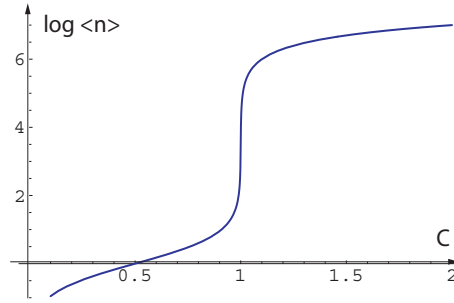


Figure 4.7: The photon number of the laser mode as a function of the parameter  $C = NR/(n_s \Gamma_{cav})$ . The curve corresponds to a saturation photon number  $n_s = 10^7$ .

$c|\mathcal{T}|^2/L$ . By multiplying the equation with  $n$  and averaging over the probability distribution, we find the following expression for the photon expectation value<sup>10</sup>,

$$N_2 \Gamma_{st}(1 + \langle n \rangle) = \Gamma_{cav} \langle n \rangle \quad (4.140)$$

This equation relates the number  $N_2$  of atoms in level 2 to the average photon number in the laser mode. We insert this in the steady state equation (4.138), with  $n$  replaced by  $\langle n \rangle$ , and we also replace  $N_0$  by the total number of atoms  $N$ ,

$$\Gamma_{st} \Gamma_{cav} \langle n \rangle^2 - (NR \Gamma_{st} - \Gamma_{sp} \Gamma_{cav}) \langle n \rangle - NR \Gamma_{st} = 0 \quad (4.141)$$

By introducing the coefficient

$$C = \frac{NR \Gamma_{st}}{\Gamma_{sp} \Gamma_{cav}} \quad (4.142)$$

the equation simplifies to

$$\langle n \rangle^2 - (C - 1)n_s \langle n \rangle - C n_s = 0 \quad (4.143)$$

with solution

$$\langle n \rangle = \frac{1}{2} \left[ (C - 1)n_s + [(C - 1)^2 n_s^2 + 4C n_s]^{\frac{1}{2}} \right] \quad (4.144)$$

The expectation value for the photon number is in Fig. (4.7) shown as a function of the parameter  $C$  for  $n_s = 10^7$ . As a characteristic feature one notes that around  $C = 1$  the photon number rapidly increases from a small number to a number of the order of  $n_s$ . After this rapid increase there is a continued less dramatic increase where  $\langle n \rangle$  changes linearly with  $C$ .

The curve demonstrates the presence of a threshold for the laser around  $C = 1$ . For smaller values the effects of spontaneous emission and emission from the cavity prevents the build up of the laser mode, while for larger values of  $C$  there is a net input of photons into the mode which allows the photon number to grow to a large number.

<sup>10</sup>Correlations between quantum fluctuations in  $N_2$  and  $n$  are then assumed to be unimportant

### 4.4.2 Quantum coherence

So far we have considered the *expectation value* of the photon number, which can increase to a large value for  $C > 1$ . This implies that the mode is strongly excited, but does not necessarily mean that it is in a coherent state that can be described by a (classical) monochromatic wave. For this to be the case *fluctuations* of the field variables have to be restricted. The fluctuations in the photon number can be determined from the evolution equation of the probability distribution (4.139). This should be satisfied for all  $n$ , including  $n = 0$  with  $p_{-1} = 0$ , and from this we conclude that following simpler equation has to be satisfied

$$N_2 \Gamma_{st} p_{(n-1)} = \Gamma_{cav} p_n \quad (4.145)$$

With the occupation number  $N_2$  determined by (4.138), we get

$$\begin{aligned} p_n &= \frac{NR\Gamma_{st}}{\Gamma_{cav}(\Gamma_{sp} + \Gamma_{st}n)} p_{(n-1)} \\ &= \frac{Cn_s}{n_s + n} p_{(n-1)} \end{aligned} \quad (4.146)$$

By repeated use of the equation we find

$$p_n = \frac{(Cn_s)^n n_s!}{(n_s + n)!} p_0 \quad (4.147)$$

where  $p_0$  is determined by the normalization of the probability distribution.

Well above the laser threshold,  $C \gg 1$ , then we have

$$\langle n \rangle = (C - 1)n_s \quad (4.148)$$

as follows from Eq. (4.144). By use of this expression for  $C$ , the distribution can be re-written as

$$p_n = \frac{(n_s + \langle n \rangle)^n}{(n + n_s)!} n_s! p_0 \quad (4.149)$$

We note that this distribution has a form very similar to that of a coherent state, which we can write as

$$p_n^{cs} = \frac{\langle n \rangle^n}{(n)!} e^{-\langle n \rangle} \quad (4.150)$$

The  $n$ -dependence is the same, except for a shift  $n \rightarrow n + n_s$ . For the coherent state the width of the distribution is given by the variance

$$(\Delta n)_{cs}^2 = \langle n \rangle \quad (4.151)$$

whereas, due to the shift, the width of the probability distribution (4.149) is

$$(\Delta n)^2 = \langle n \rangle + n_s \quad (4.152)$$

For large photon numbers,  $\langle n \rangle \gg n_s$  the last term can be neglected and the variance is the same as expected for a coherent state. However, for smaller values  $n_s$  introduces a non-negligible contribution to the fluctuation in the photon number. This can be interpreted as the influence of spontaneous emission: It affects the fluctuations in the occupation number  $N_2$  which in turn influences the fluctuations in the photon number of the laser mode through stimulated emission.

The fluctuation in photon number only describes a part of the fluctuations of the laser field. If we compare with a coherent state, of the form

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_n \frac{\alpha^n}{\sqrt{n!}} \quad (4.153)$$

the probability distribution  $p_n$  gives information about the absolute square of the  $n$ -components, here given by  $|\alpha|^{2n}$ , but there is no information about the relative phases of the components. To get information about the fluctuations both in absolute value and in phase, we apply the coherent state representation, which for a general state  $|\psi\rangle$  defines a (phase space) probability distribution in terms of the overlap of  $|\psi\rangle$  with a coherent state  $|z\rangle$ ,

$$f_\psi(z) = |\langle z|\psi\rangle|^2 \quad (4.154)$$

For the coherent state  $|\alpha\rangle$  the function is

$$f_\alpha(z) = e^{-|z-\alpha|^2} \quad (4.155)$$

which means that it is strongly localized around the point  $\alpha$  in the complex (phase) plane. A Fock state, with a well defined photon number is on the other hand given by

$$f_n(z) = e^{-|z|^2} \frac{|z|^{2n}}{n!} \quad (4.156)$$

which depends only on the modulus of  $z$ , and which therefore is localized in a ring in the complex plane.

Even if the photon probability distribution of the laser mode approaches that of a coherent state for large photon numbers, this does not determine the angular distribution of the state. To have well defined values for the electric and magnetic fields, like in the case of coherent states, a restriction on the fluctuations in the angular direction is needed. We will not discuss this question in depth here, which would require that we consider the evolution of the density matrix, including its off diagonal matrix elements. Instead we shall make the coherence probable by considering the effect of the emission Hamiltonian on a state that is already coherent.

The matrix element of the emission matrix element between the two atomic states 2 and 1 is in the dipole approximation

$$\langle 1|\hat{H}_{emis}|2\rangle = -ie\sqrt{\frac{\hbar\omega}{2V}} \mathbf{r}_{12} \cdot \boldsymbol{\epsilon} \hat{a}^\dagger \equiv m \hat{a}^\dagger \quad (4.157)$$

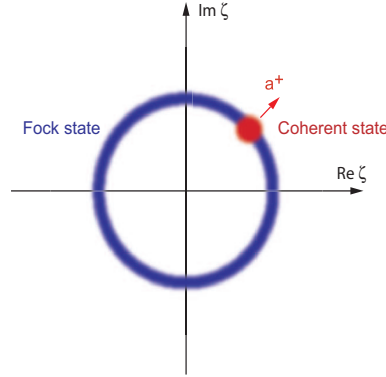


Figure 4.8: The complex phase plane of a single electromagnetic mode. A photon state is represented by the overlap with a *coherent state*  $|z\rangle$ . The radial coordinate correspond to the direction of increasing energy (or photon number), while the angular variable correspond to the phase of the electromagnetic wave. A Fock state (blue), with sharp photon number, is completely delocalized in the angular direction. A coherent state is well localized in both directions. The photon creation operator  $\hat{a}^\dagger$ , when acting on a coherent state will shift it in the radial direction.

In this expression  $V$  is the volume of the cavity, and the quantum numbers of the photon mode has been omitted since we consider only stimulated emission to a single mode. Since the prefactor of the photon creation operator is independent of the photon number they are collected in the constant  $m$ . The transition  $2 \rightarrow 1$  will therefore, when we consider this as a first order effect change the state simply by the action of  $\hat{a}^\dagger$ . If the photon state is before the transition well described by a coherent state  $\alpha$  this gives a change

$$|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle \equiv \mathcal{N} \hat{a}^\dagger |\alpha\rangle \quad (4.158)$$

where  $\mathcal{N}$  is a normalization factor.

With  $|\tilde{\alpha}\rangle$  normalized to unity, the spread of the state in the complex phase plane is

$$\begin{aligned} f_{\tilde{\alpha}}(z) &= |\mathcal{N}|^2 |\langle z | \hat{a}^\dagger | \alpha \rangle|^2 \\ &= \frac{|z|^2}{|\alpha|^2 + 1} e^{-|z-\alpha|^2} \end{aligned} \quad (4.159)$$

For large photon number, corresponding to large  $|\alpha|^2$ , it is convenient to change variable to  $\xi = z - \alpha$ , which by the gaussian factor is restricted to values of the order of unity. This gives

$$\begin{aligned} f_{\tilde{\alpha}}(\xi) &= |\mathcal{N}|^2 |\langle z | \hat{a}^\dagger | \alpha \rangle|^2 \\ &= \frac{|\alpha|^2 + \alpha \xi^* + \alpha^* \xi + |\xi|^2}{|\alpha|^2 + 1} e^{-|\xi|^2} \\ &\approx \exp \left[ -|\xi|^2 + \frac{\xi}{\alpha} + \frac{\xi^*}{\alpha^*} - \frac{1}{2} \left( \frac{\xi^2}{\alpha^2} + \frac{\xi^{*2}}{\alpha^{*2}} \right) \right] \end{aligned} \quad (4.160)$$

where the last expression is correct to order  $1/|\alpha|^2$ . The linear terms in  $\xi$  and  $\xi^*$  show that the location of the state is slightly shifted by the action of the photon creation operator,  $\xi \rightarrow \xi - 1/\alpha^*$  or  $\alpha \rightarrow \tilde{\alpha} = \alpha + 1/\alpha^*$ . This shift, which is due to the added energy, is in the radial direction in the complex plane, with the value proportional to  $1/|\alpha| = 1/\sqrt{\langle n \rangle}$ . There are also quadratic terms, which show that the width of the gaussian is slightly changed. But these are of the order of  $1/|\alpha|^2 = 1/\langle n \rangle$ , and are therefore less important than the shift for large photon numbers.

Even if this discussion does not show *how* coherence of the laser mode is created, it shows that the action of the stimulated emission on the photon state is mainly to increase its energy, and only to a lesser degree to change the coherence of the state. However, the rotational invariance in the complex shows that there is no preferred value for the complex phase of  $\alpha$ . The effect of spontaneous emission will in reality be to introduce a slow, random drift in the phase of the laser mode.