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QUANTUM OPTICS

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Contents

Part I

MAIN PART OF THE LECTURES

Chapter 1

Classical harmonic oscillator in external field

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Classical simple harmonic oscillator (SHO) is a very important model for many physical situations. When the potential energy of some interaction possesses a smooth minimum, then in the vicinity of this minimum interaction energy can be approximated by a parabola and that corresponds to the potential energy of SHO. This is the reason why SHO is such an important model and why we start our lectures with the discussion of this model.

1.1 Equation of motion

We consider a one-dimensional harmonic oscillator with mass m, frequency $\omega_0 > 0$ and electric charge q. The forces acting on the oscillator are as follows. The elastic force $F_e = -kx = -m\omega_0^2 x$ obeys Hooke's law. The friction $F_f = -m\Gamma\dot{x}$ is proportional to velocity and directed in the opposite direction, this allows us to take $\Gamma \geq 0$. Moreover, we assume that the oscillator is driven by a classical time–dependent electric field $E(t)$ which exerts the force $F_q = qE(t)$. The corresponding equation of motion follows immediately from second law of dynamics and is of the form

$$m\ddot{x} = -m\omega_0^2 x - m\Gamma\dot{x} + qE(t). \tag{1.1}$$ os1a

We rewrite Eq. (1.1) as

$$\ddot{x} + \Gamma\dot{x} + \omega_0^2 x = f(t), \qquad \text{with} \qquad f(t) = (q/m)E(t). \tag{1.2}$$ os1b

Equation (1.2) is an inhomogeneous one. Whatever the method used for finding its solution we need initial conditions. We will assume general initial conditions, that is

$$x(t=0) = x_0, \qquad \dot{x}(t=0) = v(t=t_0) = v_0. \tag{1.3}$$ os2

In some particular cases, we shall use more specific initial conditions.

1.2 Solution to homogeneous equation

Solution to Eq. (1.2) is a sum of a general solution to the homogeneous equation and of a particular solution to the inhomogeneous one. Thus, we first consider the homogeneous

equation, which reads

$$\ddot{x} + \Gamma\dot{x} + \omega_0^2 x = 0. \tag{1.4}$$ os4

We will seek the solution in the form $e^{-i\omega t}$. It is as well possible to look for a solution in another form, for example $e^{\lambda t}$. We, however adopt the former form, which is due to the fact that we will further use the Fourier transform of the Green's function. The Fourier components of the time-dependent functions are taken to have time dependence $e^{-i\omega t}$. This explains the adopted form of the solution to the homogeneous equation. Substituting our ansatz into equation (1.4) we find the quadratic characteristic equation

$$-\omega^2 - i\Gamma\omega + \omega_0^2 = 0. \tag{1.5}$$ os6a

The discriminant is equal to $4\omega_0 - \Gamma^2$. At present, we assume that damping is weak, so that the inequality $\frac{1}{2}\Gamma < \omega_0$ is satisfied, and then the discriminant is positive and the characteristic roots are

$$\omega_{1,2} = -\frac{i\Gamma}{2} \pm \Omega, \tag{1.6}$$ os6d

where we have introduced a new parameter

$$\Omega = \sqrt{\omega_0^2 - \frac{1}{4}\Gamma^2}. \tag{1.7}$$ os6e

These roots are discussed in more detail in *Auxiliary Chapters* (see the corresponding chapter). There, we will drop the assumption that damping constant is sufficiently small and discuss the physical consequences of $\frac{1}{2}\Gamma \geq \omega_0$ which entails Ω being purely imaginary which has quite interesting consequences.

Having found the characteristic roots, we write the solution to the homogeneous equation as a combination of two (linearly independent) exponentials

$$x(t) = Ae^{-i\omega_1 t} + Be^{-i\omega_2 t} = \exp\left(-\tfrac{1}{2}\Gamma t\right)\left[Ae^{i\Omega t} + Be^{-i\Omega t}\right], \tag{1.8}$$ os8

with A and B being the constants to be fixed by initial conditions.

Differentiating relation (1.8) and using the initial conditions (1.3) we arrive at the set of equations for constants A and B os10

$$x_0 = A + B, \tag{1.9a}$$ os10a

$$v_0 = \left(-\tfrac{1}{2}\Gamma + i\Omega\right)A + \left(-\tfrac{1}{2}\Gamma - i\Omega\right)B. \tag{1.9b}$$ os10b

It is a straightforward matter to solve this set of equations. The solutions are

$$A = \frac{1}{2i\Omega}\left[v_0 + \left(\tfrac{1}{2}\Gamma + i\Omega\right)x_0\right], \qquad B = -\frac{1}{2i\Omega}\left[v_0 - \left(\tfrac{1}{2}\Gamma + i\Omega\right)x_0\right]. \tag{1.10}$$ os11

Substituting the obtained constants into Eq. (1.8), after minor rearrangement we arrive at the general solution to the homogeneous equation of motion, which satisfies general initial conditions and is of the form

$$x(t) = \exp\left(-\tfrac{1}{2}\Gamma t\right)\left[x_0\cos(\Omega t) + \frac{v_0 + \frac{1}{2}\Gamma x_0}{\Omega}\sin(\Omega t)\right]. \tag{1.11}$$ os12

This solution corresponds to simple damped oscillations, since the parameter Ω is real. This is so, because the damping is small, in the sense that $\frac{1}{2}\Gamma < \omega_0$.

1.3 Driven oscillator

1.3.1 General remarks

The oscillator driven by the external electric field is described by the equation of motion as in (1.2), that is

$$\ddot{x} + \Gamma\dot{x} + \omega_0^2 x = f(t), \qquad \text{with} \qquad f(t) = (q/m)E(t). \tag{1.12}$$ os25

Its general solution is the sum

$$x(t) = x_{hom}(t) + x_{inh}(t), \tag{1.13}$$ os26

where x_{hom} is a general solution to the homogeneous equation. This solution (for weak damping which we still assume to be the case so that $\Omega \in \mathbb{R}$) is given in (1.11) with the notation introduced in the previous section. On the other hand x_{inh} is a particular solution to the inhomogeneous equation and is still unknown. Finding the solution to the inhomogeneous equation with arbitrary driving force $f(t)$ is certainly possible, but difficult. The very elegant method to find the solution is to construct and use the Green's function for equation (1.12). However, it is rather a mathematical question, therefore it is discussed in the *Auxiliary chapters* where we derive the necessary Green's function. Here we will simply employ the results obtained in these chapters.

One can show that the solution to the inhomogeneous equation can be written as

$$x_{inh}(t) = \int_{-\infty}^{\infty} dt'\ g(t-t')\, f(t'), \tag{1.14}$$ os28a

Where $g(\tau)$ is the Green's function and is given as

$$g(\tau) = \Theta(\tau)\,\frac{1}{\Omega}\,\exp\left(-\tfrac{1}{2}\Gamma\tau\right)\,\sin\left(\Omega\tau\right), \tag{1.15}$$ os28b

where $\Theta(\tau)$ is the Heaviside function, defined as

$$\Theta(\tau) = \begin{cases} 1 & \text{for } \tau \geq 0, \\ 0 & \text{for } \tau < 0. \end{cases} \tag{1.16}$$ os28c

The presence of the Heaviside function ensures that the integral in (1.14) has the upper limit actually equal to t and not to infinity. This, in turn, ensures the causality of the solution, that is $x_{inh}(t)$ depends on the force $f(t')$ taken at the moments earlier that the current moment t. (this is discussed in *Auxiliary chapters*). Then, given the driving force $f(t)$ we can compute the integral in (1.14) thereby finding the sought solution to the inhomogeneous equation of motion.

We can now construct a general solution to the driven oscillator equation (1.2) by summing the general solution to the homogeneous equation (1.11) and the solution to the inhomogeneous equation (1.14)) with the Green's function given in (1.15). We restrict our attention to the case of standard damped oscillations, that is to $\frac{1}{2}\Gamma < \omega_0$. The obtained

solution satisfies arbitrary initial conditions and can be written down for arbitrary driving force $f(t)$. The obtained result is thus, as follows

$$x(t) = \exp\left(-\frac{\Gamma t}{2}\right)\left[x_0\cos(\Omega t) + \frac{v_0 + \frac{1}{2}\Gamma x_0}{\Omega}\sin(\Omega t)\right] + \frac{1}{\Omega}\int_{-\infty}^{t} dt'\ \exp\left(-\frac{\Gamma(t-t')}{2}\right)\sin\left(\Omega(t-t')\right) f(t'). \tag{1.17}$$ os28d

We see that $x(t)$ depends only on the driving force for times earlier than the current moment. This conforms with the causality requirement.

It is interesting to note, that when the oscillator is initially at rest $x_0 = 0$ and $v_0 = 0$, then the first term in (1.17) vanishes. Only the driving force governs its evolution. In the general case (arbitrary initial conditions), if time t is sufficiently long then all the transients depending on initial conditions decay and again the evolution is determined only by the second term in (1.17)). This is a stationary regime which we will discuss in the next sections. In this regime only the influence of the external force is of interest. Hence it remains to investigate special cases for which we can take the evolution of the displacement as

$$x(t) \xrightarrow[no\ transients]{} \int_{-\infty}^{t} dt'\ \frac{1}{\Omega}\ \exp\left(-\frac{\Gamma(t-t')}{2}\right)\ \sin\left[\Omega(t-t')\right]\ f(t'). \tag{1.18}$$ os28e

Moreover, in most of the practical cases, the electric field is switched on at the moment $t = 0$. Thus we take

$$E(t) = \begin{cases} 0 & \text{for } t < 0, \\ E(t) & \text{for } t > 0, \end{cases} \tag{1.19}$$ os28f

with the concrete form of the time dependence of the field to be specified later. If the driving field satisfies the above requirement, then the driving force $f(t) = (q/m)E(t)$ has the same property. In such a case the lower limit of the integral in (1.17) or (1.18) effectively becomes zero instead of minus infinity.

1.3.2 Harmonic driving force

In the following we will consider a quite special type of the driving force, namely, the harmonic driving force, that is

$$f(t) = \frac{qE_0}{m}\ \cos(\omega t) = \frac{qE_0}{2m}\ \left(e^{i\omega t} + e^{-i\omega t}\right). \tag{1.20}$$ os30

We assume that the force is turned on at $t = 0$, hence $f(t) = 0$ for $t < 0$ as indicated in (1.19), so that the lower limit of integration in (1.14) is zero. This case is important because it corresponds to the oscillator placed in the field of the electromagnetic wave the time behavior of which is given as above. This especially true when the oscillator is much smaller than the wavelength, so that the position dependence is unimportant.

It is now straightforward to find the solution to inhomogeneous equation for the oscillator driven by a harmonic force. Inserting (1.20) and (1.15) into the integral (1.14)

and taking into account the remarks on the limits of integration, we get

$$x_{inh}(t) = \frac{qE_0}{2m\Omega} \int_0^t dt' \; e^{-\frac{1}{2}\Gamma(t-t')} \; \sin\left[\Omega(t-t')\right] \left(e^{i\omega t'} + e^{-i\omega t'}\right). \tag{1.21}$$ os31

This relation can be rewritten as

$$x_{inh}(t) = \frac{f_0}{\Omega}\left[\, I(t) + \text{C.C} \,\right] = \frac{2f_0}{\Omega} \; \text{Re}\{I(t)\}, \tag{1.22}$$ os32

with $f_0 = qE_0/2m$, and where C.C denotes complex conjugation. $I(t)$ is the integral

$$I(t) = \int_0^t dt' \; e^{i\omega t - \frac{1}{2}\Gamma(t-t')} \; \sin\left[\Omega(t-t')\right]. \tag{1.23}$$ os33

The problem, as for now, is reduced to the computation of the integral (1.23). This computation is not difficult but somewhat tedious. We present the major steps. First one expresses the sine by complex exponentials, then one changes the integration variable from t' to $x = t - t'$. Thus one has

$$I(t) = e^{i\omega t} \int_0^t dx \; e^{-i\omega x - \frac{1}{2}\Gamma x} \; \frac{1}{2i} \left(e^{i\Omega x} - e^{-i\Omega x}\right). \tag{1.24}$$ os34a

Computation of the integrals is simple. The result is

$$I(t) = \frac{e^{i\omega t}}{2i} \left[\; \frac{e^{i(\Omega-\omega)t - \frac{1}{2}\Gamma t} - 1}{i(\Omega-\omega) - \frac{1}{2}\Gamma} \; - \; \frac{e^{-i(\Omega+\omega)t - \frac{1}{2}\Gamma t} - 1}{-i(\Omega+\omega) - \frac{1}{2}\Gamma} \; \right]. \tag{1.25}$$ os34c

Next one separates terms proportional to $e^{i\omega t}$ and to $e^{-\frac{1}{2}\Gamma t}$. Using relation (1.7) one finds the final result, which is

$$x_{inh}(t) = \frac{\Omega e^{i\omega t}}{\omega_0^2 - \omega^2 + i\Gamma\omega} \; - \; e^{-\frac{1}{2}\Gamma t} \; \frac{\Omega\cos(\Omega t) + (\frac{1}{2}\Gamma + i\omega)\sin(\Omega t)}{\omega_0^2 - \omega^2 + i\Gamma\omega}. \tag{1.26}$$ os35

To find the solution $x_{inh}(t)$ according to (1.22) it remains to find the real part of the integral (1.26). This is a simple matter, so we just give the final form of (1.22). It is

$$\begin{aligned} x_{inh}(t) = {} & 2f_0 \; \frac{(\omega_0^2 - \omega^2) \; \cos(\omega t) + \omega\Gamma \sin(\omega t)}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\omega^2} \\ & - \; 2f_0 \; e^{-\frac{1}{2}\Gamma t} \; \frac{(\omega_0^2 - \omega^2) \; \cos(\Omega t) + \frac{1}{2}(\Gamma/\Omega)(\omega_0^2 + \omega^2)\sin(\Omega t)}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\omega^2}. \end{aligned} \tag{1.27}$$ os38

Examining this expression, we can say that the first term is a driven one, while the second is the damped one. In the long time limit only the first term survives. We note also that the full solution to the equations of motion for the oscillator driven by harmonic force is given by the sum of homogeneous solution (1.11) and of (1.27). However, homogeneous solution does not survive in the long time limit.

1.4 Stationary behavior

1.4.1 General discussion

Stationary behavior occurs when all the initial transients die out. This certainly occurs when the time t is long enough. Clearly, from (1.11) and (1.27) we see that the damped motion is the mentioned transient. For t large enough the terms proportional to $\exp(-\frac{1}{2}\Gamma t)$ become insignificant and do not contribute in the stationary regime. Hence, the long time behavior means $t \gg \Gamma^{-1}$, and in this regime we conclude that only the first term in the inhomogeneous solution (1.27) is of importance. Hence, the evolution of the harmonically driven oscillator in the stationary regime is given as

$$x_s(t) = \frac{qE_0}{m} \frac{(\omega_0^2 - \omega^2)\,\cos(\omega t) + \omega\Gamma \sin(\omega t)}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\omega^2}, \tag{1.28}$$ os42a

which may be called the stationary solution. It consists of two terms. The first one is in-phase with the driving force (which is proportional to $\cos(\omega t)$)

$$x_s^{(in)}(t) = \frac{qE_0}{m} \frac{(\omega_0^2 - \omega^2)\,\cos(\omega t)}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\omega^2}, \tag{1.29}$$ os42b

while the second is shifted in phase by $\pi/2$ and has the form

$$x_s^{(out)}(t) = \frac{qE_0}{m} \frac{\omega\Gamma \sin(\omega t)}{(\omega_0^2 - \omega^2)^2 + \Gamma^2\omega^2}, \tag{1.30}$$ os42c

For future purposes it is worth noting that the stationary solution can also be written as

$$x_s(t) = \frac{qE_0}{2m} \left(\frac{e^{i\omega t}}{\omega_0^2 - \omega^2 + i\Gamma\omega} + \text{C.C} \right), \tag{1.31}$$ os43

It is interesting to note that the stationary solution (1.31) can be obtained in a much simpler way. To see this, let us consider a simplified equation of motion

$$\ddot{x} + \Gamma\dot{x} + \omega_0^2 x = f_0 e^{i\omega t}. \tag{1.32}$$ os44a

We postulate the particular solution in the form $Ae^{i\omega t}$, which plugged into the above equation yields

$$\left(-\omega^2 + i\Gamma\omega + \omega_0^2\right) A e^{i\omega t} = f_0 e^{i\omega t}. \tag{1.33}$$ os44c

This equation is clearly satisfied when we take

$$A = \frac{f_0}{\omega_0^2 - \omega^2 + i\Gamma\omega}. \tag{1.34}$$ os44d

This reasoning reproduces stationary solution (1.31), since the second term in this relation follows by replacing ω by $-\omega$ in (1.34) and by combining corresponding two results.

1.4.2 Resonance approximation

This approximation consists in the assumption that $\omega_0 \simeq \omega$. This allows us to write

$$\omega_0^2 - \omega^2 \;=\; (\omega_0 + \omega)\,(\omega_0 - \omega) \;\approx\; 2\omega(\omega_0 - \omega) \tag{1.35}$$ os46

In such a case (os42a 1.28) gives

$$x_s(t) = \frac{qE_0}{m}\;\frac{2\omega(\omega_0-\omega)\;\cos(\omega t) + \omega\Gamma\sin(\omega t)}{4\omega^2(\omega_0-\omega)^2 + \Gamma^2\omega^2}. \tag{1.36}$$ os46x

Some simple rearrangement and substitution of ω_0 instead of ω in the common factors (which is allowed in the resonance approximation) leads to the expression

$$x_s(t) = \frac{qE_0}{2m\omega_0}\left(\;\frac{\omega_0-\omega}{(\omega_0-\omega)^2 + \frac{1}{4}\Gamma^2}\;\cos(\omega t)\;+\;\frac{\frac{1}{2}\Gamma}{(\omega_0-\omega)^2 + \frac{1}{4}\Gamma^2}\;\sin(\omega t)\;\right). \tag{1.37}$$ os47a

Let us discuss briefly the behavior of the oscillator within the resonance approximation. We see that the in-phase term (proportional to $\cos(\omega t)$, as the driving field) has dispersive character. Its amplitude is

$$A_{disp} \;=\; \frac{f_0}{2\omega_0}\;\frac{\omega_0-\omega_d}{(\omega_0-\omega_d)^2 + (\Gamma/2)^2}. \tag{1.38}$$ os47b

It is sketched by a broken line in the figure below.

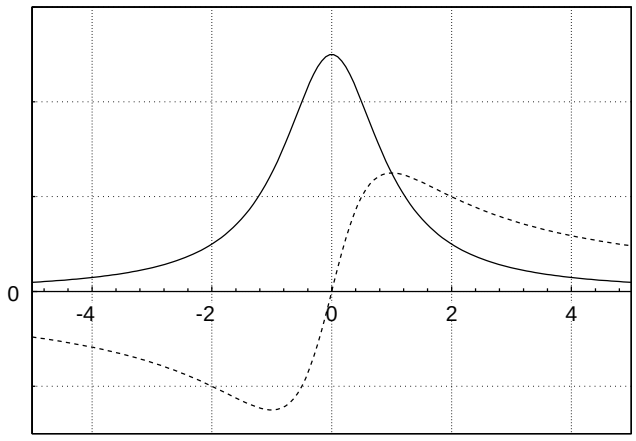

Fig. 1.1: Shapes of dispersive (broken line) and absorptive (solid line) curves. Zero on the horizontal axis corresponds to strict resonance $\omega = \omega_0$. The units are arbitrary. It should be noted that the curves are out of proportion.

fig:dabs

On the other hand, the out-of-phase term (proportional to $\sin(\omega t)$] is absorptive, and its amplitude is

$$A_{abs} \;=\; \frac{f_0}{2\omega_0}\;\frac{\Gamma/2}{(\omega_0-\omega_d)^2 + (\Gamma/2)^2}. \tag{1.39}$$ os47c

Figure (fig:dabs 1.1) (solid line) illustrates the behavior of this amplitude a functions of frequency. The terminology used here may be somewhat unclear. It will be fully clarified when we

employ the oscillator model to describe some phenomena which occur in the atomic media irradiated by electromagnetic waves.

When the damping is weak, then apart from the close vicinity of the resonance we have

$$\left| \frac{A_{disp}}{A_{abs}} \right| = \left| \frac{\omega_0 - \omega_d}{\Gamma/2} \right| \gg 1, \quad \text{off resonance.} \tag{1.40}$$ 1aaoff

This allows some interesting conclusions.

1. Off resonance, (1.37) os47a implies that

$$x_s(t) \approx x_s^{(in)}(t) = \pm \left(\frac{qE_0}{2m\omega_0} \right) \frac{|\omega_0 - \omega|}{(\omega_0 - \omega)^2 + (\Gamma/2)^2} \cos(\omega t), \tag{1.41}$$ os47d

where we have plus for $\omega < \omega_0$ and minus when $\omega_d > \omega_0$. This means that off resonance the oscillator is in phase with the driving force.

2. Close to the resonance (or just on resonance), the absorptive term dominates, and in this case we have

$$x_s(t) \approx x_s^{(out)}(t) = \left(\frac{f_0}{2\omega_0} \right) \frac{\Gamma/2}{(\omega_0 - \omega_d)^2 + (\Gamma/2)^2} \sin(\omega_d t + \phi). \tag{1.42}$$ os47e

This indicates, that in resonance the motion of the oscillator is out of phase. It motion is shifted in phase (with respect to the driving force) by a factor of $\pi/2$.

The discussed features of the driven oscillator are useful in the discussion of some atomic or molecular phenomena.

1.5 Nonlinear perturbation

1.5.1 Description of the problem

Harmonic oscillator models physical situation in which potential energy has a minimum. It is a good approximation only in the close neighborhood of the minimum. The farther we get the poorer the approximation and we need to take into account the nonlinear corrections.

To facilitate further discussion we will now adopt the following model. As previously we consider weakly damped oscillator driven by two external fields with different amplitudes and different frequencies. But now we will include a small anharmonic (quadratic) correction to the Hooke's force. The corresponding equation of motion now becomes

$$\ddot{x} + \Gamma\dot{x} + \omega_0^2 x + bx^2 = F_1(t) + F_2(t), \tag{1.43}$$ os51a

where b is a small parameter controlling the strength of the nonlinear perturbation. The force $F_k(t)$ are specified as previously, that is

$$F_k(t) = \frac{qE_k}{2m} \left(e^{i\omega_k t} + e^{-i\omega_k t} \right). \tag{1.44}$$ os51b

From now on we will consider only the stationary solutions, since only they survive in the long-time limit. Moreover, the nonlinear correction is small so that we can seek approximate solutions. It is easy to find the stationary solution to the unperturbed case ($b = 0$). In such a case equation (1.43) is linear so its solution is just the sum of two solutions each for one of the external force. So, following the results of the previous section, we can write the unperturbed solution as

$$x^{(0)}(t) = \frac{f_1\, e^{i\omega_1 t}}{\omega_0^2 - \omega_1^2 + i\Gamma\omega_1} + \frac{f_2\, e^{i\omega_2 t}}{\omega_0^2 - \omega_2^2 + i\Gamma\omega_2} + \text{C.C}, \tag{1.45}$$

where $f_k = qE_k/2m,\ (k = 1, 2)$. To simplify the equations we denote

$$\alpha_k(t) = \frac{f_1\, e^{i\omega_1 t}}{\omega_0^2 - \omega_1^2 + i\Gamma\omega_1}, \tag{1.46}$$

so the unperturbed solution (1.45) is shortly written as

$$x^{(0)}(t) = \alpha_1 + \alpha_2 + \alpha_1^* + \alpha_2^*. \tag{1.47}$$

1.5.2 Iterative solution

We return to the perturbed case, that is to Eq.(1.43). As we noted we treat the nonlinear correction as a small perturbation. We look for the solution in the form

$$x(t) = x^{(0)}(t) + y(t), \tag{1.48}$$

where $x^{(0)}(t)$ is the unperturbed solution (1.47) and $y(t)$ is a small correction due to the perturbation. Inserting our ansatz into (1.43) and moving the nonlinear term to the right hand side we obtain

$$\ddot{x}^{(0)} + \Gamma\dot{x}^{(0)} + \omega_0^2 x^{(0)} + \ddot{y} + \Gamma\dot{y} + \omega_0^2 y = F_1(t) + F_2(t) - b\big(x^{(0)} + y\big)^2. \tag{1.49}$$

Iterative solution of this equation consists in neglecting the correction $y(t)$ in the nonlinear term. Thus, we approximate (1.49) by the following equation

$$\ddot{x}^{(0)} + \Gamma\dot{x}^{(0)} + \omega_0^2 x^{(0)}\ddot{y} + \Gamma\dot{y} + \omega_0^2 y = F_1(t) + F_2(t) - b\big(x^{(0)}\big)^2. \tag{1.50}$$

Noting that $x^{(0)}(t)$ is the (stationary) solution of the unperturbed equation we see that the first three terms in the left hand side cancel out with the forces in right hand side. Therefore, we finally get an equation for correction $y(t)$ only. We get

$$\ddot{y} + \Gamma\dot{y} + \omega_0^2 y = -b\left(\alpha_1 + \alpha_2 + \alpha_1^* + \alpha_2^*\right)^2, \tag{1.51}$$

where auxiliary functions $\alpha_k(t)$ are specified in (1.46) and (1.47). Performing the multiplication an regrouping we find

$$\begin{aligned}\ddot{y} + \Gamma\dot{y} + \omega_0^2 y = -b\Big[&\big(\alpha_1^2 + \text{C.C}\big) + \big(\alpha_2^2 + \text{C.C}\big) + 2\big(\alpha_1\alpha_2 + \text{C.C}\big) \\ &+ 2\big(\alpha_1\alpha_2^* + \text{C.C}\big) + 2\big|\alpha_1\big|^2 + 2\big|\alpha_1\big|^2\Big],\end{aligned} \tag{1.52}$$

This equation looks pretty complicated, but this is misleading. It is sufficient to examine its structure, to note that it is linear. Linearity implies that we can consider each inhomogeneity (the terms in the right hand side) separately. Hence our solution has the form of the sum

$$y(t) = y_1(t) + y_2(t) + y_3(t) + y_4(t) + y_5(t), \tag{1.53}$$ os61

where each of the terms satisfies the equation of motion

$$\ddot{y}_k + \Gamma\dot{y}_k + \omega_0^2 y_k = -b\left(A_k e^{i\Omega_k t} + A_k^* e^{-i\Omega_k t}\right), \qquad k = 1,2,3,4,5. \tag{1.54}$$ os62

The structure of the rhs follows from inspection of the rhs of (1.52) compared to the form of α_k's as they are given in (1.46). Since we are interested only in the stationary solutions, we see that we have special cases of equations (1.32) to (1.34). The only point is to correctly recognize the amplitudes A_k and frequencies Ω_k. Now we will briefly discuss the particulars.

First term in (1.52)

The first part of (1.52) is as follows

$$\ddot{y}_1 + \Gamma\dot{y}_1 + \omega_0^2 y_1 = -b\left(\,\alpha_1^2 + \text{C.C}\,\right). \tag{1.55}$$ os65a

By means of (1.46) we read that

$$\Omega_1 = 2\omega_1, \qquad A_1 = \frac{f_1^2}{\left(\omega_0^2 - \omega_1^2 + i\Gamma\omega_1\right)^2}. \tag{1.56}$$ os65b

Therefore the first contribution to the correction $y(t)$ is of the form

$$y_1(t) = \frac{-b\, f_1^2\, e^{2i\omega_1 t}}{\left(\omega_0^2 - \omega_1^2 + i\Gamma\omega_1\right)^2\left(\omega_0^2 - 4\omega_1^2 + 2i\Gamma\omega_1\right)} \;+\; \text{C.C.} \tag{1.57}$$ os65d

This corresponds to stationary oscillations with the doubled frequency of the first driving field. In other words, it can be associated with second harmonic generation.

Second term in (1.52)

Clearly the second terms differs from the previous one only by the index: 2 instead of 1. Hence from (1.57) we immediately get

$$y_2(t) = \frac{-b\, f_2^2\, e^{2i\omega_2 t}}{\left(\omega_0^2 - \omega_2^2 + i\Gamma\omega_2\right)^2\left(\omega_0^2 - 4\omega_2^2 + 2i\Gamma\omega_2\right)} \;+\; \text{C.C.} \tag{1.58}$$ os66

This terms, thus describes the generation of the second harmonic of the second external field.

Third term in (1.52)

The third contribution to (1.52) is

$$\ddot{y}_3 + \Gamma\dot{y}_3 + \omega_0^2 y_3 = -b\,\big(\,2\alpha_1\alpha_2 + \text{C.C}\,\big). \tag{1.59}$$ os67a

As previously, from (1.46) we read that

$$\Omega_3 = \omega_1 + \omega_2, \qquad A_3 = \frac{2f_1 f_2}{\big(\omega_0^2 - \omega_1^2 + i\Gamma\omega_1\big)\big(\omega_0^2 - \omega_2^2 + i\Gamma\omega_2\big)}. \tag{1.60}$$ os67b

This part of the correction $y(t)$ is, thus, of the form

$$y_3(t) = \frac{-2\,b\;f_1\;f_2\;e^{i(\omega_1+\omega_2)t}}{\big(\omega_0^2 - \omega_1^2 + i\Gamma\omega_1\big)\big(\omega_0^2 - \omega_2^2 + i\Gamma\omega_2\big)\big[\omega_0^2 - (\omega_1+\omega_2)^2 + i\Gamma(\omega_1+\omega_2)\big]} \;+\; \text{C.C.} \tag{1.61}$$ os67c

This describes stationary oscillations with the frequency being the sum of the frequencies of two driving fields. Hence, it can be associated with the so-called sum-frequency generation.

Fourth term in (1.52)

The next contribution to (1.52) follows

$$\ddot{y}_4 + \Gamma\dot{y}_4 + \omega_0^2 y_4 = -b\,\big(\,2\alpha_1\alpha_2^* + \text{C.C}\,\big). \tag{1.62}$$ os68a

Due to the presence of α_2^* it differs from the previous case only by replacing $+\omega_2$ by $-\omega_2$ Therefore (1.61) allows us to write

$$y_4(t) = \frac{-2\,b\;f_1\;f_2\;e^{i(\omega_1-\omega_2)t}}{\big(\omega_0^2 - \omega_1^2 + i\Gamma\omega_1\big)\big(\omega_0^2 - \omega_2^2 + i\Gamma\omega_2\big)\big[\omega_0^2 - (\omega_1-\omega_2)^2 + i\Gamma(\omega_1-\omega_2)\big]} \;+\; \text{C.C.} \tag{1.63}$$ os68c

These are stationary oscillations with the frequency being the difference of the frequencies of two driving fields. Hence, it can be associated with the so-called difference-frequency generation.

Fifth term in (1.52)

In this, last, case we have an equation of motion (as it follows from (1.52))

$$\ddot{y}_5 + \Gamma\dot{y}_5 + \omega_0^2 y_5 = -b\,\big(\,2\big|\alpha_1\big|^2 + 2\big|\alpha_2\big|^2\,\big). \tag{1.64}$$ os69a

As we see from inspection of (1.46) rhs in this case is time-independent. It is straightforward to check the particular solution to the above equation is also constant. Namely it is

$$y_5(t) = -\,\frac{2\,b}{\omega_0^2}\,\Big(\big|\alpha_1\big|^2 + \big|\alpha_1\big|^2\Big)\,. \tag{1.65}$$ os69b

Taking α's from (1.46) os54 we obtain

$$y_5(t) = -\frac{2\,b}{\omega_0^2}\left(\frac{f_1^2}{\left|\omega_0^2-\omega_1^2+i\Gamma\omega_1\right|^2} + \frac{f_2^2}{\left|\omega_0^2-\omega_2^2+i\Gamma\omega_2\right|^2}\right). \tag{1.66}$$ os69c

This term describes a constant shift due to the nonlinearity of the potential energy. Simple harmonic oscillator has quadratic potential energy, hence symmetric . Introduced nonlinearity results in the term in potential energy proportional to x^3 thereby inducing asymmetry which entails the constant shift of the stationary oscillations.

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Chapter 2

Classical electrodynamics

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It is not our aim to give a lecture on electrodynamics. There is a book by Griffith which gives an excellent presentation of the subject. We only briefly review the fundamentals of the subject necessary to perform the quantization in a simple and convenient manner. This chapter only summarizes the main aspects of classical electrodynamics. Some other ones, useful in more restricted applications will be dealt with when such a need arises.

2.1 Maxwell's equations

We will use the SI system of units. In this system, the general Maxwell's equations in presence of free charges and currents are as follows

ce1

$$\text{div}\,\vec{\mathbf{D}}(\vec{\mathbf{r}},t) = \rho(\vec{\mathbf{r}},t), \qquad (Gauss'\ law), \tag{2.1a}$$ ce1a

$$\text{div}\,\vec{\mathbf{B}}(\vec{\mathbf{r}},t) = 0, \qquad (no\ magnetic\ monopoles), \tag{2.1b}$$ ce1b

$$\text{rot}\,\vec{\mathbf{E}}(\vec{\mathbf{r}},t) = -\frac{\partial}{\partial t}\vec{\mathbf{B}}(\vec{\mathbf{r}},t), \qquad (Faraday's\ law), \tag{2.1c}$$ ce1c

$$\text{rot}\,\vec{\mathbf{H}}(\vec{\mathbf{r}},t) = \vec{\mathbf{j}}(\vec{\mathbf{r}},t) + \frac{\partial}{\partial t}\vec{\mathbf{D}}(\vec{\mathbf{r}},t), \qquad (modified\ Ampere's\ law), \tag{2.1d}$$ ce1d

where ρ and $\vec{\mathbf{j}}$ are charge and current densities. The pairs of the fields $\vec{\mathbf{E}}$, $\vec{\mathbf{D}}$ and $\vec{\mathbf{B}}$, $\vec{\mathbf{H}}$ are connected by the material relations, which may be written as

$$D_i = \epsilon_o \epsilon_{ij} E_j, \qquad B_i = \mu_o \mu_{ij} H_j, \qquad \text{with} \quad \frac{1}{\mu_o \epsilon_o} = c^2. \tag{2.2}$$ ce2

with ϵ_o and μ_o the permeabilities of vacuum. The tensors ϵ_{ij} and μ_{ij} are the dielectric and magnetic susceptibilities of the medium in which the fields propagate. For linear and isotropic media these tensors reduce to constants. In general, susceptibilities ϵ_{ij} and μ_{ij} may be position and time dependent, they may also be the functions of the fields $\vec{\mathbf{E}}$ and $\vec{\mathbf{H}}$. In the latter case we arrive at the problems of nonlinear optics, which in itself, can be a subject of a separate lecture. In this notes, however, we will not address such questions.

Moreover, we note (for linear and isotropic media) that the fields $\vec{\mathbf{D}}$ and $\vec{\mathbf{B}}$ can be expressed via the electric polarization and magnetization

$$\vec{\mathbf{D}} = \epsilon\epsilon_o\vec{\mathbf{E}} = \epsilon_o\vec{\mathbf{E}} + \vec{\mathbf{P}}, \qquad \vec{\mathbf{B}} = \mu\mu_o\vec{\mathbf{H}} = \mu_o(\vec{\mathbf{H}} + \vec{\mathbf{M}}), \tag{2.3}$$ ce3

Equivalently, polarization and magnetization can be written as

$$\vec{\mathbf{P}} = (\epsilon - 1)\epsilon_o \vec{\mathbf{E}}, \qquad \vec{\mathbf{M}} = (\mu - 1)\vec{\mathbf{H}} = \frac{\mu - 1}{\mu\mu_o}\vec{\mathbf{B}} = \frac{1}{\mu_o}\vec{\mathbf{B}} - \vec{\mathbf{H}}. \tag{2.4}$$ ce4

Two additional remarks seem to be in place. Firstly, we note that Maxwell's equations automatically account for charge conservation. To see this, let us take the time derivative of the Gauss' law (2.1a) (we assume that spatial and temporal derivatives commute)

$$\operatorname{div} \frac{\partial}{\partial t}\, \vec{\mathbf{D}}(\vec{\mathbf{r}}, t) \;=\; \frac{\partial}{\partial t}\, \rho(\vec{\mathbf{r}}, t). \tag{2.5}$$ ce5a

Then we eliminate time derivative of $\vec{\mathbf{D}}$ by employing modified Ampere's law (2.1d). Thus, we get

$$\frac{\partial}{\partial t}\, \rho = \operatorname{div}\left(\operatorname{rot} \vec{\mathbf{H}} - \vec{\mathbf{j}}\right). \tag{2.6}$$ ce5b

Since we have the vector identity $\operatorname{div}\operatorname{rot} \equiv 0$, it follows that

$$\frac{\partial}{\partial t}\rho + \operatorname{div} \vec{\mathbf{j}} = 0. \tag{2.7}$$ ce6

which is an equation of charge continuity written in a local form. charge conservation requirement. It is a local law. Its integral counterpart reads

$$\int_V d^3r\, \frac{\partial}{\partial t}\, \rho = -\int_V d^3r\, \operatorname{div} \vec{\mathbf{j}} = -\int_{\partial V} d\vec{\mathbf{S}} \cdot \vec{\mathbf{j}}, \tag{2.8}$$ ce7

where the Gauss' theorem was used. Relation (2.8) means that the charge within certain volume may change only due to the current flowing across its surface.

Second remark concerns the so-called displacement current. This is a concept introduced by Maxwell himself. To understand it let us recall that the original Ampere's law states that circulation of the magnetic field along a closed contour is equal to the current flowing across an arbitrary surface spanned on this contour.

$$\oint d\vec{\mathbf{l}} \cdot \vec{\mathbf{H}} = \int d\vec{\mathbf{S}} \cdot \vec{\mathbf{j}}. \tag{2.9}$$ ce11

Then, due to Stokes' theorem, this can be written in a local form

$$\operatorname{rot} \vec{\mathbf{H}} = \vec{\mathbf{j}}. \tag{2.10}$$ ce12

The term $\partial\vec{\mathbf{D}}/\partial t$ is missing. It is just the displacement current introduced by Maxwell. This is a misnomer, since this term has nothing to do with current – the flow of charges. $\partial\vec{\mathbf{D}}/\partial t$ can be nonzero in vacuum, where any charges are absent. Let us see what would happen if the displacement current were not accounted for, that is if the fourth Maxwell's equation were reduced to (2.10). Taking divergence of both sides of this equation, we get

$$0 = \operatorname{div}\operatorname{rot} \vec{\mathbf{H}} = \operatorname{div} \vec{\mathbf{j}}. \tag{2.11}$$ ce13

where the left hand side vanishes identically. On the other hand $\operatorname{div} \vec{\mathbf{j}}$ need not be zero. For example, where the charges accumulate (capacitors) $\operatorname{div} \vec{\mathbf{j}} = -\partial\, \rho/\partial t \neq 0$, according

to charge conservation. So, Eq.(2.11) is wrong, and thus (2.10) must be wrong too. This is why the displacement current is indeed necessary. Obviously, we can correct (2.11) writing

$$0 \;=\; \mathrm{div}\,\mathrm{rot}\,\vec{\mathbf{H}} \;=\; \mathrm{div}\,\vec{\mathbf{j}} + \frac{\partial \rho}{\partial t} \;=\; \mathrm{div}\,\vec{\mathbf{j}} \;+\; \mathrm{div}\,\frac{\partial \vec{\mathbf{D}}}{\partial t}. \tag{2.12}$$

"Taking off" the divergence (we note that left hand side can be then nonzero) we get

$$\mathrm{rot}\,\vec{\mathbf{H}} \;=\; \vec{\mathbf{j}} \;+\; \frac{\partial \vec{\mathbf{D}}}{\partial t}. \tag{2.13}$$

which is exactly the fourth Maxwell's equation, called also the modified Ampere's law. We see that the introduction of the displacement current is indeed necessary.

It is worth noting that there are no such problem with Faraday's law (2.1c).Indeed, taking divergence of both sides of (2.1c) we get

$$0 \;=\; \mathrm{div}\,\mathrm{rot}\,\vec{\mathbf{E}} \;=\; -\,\frac{\partial}{\partial t}\,\mathrm{div}\,\vec{\mathbf{B}} \;=\; 0, \tag{2.14}$$

due to the second Of Maxwell's equations.

Finally we note that in vacuum there is no medium, hence polarization and magnetization vanish. There is no need to distinguish fields $\vec{\mathbf{D}}$ and $\vec{\mathbf{E}}$, $\vec{\mathbf{B}}$ and $\vec{\mathbf{H}}$, so we write Maxwell's equation for the free space as

$$\mathrm{div}\,\vec{\mathbf{E}}(\vec{\mathbf{r}},t) \;=\; \frac{1}{\epsilon_o}\,\rho(\vec{\mathbf{r}},t), \qquad (Gauss'\ law), \tag{2.15a}$$

$$\mathrm{div}\,\vec{\mathbf{B}}(\vec{\mathbf{r}},t) \;=\; 0, \qquad (no\ magnetic\ monopoles), \tag{2.15b}$$

$$\mathrm{rot}\,\vec{\mathbf{E}}(\vec{\mathbf{r}},t) \;=\; -\,\frac{\partial}{\partial t}\,\vec{\mathbf{B}}(\vec{\mathbf{r}},t), \qquad (Faraday's\ law), \tag{2.15c}$$

$$\mathrm{rot}\,\vec{\mathbf{B}}(\vec{\mathbf{r}},t) \;=\; \frac{1}{\epsilon_o c^2}\,\vec{\mathbf{j}}(\vec{\mathbf{r}},t) + \frac{1}{c^2}\frac{\partial}{\partial t}\,\vec{\mathbf{E}}(\vec{\mathbf{r}},t), \qquad (modified\ Ampere's\ law), \tag{2.15d}$$

This is the set of fundamental equations with which we will mainly deal in subsequent discussion.

2.2 Potentials

2.2.1 Introduction and basic definitions

Maxwell's equations may be formulated in terms of potentials. To define the potentials, we refer to general Maxwell's equations (2.1). We also recall the identities known from vector analysis

$$\mathrm{div}\,\mathrm{rot} \equiv 0, \qquad \mathrm{rot}\,\mathrm{grad} \equiv 0. \tag{2.16}$$

The second Maxwell's equation $\mathrm{div}\,\vec{\mathbf{B}} = 0$ is always satisfied, since it signifies that there are no magnetic monopoles. Hence, due to the first of the identities (2.16) we can always write

$$\vec{\mathbf{B}}(\vec{\mathbf{r}},t) = \mathrm{rot}\,\vec{\mathbf{A}}(\vec{\mathbf{r}},t). \tag{2.17}$$

We conclude that, when the vector potential $\vec{\mathbf{A}}$ is specified so that the magnetic field $\vec{\mathbf{B}}$ is determined by Eq.(2.17), the Maxwell's equation (2.1b) is automatically satisfied. Introducing (2.17) into the Faraday's law (2.1c) we obtain $\mathrm{rot}\,\vec{\mathbf{E}} = -\partial\,\mathrm{rot}\,\vec{\mathbf{A}}/\partial t$, which suggests that the electric field is given as $\vec{\mathbf{E}} = -\partial\,\vec{\mathbf{A}}/\partial t$. This is not sufficient, for two reasons. In the static case, it would imply that $\vec{\mathbf{E}} = 0$, which is clearly wrong – static fields do exist. Secondly, due to the second of relations (2.16) we can always add a gradient of arbitrary function, writing

$$\vec{\mathbf{E}}(\vec{\mathbf{r}},t) \;=\; -\;\mathrm{grad}\,\phi(\vec{\mathbf{r}},t) \;-\; \frac{\partial}{\partial t}\,\vec{\mathbf{A}}(\vec{\mathbf{r}},t), \tag{2.18}$$ ce23

and the Faraday's equation (2.1c) is still automatically satisfied.

Therefore, we may formulate the problem of specifying the electromagnetic field as follows. We postulate the existence of a scalar field $\phi(\vec{\mathbf{r}},t)$ and of a vector field $\vec{\mathbf{A}}(\vec{\mathbf{r}},t)$ such that the electric field is determined by Eq.(2.18) and the magnetic field by (2.17). Then, we automatically satisfy two out of four Maxwell's equations (namely, Eqs. (2.1b) and (2.1c) There are still two other Maxwell's equations to consider

$$\mathrm{div}\,\vec{\mathbf{D}} = \rho, \qquad\qquad \mathrm{rot}\,\vec{\mathbf{H}} = \vec{\mathbf{j}} + \frac{\partial}{\partial t}\,\vec{\mathbf{D}}, \tag{2.19}$$ ce24

which also must be satisfied. It remains to check what are the conditions imposed on potentials by equations (2.19).

2.2.2 Wave equations for potentials

We now look for the restrictions imposed on the potentials by two remaining Maxwell's equations (2.19).

We note that there arises a serious problem. Namely, the potentials $\vec{\mathbf{A}}$ and ϕ specify the fields $\vec{\mathbf{E}}$ and $\vec{\mathbf{B}}$, while equations (2.19) contain fields $\vec{\mathbf{D}}$ and $\vec{\mathbf{H}}$. The latter and the former fields are connected by material relations (2.3). The dielectric and magnetic susceptibilities may be complicated functions of position, time and also of the fields themselves. Thus, equations (2.19) after insertion of material relations and potentials can be expected to be very complicated. To avoid such problems, we shall restrict our attention to fields in vacuum. The relations between fields $\vec{\mathbf{E}}$, $\vec{\mathbf{B}}$ and potentials $\vec{\mathbf{A}}$, ϕ remain unchanged, because the second and the third Maxwell's equations (2.1b) and (2.1c) in vacuum are the same as in media. On the other hand, equations (2.19) become simpler, and in vacuum they are

$$\mathrm{div}\,\vec{\mathbf{E}} = \frac{\rho}{\epsilon_0}, \qquad\qquad \mathrm{rot}\,\vec{\mathbf{B}} = \frac{1}{\epsilon_0 c^2}\,\vec{\mathbf{j}} + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\vec{\mathbf{E}}, \tag{2.20}$$ ce25

Introducing electric field specified by (2.19) into the first of the above equations we get

$$\mathrm{div}\left(-\mathrm{grad}\,\phi - \frac{\partial\vec{\mathbf{A}}}{\partial t}\right) \;=\; \frac{\rho}{\epsilon_0} \qquad\Longrightarrow\qquad \boldsymbol{\nabla}^2\phi = -\frac{1}{\epsilon_0}\,\rho - \frac{\partial}{\partial t}\,\boldsymbol{\nabla}\cdot\vec{\mathbf{A}}, \tag{2.21}$$ ce26

which is the wave equation (in vacuum) for scalar potential. This wave equation is not, strictly speaking, an equation of motion for ϕ since it does not include its time derivative.

It is rather a relation between ϕ and the time derivative of vector potential $\partial\vec{\mathbf{A}}/\partial t$ at a certain moment of time.

It remains to make use of the second of equations (2.20). We replace the fields by the corresponding expressions for potentials and obtain

$$\text{rot rot}\,\vec{\mathbf{A}} = \frac{1}{\epsilon_0\, c^2}\,\vec{\mathbf{j}} + \frac{1}{c^2}\,\frac{\partial}{\partial t}\left(-\boldsymbol{\nabla}\,\phi - \frac{\partial}{\partial t}\,\vec{\mathbf{A}}\right). \tag{2.22}$$ ce27a

Using the vector analysis identity

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\vec{\mathbf{A}}) = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\vec{\mathbf{A}}) - \boldsymbol{\nabla}^2\vec{\mathbf{A}}, \tag{2.23}$$ ce27b

we get

$$\left[\frac{1}{c^2}\,\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2\right]\vec{\mathbf{A}} \;=\; \frac{1}{c^2\,\epsilon_0}\,\vec{\mathbf{j}} - \boldsymbol{\nabla}\left[\boldsymbol{\nabla}\cdot\vec{\mathbf{A}} + \frac{1}{c^2}\,\frac{\partial\,\phi}{\partial t}\right]. \tag{2.24}$$ ce28

We may conclude, restricting our considerations to vacuum, that the introduction of potentials by (2.17) and (2.18) guarantees that two of the Maxwell's equations (2.1b) and (2.1c) are automatically satisfied, while the other two are equivalent to wave equations (2.21) and (2.24).

2.2.3 Potentials – gauge invariance

We recall the relations between the fields and potentials

$$\vec{\mathbf{E}}(\vec{\mathbf{r}},t) = -\text{grad}\,\phi(\vec{\mathbf{r}},t) - \frac{\partial}{\partial t}\,\vec{\mathbf{A}}(\vec{\mathbf{r}},t), \qquad \vec{\mathbf{B}}(\vec{\mathbf{r}},t) = \text{rot}\,\vec{\mathbf{A}}(\vec{\mathbf{r}},t). \tag{2.25}$$ ce31

The fields are the true physical quantities measured and observed in a variety of experiments. The role of the potentials is rather auxiliary since they are not uniquely determined. To see this we recall that rot grad $\equiv 0$, hence the redefinition (called gauge transformation) of the vector potential

$$\vec{\mathbf{A}}(\vec{\mathbf{r}},t) \;\xrightarrow[gauge]{}\; \vec{\mathbf{A}}'(\vec{\mathbf{r}},t) = \vec{\mathbf{A}}(\vec{\mathbf{r}},t) + \boldsymbol{\nabla}\,F(\vec{\mathbf{r}},t), \tag{2.26}$$ ce32

does not change the magnetic field $\vec{\mathbf{B}}$ for arbitrary function $F(\vec{\mathbf{r}},t)$. Let us now express the electric field via a new vector potential

$$\begin{aligned}\vec{\mathbf{E}}(\vec{\mathbf{r}},t) &= -\text{grad}\,\phi(\vec{\mathbf{r}},t) - \frac{\partial}{\partial t}\left[\vec{\mathbf{A}}'(\vec{\mathbf{r}},t) - \boldsymbol{\nabla}F\right] \\ &= -\text{grad}\left[\phi(\vec{\mathbf{r}},t) - \frac{\partial}{\partial t}\,F(\vec{\mathbf{r}},t)\right] - \frac{\partial}{\partial t}\,\vec{\mathbf{A}}'(\vec{\mathbf{r}},t).\end{aligned} \tag{2.27}$$

We see that the expression in the square brackets plays a role of a new scalar potential. We conclude that the joint transformation ce34

$$\vec{\mathbf{A}}(\vec{\mathbf{r}},t) \;\xrightarrow[gauge]{}\; \vec{\mathbf{A}}'(\vec{\mathbf{r}},t) \;=\; \vec{\mathbf{A}}(\vec{\mathbf{r}},t) + \boldsymbol{\nabla}F(\vec{\mathbf{r}},t), \tag{2.28a}$$ ce34a

$$\phi(\vec{\mathbf{r}},t) \;\xrightarrow[gauge]{}\; \phi'(\vec{\mathbf{r}},t) \;=\; \phi(\vec{\mathbf{r}},t) - \frac{\partial}{\partial t}\,F(\vec{\mathbf{r}},t), \tag{2.28b}$$ ce34b

leaves the physical quantities, that is the fields $\vec{\mathbf{E}}$ and $\vec{\mathbf{B}}$, unchanged. This means that for "old" potentials we had relations (2.25), while for the "new" ones we similarly have

$$\vec{\mathbf{E}}(\vec{\mathbf{r}},t) = -\text{grad}\,\phi'(\vec{\mathbf{r}},t) - \frac{\partial}{\partial t}\,\vec{\mathbf{A}}'(\vec{\mathbf{r}},t), \qquad \vec{\mathbf{B}}(\vec{\mathbf{r}},t) = \text{rot}\,\vec{\mathbf{A}}'(\vec{\mathbf{r}},t). \tag{2.29}$$ ce35

The fields are unchanged though the potentials are. It is straightforward to check that introducing the "new" potentials (2.28) into relations (2.29) we will arrive at the fields given by (2.25).

This fact is called the gauge invariance of the fields. We have some freedom at the choice of potentials in a convenient way, best suited to particular applications. At present, we will not discuss this subject. We will only briefly indicate two most commonly used gauges – methods of choosing the potentials.

2.2.4 Lorentz gauge

Lorentz gauge consists in such a choice of the potentials, that the relation

$$\text{div}\,\vec{\mathbf{A}}(\vec{\mathbf{r}},t) + \frac{1}{c^2}\frac{\partial}{\partial t}\,\phi(\vec{\mathbf{r}},t) = 0, \tag{2.30}$$ ce37

is satisfied. This requirement still leaves some freedom. Namely, let us assume that the "old" potentials satisfy the Lorentz gauge (2.30). We make a gauge transformation by adopting "new" potentials

$$\vec{\mathbf{A}}' = \vec{\mathbf{A}} + \boldsymbol{\nabla} G, \qquad \phi' = \phi - \frac{\partial}{\partial t}\,G, \tag{2.31}$$ ce38

Inserting "new" potentials into (2.30) we obtain

$$\text{div}\,\vec{\mathbf{A}}' - \nabla^2\,G + \frac{1}{c^2}\frac{\partial\phi'}{\partial t} + \frac{1}{c^2}\frac{\partial^2 G}{\partial t^2} = 0. \tag{2.32}$$ ce39a

We see that if the function G satisfies the wave equation

$$\boldsymbol{\nabla}^2 G - \frac{1}{c^2}\,\frac{\partial^2\,G}{\partial t^2} = 0, \tag{2.33}$$ ce39b

then the "new" potentials still fulfill Lorentz requirement (2.30). Conversely, if we assume that "new potentials must also satisfy the Lorentz gauge (2.30) then we conclude that an arbitrary function G satisfying (2.33) will preserve Lorentz gauge. This indicates some arbitrariness in the choice of the gauge function G.

ce42 Let us return to wave equations (2.21) and (2.24). Assuming Lorentz gauge, we get

$$\left[\boldsymbol{\nabla}^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\phi(\vec{\mathbf{r}},t) \;=\; -\frac{1}{\epsilon_0}\,\rho(\vec{\mathbf{r}},t) \tag{2.34a}$$ ce42a

$$\left[\boldsymbol{\nabla}^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\vec{\mathbf{A}}(\vec{\mathbf{r}},t) \;=\; -\frac{1}{\epsilon_0\,c^2}\,\vec{\mathbf{j}}(\vec{\mathbf{r}},t). \tag{2.34b}$$ ce42b

As a result, we obtain uncoupled, symmetric wave equations for the potentials.

Finally, we note the Lorentz gauge can be shown to be invariant with respect to Lorentz transformation, and as such is particularly useful in relativistic considerations. It is not difficult to recast wave equations (2.34)) into four-dimensional (space-time) notation. This is, however, beyond the scope of our present interests.

2.2.5 Coulomb gauge

Coulomb gauge is specified by the requirement

$$\text{div}\,\vec{\mathbf{A}}(\vec{\mathbf{r}},t)=0. \tag{2.35}$$ ce45

So, there is no conditions imposed on the scalar potential. Unfortunately, relativistic invariance is thus lost. Nevertheless, this gauge is extremely useful.

In this case wave equations (2.21) and (2.24) are also simplified and they are of the form ce46

$$\boldsymbol{\nabla}^2\,\phi(\vec{\mathbf{r}},t) \;=\; -\frac{1}{\epsilon_0}\,\rho(\vec{\mathbf{r}},t), \tag{2.36a}$$ ce46a

$$\left[\boldsymbol{\nabla}^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\vec{\mathbf{A}}(\vec{\mathbf{r}},t) \;=\; -\frac{1}{\epsilon_0\,c^2}\,\vec{\mathbf{j}}(\vec{\mathbf{r}},t)+\frac{1}{c^2}\,\frac{\partial}{\partial t}\;\text{grad}\,\phi(\vec{\mathbf{r}},t). \tag{2.36b}$$ ce46b

The symmetry of the wave equations is lost. Scalar potential must satisfy Poisson's equation (2.36a) and it is due to the instantaneous charge distribution. Then we can write

$$\phi(\vec{\mathbf{r}},t) \;=\; \frac{1}{4\pi\epsilon_o}\int d^3r'\;\frac{\rho(\vec{\mathbf{r}}',t)}{|\vec{\mathbf{r}}-\vec{\mathbf{r}}'|} \tag{2.37}$$ ce47

as it is known from the course on electrodynamics. This may lead to the conclusion that there is some kind of an interaction which spreads with infinite velocity. It can be shown, that this is not really a problem. At present, we only state that the discussion of this problem can be found elsewhere.

2.3 Longitudinal and transverse fields

2.3.1 Introduction

In many practical applications it is convenient to split vector fields in a longitudinal part, for which the rotation is zero, and a transverse part, which has a vanishing divergence (it is a sourceless field). For example, for the electric field we write

$$\vec{\mathbf{E}}(\vec{\mathbf{r}})=\vec{\mathbf{E}}_{\parallel}(\vec{\mathbf{r}})+\vec{\mathbf{E}}_{\perp}(\vec{\mathbf{r}}),\qquad\text{and}\qquad\vec{\mathbf{E}}_{\parallel}\perp\vec{\mathbf{E}}_{\perp}, \tag{2.38}$$ ce51

with

$$\boldsymbol{\nabla}\times\vec{\mathbf{E}}_{\parallel}(\vec{\mathbf{r}})=0,\qquad\qquad\boldsymbol{\nabla}\cdot\vec{\mathbf{E}}_{\perp}(\vec{\mathbf{r}})=0. \tag{2.39}$$ ce52

For any square integrable field such a separation is unique when we also require that the transverse and longitudinal parts vanish separately at infinity. This statement is known as Helmholtz's theorem. The given separation is non-local, in the sense that knowledge of the values of $\vec{\mathbf{E}}(\vec{\mathbf{r}})$ at a certain position is not sufficient to determine the values of $\vec{\mathbf{E}}_{\perp}$ and $\vec{\mathbf{E}}_{\parallel}$ at that position. The differential operators do not specify the field in a unique way, some integration is necessary.

The separation of the fields into transverse and longitudinal parts seems to be more transparent in Fourier space – the space of spatial Fourier transforms.We shall, however, address these problems in the *Auxiliary Chapters*.

Here we will study the question why do we introduce the concepts of transverse and longitudinal fields. The answer is – this leads to the separation of Maxwell's equations.

2.3.2 Longitudinal Maxwell's equations

First of all we note that $\operatorname{div}\vec{\mathbf{B}} = \operatorname{div}\left(\vec{\mathbf{B}}_\perp + \vec{\mathbf{B}}_\parallel\right) = 0$. Since $\operatorname{div}\vec{\mathbf{B}}_\perp = 0$ (by definition of the transverse field) we have $\operatorname{div}\vec{\mathbf{B}}_\parallel = 0$. This is most easily satisfied by demanding

$$\vec{\mathbf{B}}_\parallel(\vec{\mathbf{r}}, t) = 0. \tag{2.40}$$ ce55

This is the first of longitudinal Maxwell's equations. It simply states that magnetic field has no longitudinal components. In other words, magnetic field is purely transverse (or sourceless, its divergence always vanishes).

Then, the Gauss' law gives

$$\operatorname{div}\left(\vec{\mathbf{E}}_\perp + \vec{\mathbf{E}}_\parallel\right) = \frac{\rho}{\epsilon_o}. \tag{2.41}$$ ce56a

Since $\operatorname{div}\vec{\mathbf{E}}_\perp = 0$, we are left with

$$\operatorname{div}\vec{\mathbf{E}}_\parallel = \frac{\rho}{\epsilon_o}, \tag{2.42}$$ ce56b

which is the second longitudinal Maxwell's equation. By definition $\operatorname{rot}\vec{\mathbf{E}}_\parallel = 0$, so we can always write

$$\vec{\mathbf{E}}_\parallel = -\operatorname{grad}\phi, \tag{2.43}$$ ce57

which, together with (2.42) yield

$$\boldsymbol{\nabla}^2\phi = -\frac{\rho}{\epsilon_o}, \tag{2.44}$$ ce58

that is the Poisson's equation as it was the case in the Coulomb gauge (see (2.36a) and (2.37)). Hence, we conclude that the longitudinal electric field is due to instantaneous charge distribution. In other words, longitudinal Maxwell's equations reduce to ce59

$$\vec{\mathbf{B}}_\parallel(\vec{\mathbf{r}}, t) = 0, \tag{2.45a}$$ ce59a

$$\vec{\mathbf{E}}_\parallel(\vec{\mathbf{r}}, t) = \frac{-1}{4\pi\epsilon_0}\boldsymbol{\nabla}\int d^3r'\ \frac{\rho(\vec{\mathbf{r}}', t)}{|\vec{\mathbf{r}} - \vec{\mathbf{r}}'|} = \frac{1}{4\pi\epsilon_0}\int d\vec{\mathbf{r}}'\ \rho(\vec{\mathbf{r}}', t)\ \frac{\vec{\mathbf{r}} - \vec{\mathbf{r}}'}{|\vec{\mathbf{r}} - \vec{\mathbf{r}}'|^3}. \tag{2.45b}$$ ce59b

2.3.3 Transverse Maxwell's equations

Now we consider the remaining Maxwell's equations, that is Faraday's and Ampere's laws. First we write the Faraday's law

$$\operatorname{rot}\left(\vec{\mathbf{E}}_\parallel + \vec{\mathbf{E}}_\perp\right) = -\frac{\partial\vec{\mathbf{B}}}{\partial t}. \tag{2.46}$$ ce62

By definition $\operatorname{rot}\vec{\mathbf{E}}_\parallel = 0$, so Faraday's law is transverse because so is the magnetic field $\vec{\mathbf{B}} = \vec{\mathbf{B}}_\perp$. Hence we have

$$\operatorname{rot}\vec{\mathbf{E}}_\perp = -\frac{\partial}{\partial t}\vec{\mathbf{B}}_\perp, \tag{2.47}$$ ce63

which is the first of transverse Maxwell's equations. It contains no information on the longitudinal fields because longitudinal component of $\vec{\mathbf{E}}$ does not contribute to left hand side, and magnetic field $\vec{\mathbf{B}}$ is purely transverse so there is no magnetic longitudinal contribution.

It remains to discuss the modified Ampere's law (2.1d). We take into account transversality of magnetic field and we have

$$\operatorname{rot} \vec{\mathbf{B}}_\perp \;=\; \frac{1}{\epsilon_o\, c^2}\left(\vec{\mathbf{j}}_\parallel + \vec{\mathbf{j}}_\perp\right) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\left(\vec{\mathbf{E}}_\parallel + \vec{\mathbf{E}}_\perp\right). \tag{2.48}$$

ce64

ce65 This equation splits into two parts: the transverse and longitudinal ones

$$\operatorname{rot} \vec{\mathbf{B}}_\perp \;=\; \frac{1}{\epsilon_o\, c^2}\,\vec{\mathbf{j}}_\perp + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\vec{\mathbf{E}}_\perp, \tag{2.49a}$$

$$0 \;=\; \frac{1}{\epsilon_o\, c^2}\,\vec{\mathbf{j}}_\parallel + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\vec{\mathbf{E}}_\parallel. \tag{2.49b}$$

We will now argue that equation (2.49b) does not bring any new information, and therefore, usually can be discarded. Taking the divergence of (2.49b) we get

$$0 \;=\; \operatorname{div} \vec{\mathbf{j}}_\parallel + \epsilon_o \operatorname{div} \frac{\partial}{\partial t}\,\vec{\mathbf{E}}_\parallel. \tag{2.50}$$

ce66a

But $\operatorname{div} \vec{\mathbf{j}}_\perp = 0$, by definition, so transverse component of the current can be added. Moreover, we use longitudinal equation (2.42) which allows us to write

$$0 \;=\; \operatorname{div} \vec{\mathbf{j}}_\parallel + \frac{\partial}{\partial t}\,\rho \;=\; \operatorname{div}\left(\vec{\mathbf{j}}_\parallel + \vec{\mathbf{j}}_\perp\right) + \frac{\partial}{\partial t}\,\rho. \tag{2.51}$$

ce66b

which is clearly seen to be the charge continuity equation. We conclude that (2.49b) does not bring any new information. It can indeed be discarded.

ce67 Hence, the two transverse Maxwell's equations are of the form

$$\operatorname{rot} \vec{\mathbf{E}}_\perp \;=\; -\frac{\partial}{\partial t}\,\vec{\mathbf{B}}_\perp, \tag{2.52a}$$

$$\operatorname{rot} \vec{\mathbf{B}}_\perp \;=\; \frac{1}{\epsilon_o\, c^2}\,\vec{\mathbf{j}}_\perp + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\vec{\mathbf{E}}_\perp, \tag{2.52b}$$

It is worth remembering that the longitudinal equation (2.49b) of the modified Ampere's law reduces to charge conservation requirement (2.51).

2.3.4 Discussion of the potentials

As we already mentioned the analysis of the longitudinal and transverse parts of the vector fields seems to be easier and more transparent in the Fourier domain. In this domain it is straightforward to see that grad $F(\vec{\mathbf{r}}, t)$ is a purely longitudinal vector (for arbitrary function $F(\vec{\mathbf{r}}, t)$). We shall take this fact for granted and use it in this section.

We start the discussion of potentials with the vector one. From the definition (2.17) we certainly have

$$\vec{\mathbf{B}} = \vec{\mathbf{B}}_\perp = \operatorname{rot}\left(\vec{\mathbf{A}}_\parallel + \vec{\mathbf{A}}_\perp\right) = \operatorname{rot} \vec{\mathbf{A}}_\perp, \tag{2.53}$$

ce71

since, by definition, rot $\vec{\mathbf{A}}_\parallel = 0$. The transverse part of vector potential is sufficient to specify the magnetic field. Moreover, from our discussion of longitudinal and transverse Maxwell's equations it follows that

$$\vec{\mathbf{E}}_\perp \;=\; \frac{\partial}{\partial t}\,\vec{\mathbf{A}}_\perp, \qquad \vec{\mathbf{E}}_\parallel \;=\; -\,\mathrm{grad}\,\phi\frac{\partial}{\partial t}\,\vec{\mathbf{A}}_\parallel. \tag{2.54}$$ ce72

No gradient (it is purely longitudinal) contributes to $\vec{\mathbf{E}}_\perp$. The question is, what is the role played by the longitudinal vector potential $\vec{\mathbf{A}}_\parallel$? Can we (for simplicity) put $\vec{\mathbf{A}}_\parallel = 0$. We shall discuss this problem, but before doing so, we return for a while to wave equations ce73 (ce26 2.21) and (ce28 2.24)

$$\boldsymbol{\nabla}^2\phi = -\frac{1}{\epsilon_0}\,\rho - \frac{\partial}{\partial t}\,\mathrm{div}\,\vec{\mathbf{A}}_\parallel, \tag{2.55a}$$ ce73a

$$\left[\frac{1}{c^2}\,\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2\right]\vec{\mathbf{A}} = \frac{1}{c^2\,\epsilon_o}\,\vec{\mathbf{j}} - \mathrm{grad}\left[\mathrm{div}\,\vec{\mathbf{A}}_\parallel + \frac{1}{c^2}\,\frac{\partial\,\phi}{\partial t}\right]. \tag{2.55b}$$ ce73b

$\vec{\mathbf{A}}_\perp$ does not appear in right hand sides because div $\vec{\mathbf{A}}_\perp = 0$, by definition. The gradient ce74 is longitudinal, so Eq.(ce73b 2.55b) clearly splits into two parts

$$\left[\frac{1}{c^2}\,\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2\right]\vec{\mathbf{A}}_\parallel = \frac{1}{c^2\,\epsilon_o}\,\vec{\mathbf{j}}_\parallel - \mathrm{grad}\left[\mathrm{div}\,\vec{\mathbf{A}}_\parallel + \frac{1}{c^2}\,\frac{\partial\,\phi}{\partial t}\right]. \tag{2.56a}$$ ce74a

$$\left[\frac{1}{c^2}\,\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2\right]\vec{\mathbf{A}}_\perp = \frac{1}{c^2\,\epsilon_o}\,\vec{\mathbf{j}}_\perp. \tag{2.56b}$$ ce74b

In normal space (in contrast to Fourier domain) it is not easy to show that Eq.(ce74a 2.56a) does not bring any new information and that it reduces to charge conservation requirement (ce66b 2.51). This fact, in the view of previous discussion, should not be really surprising. This is easily shown in the Fourier space and is presented in *Auxiliary chapters*. Equation (ce74a 2.56a) can be thus discarded and we remain with two wave equations (ce73a 2.55a) and (ce74a 2.56a).

Coulomb gauge requirement div $\vec{\mathbf{A}} = 0$ reduces to div $\vec{\mathbf{A}}_\parallel = 0$. The simplest way to fulfill this condition is to take $\vec{\mathbf{A}}_\parallel = 0$. In this case relations (ce71 2.53) and (ce72 2.54) still hold, so the fields remain unchanged. On the other hand, potentials now satisfy the following ce77 wave equations

$$\boldsymbol{\nabla}^2\phi = -\frac{1}{\epsilon_o}\,\rho, \tag{2.57a}$$ ce77a

$$\left[\frac{1}{c^2}\,\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2\right]\vec{\mathbf{A}}_\perp = \frac{1}{c^2\,\epsilon_o}\,\vec{\mathbf{j}}_\perp, \tag{2.57b}$$ ce77b

while the longitudinal current density is connected with charge density by Eq.(ce66b 2.51).

At the end of our discussion we shall give some additional comments (which are also discussed in *Auxiliary Chapters*.

1. Having found the scalar potential (by solving Poisson's equation (ce77a 2.57a)) we can find the longitudinal component of the electric field $\vec{\mathbf{E}}_\parallel$ according to Eq.(ce72 2.54). Moreover, it is interesting to note that in Coulomb gauge (with $\vec{\mathbf{A}}_\parallel = 0$) wave equation (ce74a 2.56a) yields

$$\frac{1}{\epsilon_o}\,\vec{\mathbf{j}}_\parallel \;=\; \frac{\partial}{\partial t}\,\mathrm{grad}\,\phi \;=\; -\,\frac{\partial}{\partial t}\,\vec{\mathbf{E}}_\parallel, \tag{2.58}$$ ce78

so the longitudinal current density can also be found.

2. The second wave equation (2.57b) gives transverse component of the vector potential as a function of the transverse part of the current density. It is sufficient to know $\vec{\mathbf{A}}_\perp$ to compute transverse components of electric and magnetic fields according to relations (2.53) and (2.54).

3. In the Coulomb gauge the transverse $\vec{\mathbf{A}}_\perp$ is the only relevant vector potential. Let us note that it is gauge invariant (this will be discussed in more detail in *Auxiliary Chapters*). To see this, we perform gauge transformation (2.28a)

$$\vec{\mathbf{A}} \xrightarrow[gauge]{} \vec{\mathbf{A}}' = \vec{\mathbf{A}} + \boldsymbol{\nabla} F. \tag{2.59}$$

ce79

Since any gradient is purely longitudinal, the transverse component is unchanged.

* *

Chapter 3

Quantization of electromagnetic field

c:fq

3.1 Introductory remarks

We will quantize electromagnetic field in a simple, intuitive manner. We consider the sourceless electromagnetic field in a cavity with Coulomb gauge, that is the field, for which the vector potential satisfies the requirement

$$\operatorname{div} \vec{\mathbf{A}} = 0. \tag{3.1}$$ fq01

As it follows from the considerations in the previous chapter, the vector potential is transverse, gauge independent, and since there are no sources, it satisfies the homogeneous wave equation

$$\frac{1}{c^2}\frac{\partial^2 \vec{\mathbf{A}}_\perp}{\partial t^2} - \boldsymbol{\nabla}^2 \vec{\mathbf{A}}_\perp(\vec{\mathbf{r}}, t) \;=\; 0. \tag{3.2}$$ fq03

Due to the Coulomb gauge and to the absence of the sources we can take the scalar potential to be identically zero. Then the fields are fully specified by the vector potential

fq05

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{r}}, t) = -\frac{\partial}{\partial t}\vec{\mathbf{A}}_\perp(\vec{\mathbf{r}}, t), \qquad \vec{\mathbf{E}}_\parallel(\vec{\mathbf{r}}, t) \;=\; 0, \tag{3.3a}$$ fq05a

$$\vec{\mathbf{B}}(\vec{\mathbf{r}}, t) = \vec{\mathbf{B}}_\perp \;=\; \boldsymbol{\nabla} \times \vec{\mathbf{A}}_\perp(\vec{\mathbf{r}}, t), \tag{3.3b}$$ fq05b

We will not go into the subtleties of the gauge problems, or other mathematical nuances. We will consider the electromagnetic field in the cavity of volume V. The procedure we will describe does not depend on the shape of the cavity, although the proof of this fact is far from trivial. We will also indicate the limiting procedure allowing the description of the fields in all space.

3.2 Expansion into normal modes

3.2.1 Statement of the problem

We seek the solution to the wave equation (3.2) in a form with separated variables

$$\vec{\mathbf{A}}_\perp(\vec{\mathbf{r}},t) \;=\; \sqrt{\frac{1}{\epsilon_0}}\;\sum_n\, q_n(t)\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}). \tag{3.4}$$

The index n may have the meaning of the multiindex (the Laplace operator in the wave equation is usually degenerate). The coefficient in the front is introduced for future convenience. We will call $q_n(t)$ the field amplitudes, while the function $\vec{\mathbf{u}}_n(\vec{\mathbf{r}})$ will be called field modes. At present we will assume that the set of field modes is linearly independent, and as such can be orthonormalized. This point will be discussed later. Since the fields are physical observables, we can for present purposes take the field amplitudes and modes to be real.

Before analyzing the wave equation let us express the fields via the adopted vector potential. From (3.3) and (3.4) we get

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{r}},t) = -\sqrt{\frac{1}{\epsilon_0}}\;\sum_n\, \dot{q}_n(t)\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}), \tag{3.5a}$$

$$\vec{\mathbf{B}}(\vec{\mathbf{r}},t) = \sqrt{\frac{1}{\epsilon_0}}\;\sum_n\, q_n(t)\,\mathrm{rot}\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \tag{3.5b}$$

Let us also note, that the Coulomb gauge implies the relation

$$0 \;=\; \mathrm{div}\,\vec{\mathbf{A}}(\vec{\mathbf{r}},t) \;=\; \sqrt{\frac{1}{\epsilon_0}}\;\sum_n\, q_n(t)\,\mathrm{div}\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \tag{3.6}$$

We return to the wave equation. Substituting (3.4) into the wave equation (3.2) we employ the linear independence of the field modes to obtain

$$\frac{1}{c^2}\,\ddot{q}_n(t)\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \;-\; q_n(t)\,\boldsymbol{\nabla}^2\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \;=\; 0. \tag{3.7}$$

We can add and subtract the same quantity. Then we get

$$\frac{1}{c^2}\,\left[\,\ddot{q}_n(t) \;+\; \omega_n^2 q_n(t)\,\right]\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \;-\; q_n(t)\,\left[\,\boldsymbol{\nabla}^2\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \;+\; \frac{\omega_n^2}{c^2}\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}})\,\right] \;=\; 0. \tag{3.8}$$

This procedure is fully equivalent to usual variable separation. This equation must be satisfied identically for any time instant and at any point within the cavity, therefore, the coefficients in square brackets must vanish separately. Hence, our wave equation is equivalent to the set of equations

$$\ddot{q}_n(t) \;+\; \omega_n^2\, q_n(t) = 0, \tag{3.9a}$$

$$\boldsymbol{\nabla}^2\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \;+\; \frac{\omega_n^2}{c^2}\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) = 0. \tag{3.9b}$$

Equation (3.9a) has dynamical character, while (3.9b) is geometrical. First, we consider the geometrical one with the reasonable assumption that $\omega_m \neq \omega_n$.

The field within the cavity must satisfy the boundary conditions at the walls of the cavity. The tangent component of the electric field must vanish, and so must the normal component of the magnetic field. Since the fields are given via Eqs.(3.5), we see that the geometric equation (3.9b) must be solved with three conditions

fq19

$$\vec{\mathbf{u}}_n(\vec{\mathbf{r}})|_{tangent} = 0 \quad \text{on the boundary } \partial V, \tag{3.10a}$$ fq19a

$$\text{rot } \vec{\mathbf{u}}_n(\vec{\mathbf{r}})|_{normal} = 0 \quad \text{on the boundary } \partial V, \tag{3.10b}$$ fq19b

$$\text{div } \vec{\mathbf{u}}_n(\vec{\mathbf{r}}) = 0 \quad \text{in all volume } V. \tag{3.10c}$$ fq19c

The third condition follows from the Coulomb gauge (3.6) and must be satisfied within all volume of the cavity. It can be shown that relations (3.10a) and (3.10c) imply that the electric field should vanish on the cavity walls. Hence, we can say that $\vec{\mathbf{u}}_n|_{wall} = 0$. We will not solve Eq.(3.9b) with the above given conditions. We refer to mathematical handbooks, and we will only state that such a problem can be solved once the shape of the cavity is given. Moreover, the obtained cavity modes $\vec{\mathbf{u}}_n(\vec{\mathbf{r}})$ can be shown to characterize the cavity in a unique manner. Such modes are called normal modes of the cavity. Hence, normal modes fully characterize the geometry of the problem. The dynamical behavior of the fields is thus described by the amplitudes $q_n(t)$. Determination of amplitudes automatically determines the fields, since the normal (geometrical) modes are fixed once the cavity shape is given. Therefore we proceed to analyze the field amplitudes $q_n(t)$.

3.2.2 Energy of the field in a cavity

The field amplitudes $q_n(t)$ are best discussed via the field energy. We recall, that in classical electrodynamics the energy of the field in cavity (in vacuum) is given by the integral

$$\mathcal{E} \;=\; \frac{\epsilon_0}{2} \int_V d\vec{\mathbf{r}} \left[\vec{\mathbf{E}}^2 \;+\; c^2 \vec{\mathbf{B}}^2 \right] \tag{3.11}$$ fq21

Inserting the fields according to relations (3.5) we get

$$\mathcal{E} = \frac{1}{2} \int_V d\vec{\mathbf{r}} \left[\sum_{n,m} \dot{q}_m(t)\dot{q}_n(t)\; \vec{\mathbf{u}}_m(\vec{\mathbf{r}}) \cdot \vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \right.$$
$$\left. + \frac{c^2}{2} \sum_{m,n} q_m(t) q_n(t) \;\; \text{rot } \vec{\mathbf{u}}_m(\vec{\mathbf{r}}) \cdot \text{rot } \vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \right]. \tag{3.12}$$ fq23

We proceed with the analysis of the second integral, which we denote as

$$J_{mn} \;=\; \int_V d\vec{\mathbf{r}} \;\; \text{rot } \vec{\mathbf{u}}_m(\vec{\mathbf{r}}) \cdot \text{rot } \vec{\mathbf{u}}_n(\vec{\mathbf{r}}), \tag{3.13}$$ fq25

and which is obviously symmetric, that is $J_{mn} = J_{nm}$. We will now transform this integral so as to make use of the boundary conditions imposed on cavity modes. We use the vector

analysis identities ($\mathrm{rot}\,\mathrm{rot} = \mathrm{grad}\,\mathrm{div} - \nabla^2$),

$$\begin{aligned}\mathrm{rot}\,\vec{\mathbf{a}}\cdot\mathrm{rot}\,\vec{\mathbf{b}} &= \mathrm{div}\big(\,\vec{\mathbf{a}}\times\mathrm{rot}\,\vec{\mathbf{b}}\,\big) \;+\; \vec{\mathbf{a}}\cdot\mathrm{rot}\,\mathrm{rot}\,\vec{\mathbf{b}} \\ &= \mathrm{div}\big(\,\vec{\mathbf{a}}\times\mathrm{rot}\,\vec{\mathbf{b}}\,\big) \;+\; \vec{\mathbf{a}}\cdot\mathrm{grad}\,\mathrm{div}\,\vec{\mathbf{b}} \;-\; \vec{\mathbf{a}}\cdot\nabla^2\vec{\mathbf{b}},\end{aligned} \tag{3.14}$$ fq27

which allows us to rewrite the integral J_{mn}

$$J_{mn} \;=\; \int_V d\vec{\mathbf{r}}\;\left[\;\mathrm{div}\,(\vec{\mathbf{u}}_m\times\mathrm{rot}\,\vec{\mathbf{u}}_n) \;+\; \vec{\mathbf{u}}_m\cdot\mathrm{grad}\,\mathrm{div}\,\vec{\mathbf{u}}_n \;-\; \vec{\mathbf{u}}_m\cdot\nabla^2\vec{\mathbf{u}}_n\right]. \tag{3.15}$$ fq29

Firstly, we note that the second term in (3.14) does not contribute, because the fields are transverse: $\mathrm{div}\,\vec{\mathbf{u}}_n = 0$, see (3.10c). Secondly, the functions $\vec{\mathbf{u}}_n$ satisfy Helmholtz equation (3.9b). Hence, from (3.15) we obtain

$$J_{mn} \;=\; \int_V d\vec{\mathbf{r}}\;\left[\;\mathrm{div}\,(\vec{\mathbf{u}}_m\times\mathrm{rot}\,\vec{\mathbf{u}}_n) \;+\; \frac{\omega_n^2}{c^2}\;\vec{\mathbf{u}}_m\cdot\vec{\mathbf{u}}_n\right]. \tag{3.16}$$ fq31

The symmetry of the integral J_{mn} gives $J_{mn}-J_{nm}=0$, and by subtraction of the equations of the type of (3.16) we obtain

$$\int_V d\vec{\mathbf{r}}\;\left[\;\mathrm{div}\,(\vec{\mathbf{u}}_m\times\mathrm{rot}\,\vec{\mathbf{u}}_n) \;-\; \mathrm{div}\,(\vec{\mathbf{u}}_n\times\mathrm{rot}\,\vec{\mathbf{u}}_m)\right] \;=\; \frac{\omega_m^2-\omega_n^2}{c^2}\;\int_V d\vec{\mathbf{r}}\;\;\vec{\mathbf{u}}_m\cdot\vec{\mathbf{u}}_n, \tag{3.17}$$ fq33

Now, we consider the integral of the term similar to the ones appearing in the above formula. First we use the Gauss theorem and transform the volume integral into the surface one. Then we argue that, for any m and n, the resulting integral vanishes, that is we have

$$\int_V d\vec{\mathbf{r}}\;\;\mathrm{div}\,(\vec{\mathbf{u}}_m\times\mathrm{rot}\,\vec{\mathbf{u}}_n) \;=\; \oint_{\partial V} d\vec{\mathbf{S}}\cdot(\vec{\mathbf{u}}_m\times\mathrm{rot}\,\vec{\mathbf{u}}_n) \;=\; 0. \tag{3.18}$$ fq35

The scalar product in the surface integral "selects" the component of $\vec{\mathbf{u}}_m\times\mathrm{rot}\,\vec{\mathbf{u}}_n$ along the vector $d\vec{\mathbf{S}}$ which is perpendicular to the surface. This (perpendicular) part of the vector $\vec{\mathbf{u}}_m\times\mathrm{rot}\,\vec{\mathbf{u}}_n$ arises from the components which are parallel (tangent) to the surface, as it follows from the properties of the vector product of two vectors. But the tangent component of $\mathrm{rot}\,\vec{\mathbf{u}}_n$ vanishes [see the boundary conditions (3.10a)]. Hence, the normal component of the vector product vanishes. The integrand is thus zero, and the relation (3.18) is proved. Left-hand side of (3.17) is zero, and we arrive at the conclusion that

$$\frac{\omega_m^2-\omega_n^2}{c^2}\;\int_V d\vec{\mathbf{r}}\;\;\vec{\mathbf{u}}_m\cdot\vec{\mathbf{u}}_n \;=\; 0. \tag{3.19}$$ fq37

Since parameters $\omega_n \neq \omega_m$, we may write

$$\int_V d\vec{\mathbf{r}}\;\;\vec{\mathbf{u}}_m\cdot\vec{\mathbf{u}}_n \;=\; \delta_{mn}, \tag{3.20}$$ fq39

because orthogonal functions can be normalized. This fact may be explained in a different manner. Namely, we can refer to the wave equation (3.9b) and since the laplacian ∇^2 is a Hermitian operator, its eigenfunctions belonging to different eigenvalues should be

orthonormal, which is reflected by (3.20). We complete our discussion by returning to the integral (3.16) in which we use relations (3.18) and (3.20) to get

$$J_{mn} \;=\; J_{nm} \;=\; \int_V d\vec{\mathbf{r}}\;\; \mathrm{rot}\,\vec{\mathbf{u}}_m(\vec{\mathbf{r}})\cdot \mathrm{rot}\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \;=\; \frac{\omega_n^2}{c^2}\,\delta_{mn}. \tag{3.21}$$ fq41

Inserting the obtained results (3.20) and (3.21) into the expression (3.12) for the energy of the field in the cavity, we obtain

$$\begin{aligned}\mathcal{E} &= \frac{1}{2}\sum_n\; \dot{q}_n^2(t) \;+\; \frac{c^2}{2}\sum_{m,n}\; q_m(t)q_n(t)\,\frac{\omega_n^2}{c^2}\,\delta_{mn}\\ &= \frac{1}{2}\sum_n\; \big(\,\dot{q}_n^2(t) \;+\; \omega_n^2\, q^2(t)\,\big).\end{aligned} \tag{3.22}$$ fq43

This result confirms that all dynamical information on the fields is included in the field amplitudes $q_n(t)$. The obtained result clearly reminds of the harmonic oscillator. We may interpret (3.22) as the sum of the energies of the so-called field oscillators. This analogy will be very important, therefore, we will devote some attention to the harmonic oscillator.

3.2.3 Expansion in normal variables

To proceed further we introduce new, in this case complex, time dependent functions which reexpress the amplitudes q_n and associated momenta p_n as

$$q_n \;=\; \sqrt{\frac{\hbar}{2\omega_n}}\;(\,a_n \;+\; a_n^*\,), \qquad\qquad p_n \;=\; \dot{q}_n \;=\; -\,i\,\sqrt{\frac{\hbar\,\omega_n}{2}}\,(\,a_n \;-\; a_n^*\,), \tag{3.23}$$ fq45

where Planck's constant is introduced for future convenience. These relations are easily inverted to give

$$a_n \;=\; \frac{1}{\sqrt{2\hbar\omega_n}}\;(\,\omega_n\, q_n \;+\; ip_n\,), \qquad\qquad a_n^* \;=\frac{1}{\sqrt{2\hbar\omega_n}}\;(\,\omega_n\, q_n \;-\; ip_n\,). \tag{3.24}$$ fq47

The functions a_n and a_n^* are called "normal variables" of the fields which, as follows from (3.3) and (3.5) after substitution of (3.23), are now of the form fq49

$$\vec{\mathbf{A}}_\perp(\vec{\mathbf{r}},t) = \sum_n\; \sqrt{\frac{\hbar}{2\epsilon_0\,\omega_n}}\;\big(\,a_n \;+\; a_n^*\,\big)\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}). \tag{3.25a}$$ fq49a

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{r}},t) = i\sum_n\; \sqrt{\frac{\hbar\,\omega_n}{2\epsilon_0}}\;\big(\,a_n \;-\; a_n^*\,\big)\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}), \tag{3.25b}$$ fq49e

$$\vec{\mathbf{B}}(\vec{\mathbf{r}},t) = \sum_n\; \sqrt{\frac{\hbar}{2\epsilon_0\,\omega_n}}\;\big(\,a_n \;+\; a_n^*\,\big)\,\mathrm{rot}\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}). \tag{3.25c}$$ fq49m

Energy of the field, given in (3.22), can also be given in terms of the normal variables. It becomes

$$\mathcal{E} \;=\; \frac{1}{2}\sum_n \hbar\omega_n\big[\,a_n a_n^* \;+\; a_n^* a_n\,\big] \;=\; \sum_n \hbar\omega_n\, a_n^* a_n, \tag{3.26}$$ fq51

where the second equality follows from the commutation of classical normal variables.

We have already mentioned analogies to classical harmonic oscillator. The energy of the field expressed as in (3.26) by normal variables brings further associations, but this time with quantum-mechanical harmonic oscillator.

3.3 Field quantization in a cavity

3.3.1 Field oscillators – harmonic oscillator

We recall some basic facts about quantum mechanical harmonic oscillator. We consider one-dimensional harmonic oscillator with unit mass, thus we write its Hamiltonian as

$$H_{osc} \;=\; \frac{1}{2}\,p^2 \;+\; \frac{1}{2}\,\omega^2\,q^2 \tag{3.27}$$

The position and momentum operators satisfy the well-known canonical commutation relation $[q,\,p] = i\hbar$. It is straightforward to find the Heisenberg equations of motion for both operators

$$i\hbar\,\dot{q} = \left[\,q,\,H\,\right] \;=\; \frac{1}{2}\,\left[\,q,\,p^2\,\right] \;=\; i\hbar p \tag{3.28a}$$

$$i\hbar\,\dot{p} = \left[\,p,\,H\,\right] \;=\; \frac{1}{2}\,\left[\,p,\,\omega^2\,q^2\,\right] \;= -i\hbar\omega^2\,q \tag{3.28b}$$

We see that quantum-mechanical Heisenberg equations yield the same equations as classical Hamilton equations

$$\dot{q} \;=\; p \;=\; \frac{\partial H}{\partial p} \qquad\qquad \dot{p} \;=\; -\,\omega^2\,q \;=\; -\,\frac{\partial H}{\partial p} \tag{3.29}$$

We know (see the chapter 10) that the variables of the harmonic oscillator can be re-expressed in terms of the dimensionless annihilation and creation operators. Such a procedure is called second quantization. We assign the following operators to the position and momentum ones

$$q \;=\; \sqrt{\frac{\hbar}{2\omega}}\;\left(\,\hat{a} \;+\; \hat{a}^\dagger\,\right), \qquad\qquad p \;=\; -\,i\,\sqrt{\frac{\hbar\,\omega}{2}}\,\left(\,\hat{a} \;-\; \hat{a}^\dagger\,\right), \tag{3.30}$$

These relations are easily inverted to give

$$\hat{a} \;=\; \frac{1}{\sqrt{2\hbar\omega}}\;\left(\,\omega\,q \;+\; ip\,\right), \qquad\qquad \hat{a}^\dagger \;=\; \frac{1}{\sqrt{2\hbar\omega}}\;\left(\,\omega\,q \;-\; ip\,\right). \tag{3.31}$$

So far, we easily see full analogy between quantum-mechanical annihilation and creation operators and normal variables. The essential difference follows from the canonical commutation relation for position and momentum operators. It implies the canonical commutation relation for annihilation and creation operators

$$\left[\,\hat{a},\,\hat{a}^\dagger\,\right] \;=\; 1. \tag{3.32}$$

The Hamiltonian of the oscillator, rewritten in terms of annihilation and creation operators is of the form

$$H_{osc} \;=\; \hbar\omega\big(\,\hat{a}^\dagger\hat{a} \;+\; \frac{1}{2}\,\big), \tag{3.33}$$ fq65

where the term $1/2$ is due to noncommutativity of $\hat{a}$ and $\hat{a}^\dagger$.

It is also important to note, than the states of the harmonic oscillator (ie., eigenstates of the Hamiltonian) are denoted by $|\,n\,\rangle$ with $n = 0,\ 1,\ 2,\ ,\ldots\ldots$. So we have

$$H_{osc}|\,n\,\rangle = \hbar\omega\big(\,n + \frac{1}{2}\,\big)\,|\,n\,\rangle \tag{3.34}$$ fq67

The state with $n = 0$ is called the vacuum state and it has the property

$$\hat{a}\,|\,0\,\rangle \;=\; 0. \tag{3.35}$$ fq69

It is useful to remind that given the vacuum state, we can construct all states $|\,n\,\rangle$ by successive application of the creation operator

$$|\,n\,\rangle \;=\; \frac{(\hat{a}^\dagger)^n}{\sqrt{n\,!}}\,|\,0\,\rangle. \tag{3.36}$$ fq71

Obviously, we can also construct the wave functions of the oscillator. For example, in the position representation we can find the eigenfunctions $\psi_n(q) = \langle\, q\,|\,n\,\rangle$. We refer the reader to the auxiliary chapter 10. ac:ac

We can also easily derive the Heisenberg equations of motion for annihilation and creation operators. This can be done directly by the differentiation of the definitions (3.31) or in a standard way. We get fq61

fq73

$$\dot{\hat{a}} = \frac{1}{i\hbar}\big[\,\hat{a},\,H_{osc}\,\big] \;=\; -\,i\omega\big[\,\hat{a},\,\hat{a}^\dagger\hat{a}\,\big] \;=\; -\,i\omega\big[\,\hat{a},\,\hat{a}^\dagger\,\big]\,\hat{a} \;=\; -\,i\omega\hat{a}, \tag{3.37a}$$ fq73a

$$\dot{\hat{a}}^\dagger = \frac{1}{i\hbar}\big[\,\hat{a}^\dagger,\,H_{osc}\,\big] \;=\; -\,i\omega\big[\,\hat{a}^\dagger,\,\hat{a}^\dagger\hat{a}\,\big] \;=\; -\,i\omega\hat{a}^\dagger\big[\,\hat{a},\,\hat{a}\,\big] \;=\; i\omega\hat{a}^\dagger. \tag{3.37b}$$ fq73c

This summarizes all the information on the quantum mechanical harmonic oscillator. This is relevant for the context of electromagnetic fields in the cavity.

3.3.2 Field quantization

We proceed with the intuitively simple quantization of the electromagnetic field in the cavity. With each of the field oscillators we associate corresponding annihilation and creation operators which satisfy the commutation relation

$$\big[\,\hat{a}_m,\,\hat{a}_n^\dagger\,\big] \;=\; \delta_{mn}, \tag{3.38}$$ fq75

with all other commutators vanishing. This commutation relation reflects the independence of the field modes.

Quantization of the fields consists in replacing the normal variables by corresponding operators $\hat{a}$ and $\hat{a}^\dagger$. Adopting such an equivalence we now have the quantized fields in the

form identical to (3.25) only with normal variables replaced by annihilation and creation operators. We thus obtain the fields as

$$\vec{\mathbf{A}}_\perp(\vec{\mathbf{r}},t) = \sum_n \sqrt{\frac{\hbar}{2\epsilon_0\,\omega_n}}\,\left(\,\hat{a}_n \;+\; \hat{a}_n^\dagger\,\right)\vec{\mathbf{u}}_n(\vec{\mathbf{r}}). \tag{3.39a}$$

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{r}},t) = i\sum_n \sqrt{\frac{\hbar\,\omega_n}{2\epsilon_0}}\,\left(\,\hat{a}_n \;-\; \hat{a}_n^\dagger\,\right)\vec{\mathbf{u}}_n(\vec{\mathbf{r}}), \tag{3.39b}$$

$$\vec{\mathbf{B}}(\vec{\mathbf{r}},t) = \sum_n \sqrt{\frac{\hbar}{2\epsilon_0\,\omega_n}}\,\left(\,\hat{a}_n \;+\; \hat{a}_n^\dagger\,\right)\,\mathrm{rot}\,\vec{\mathbf{u}}_n(\vec{\mathbf{r}}) \tag{3.39c}$$

Thus, instead of classical functions describing the electromagnetic field we now have quantum-mechanical field operators. These operators do not commute, since the annihilation and creation operators do not commute. It is important to understand that the time dependence (or, dynamical behavior) of the fields is hidden in the annihilation and creation operators. This is evident, if we take into account that in the classical case, the dynamics was hidden in the field amplitudes $q(t)$, as it can be seen from Eq.(3.22). Since the amplitudes are, in the quantum-mechanical case, replaced by annihilation and creation operators, they must account for the dynamics of the fields.

Applying the same procedure to the field energy, we reexpress it in terms of the annihilation and creation operators. Thus, we replace the classical energy of the field by the quantum mechanical operator

$$H_{field} \;=\; \sum_n \hbar\omega_n\,\left(\,\hat{a}_n^\dagger\,\hat{a}_n \;+\; \frac{1}{2}\,\right). \tag{3.40}$$

The term 1/2, absent in the classical case, now follows from the noncommutativity of the annihilation and creation operators.

To complete the field quantization we must specify the Hilbert space of the field eigenstates. We again employ the analogy with the harmonic oscillator. First we define the vacuum state by the requirement

$$\hat{a}_n\,|\,\Omega\,\rangle = 0, \qquad \text{for any mode } n. \tag{3.41}$$

Since the field modes are independent we construct other eigenstates of the field as a tensor product

$$\begin{aligned}|\,n_{(1)},n_{(2)},\ldots,n_{(k)},\ldots\,\rangle &= |\,n_{(1)}\,\rangle\otimes|\,n_{(2)}\,\rangle\otimes\ldots\otimes|\,n_{(k)}\,\rangle\otimes\ldots\\ &= \bigotimes_{(i)}\;\frac{(\hat{a}^\dagger_{n_{(i)}})^{n_{(i)}}}{\sqrt{n_{(i)}\,!}}\;|\,\Omega\,\rangle\end{aligned} \tag{3.42}$$

where numbers $n_{(i)}$ are nonnegative integers and index (i) numbers all modes. The states defined above are called states with $n_{(i)}$ photons in the mode number (i).

We note, that in many practical cases the number of modes in the cavity is infinite. In such a case the expectation value of the energy of the vacuum state follows form (3.40)

$$\langle\,\Omega\,|\,H_{field}\,|\,\Omega\,\rangle \;=\; \sum_n \frac{1}{2}\,\hbar\omega_n \tag{3.43}$$

and is infinite. We renormalize the energy by dropping the term 1/2. Thus the free field hamiltonian is taken to be

$$H_{field} \;=\; \sum_n \hbar\omega_n \,\hat{a}_n^\dagger \hat{a}_n. \tag{3.44}$$ fq87

Omission of the 1/2 term does not change the equation of motion for field operators. They follow again by the analogy to harmonic oscillator, and we have fq89

$$\dot{\hat{a}}_n = -i\omega \hat{a}_n, \tag{3.45a}$$ fq89a

$$\dot{\hat{a}}_n^\dagger = i\omega \hat{a}_n^\dagger. \tag{3.45b}$$ fq89c

Hence the time dependence of the field annihilation and creation operators for the case of free field is simple. By direct integration we get

$$\hat{a}_n(t) \;=\; \hat{a}_n(t_0)\, e^{-i\omega_n(t-t_0)}, \qquad\qquad \hat{a}_n^\dagger(t) \;=\; \hat{a}_n^\dagger(t_0)\, e^{i\omega_n(t-t_0)}, \tag{3.46}$$ fq91

with $\hat{a}_n(t_0)$ and $\hat{a}_n^\dagger(t_0)$ being the initial values. As we already stressed, the dynamics of the fields is "hidden" in the annihilation and creation operators. If we insert relations (3.46) into the fields (3.39), we see that their time dependence is sinusoidal, as might be expected due to the oscillator analogy.

3.4 Plane wave representation

3.4.1 Discussion of our results

As we already mentioned, the index n numbering field modes should be understood as a multiindex. We generalize our results by using an additional index α explicitly. Moreover, the wave equation (3.9b) is real, but in general, it allows complex valued solutions. Therefore, we generalize the fields (3.39) by writing fq93

$$\vec{\mathbf{A}}(\vec{\mathbf{r}},t) = \sum_{n,\alpha} \sqrt{\frac{\hbar}{2\epsilon_0\,\omega_n}}\; \left(\, \hat{a}_{n\alpha}\, \vec{\mathbf{f}}_{n\alpha}(\vec{\mathbf{r}}) \;+\; \hat{a}_{n\alpha}^\dagger\, \vec{\mathbf{f}}_{n\beta}^{\,*}(\vec{\mathbf{r}}) \,\right), \tag{3.47a}$$ fq93a

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{r}},t) = i\sum_{n,\alpha} \sqrt{\frac{\hbar\,\omega_n}{2\epsilon_0}}\; \left(\, \hat{a}_{n\alpha}\, \vec{\mathbf{f}}_{n\alpha}(\vec{\mathbf{r}}) \;-\; \hat{a}_{n\alpha}^\dagger\, \vec{\mathbf{f}}_{n\alpha}^{\,*}(\vec{\mathbf{r}}) \,\right), \tag{3.47b}$$ fq93e

$$\vec{\mathbf{B}}(\vec{\mathbf{r}},t) = \sum_{n,\alpha} \sqrt{\frac{\hbar}{2\epsilon_0\,\omega_n}}\; \left(\, \hat{a}_{n\alpha}\, \mathrm{rot}\, \vec{\mathbf{f}}_{n\alpha}(\vec{\mathbf{r}}) \;+\; \hat{a}_{n\alpha}^\dagger\, \mathrm{rot}\, \vec{\mathbf{f}}_{n\alpha}^{\,*}(\vec{\mathbf{r}}) \,\right) \tag{3.47c}$$ fq93m

The functions $\vec{\mathbf{f}}_{n\alpha}(\vec{\mathbf{r}})$ possess similar properties as initial functions $\vec{\mathbf{u}}_n$. They satisfy the boundary conditions, are orthonormal, etc. We stress that the form of the fields as above ensures hermiticity of the field operators, as it should be, because the fields are most certainly the physically observable quantities.

The annihilation and creation operators satisfy the commutation relation which is an obvious generalization of (3.38), and which reads

$$\left[\, \hat{a}_{m\alpha},\, \hat{a}_{n\beta}^\dagger \,\right] \;=\; \delta_{mn}\,\delta_{\alpha\beta}. \tag{3.48}$$ fq95

Other expressions, as for example the free field Hamiltonian (3.44), are also suitably generalized in an obvious manner. It may be worth noting that our generalization can be viewed as a unitary transformation of the previous results. Unitary transformation preserve commutation relations, orthonormality etc., thus, there is no need to discuss this point in more detail.

As we also mentioned, the specific form of cavity modes $\vec{\mathbf{f}}_{n\alpha}$ depends on the geometry of the cavity. It is possible to discuss cavities of various shapes, symmetries, but we will focus attention on the simplest, but most widely used case – the plane waves.

3.4.2 Introduction of plane waves

We will now discuss the quantization of fields in a cubic box of volume V. The simplest set of orthonormal eigenfunctions of such a cavity consists of plane waves

$$\vec{\mathbf{f}}_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}}) \;=\; \frac{1}{\sqrt{V}}\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}, \tag{3.49}$$

which are labelled by the wave vector $\vec{\mathbf{k}}$ and by an additional index λ (which replace our multiindex n,α). The wave vector satisfies the dispersion relation

$$\omega_k \;= kc, \qquad \text{with} \qquad k = |\,\vec{\mathbf{k}}\,|, \tag{3.50}$$

which is a consequence of the requirement that functions $\vec{\mathbf{f}}_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}})$ satisfy the Helmholtz equation (3.9b). The vectors $\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}$ called polarization vectors are in general complex and normalized to unity

$$||\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,|| = 1. \tag{3.51}$$

In order to discuss these functions we expand the vector potential in terms of them. Adjusting the summation indices according to the present situation, from (3.47a) we get

$$\vec{\mathbf{A}}_\perp(\vec{\mathbf{x}},t) = \sum_{\vec{\mathbf{k}}\lambda}\,\sqrt{\frac{\hbar}{2\epsilon_0\omega_k V}}\,\left[\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,a_{\vec{\mathbf{k}}\lambda}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;+\; \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\,a^\dagger_{\vec{\mathbf{k}}\lambda}\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right], \tag{3.52}$$

Vector potential must satisfy the Coulomb gauge (3.1), that is we consider a transverse field $\vec{\mathbf{A}} \equiv \vec{\mathbf{A}}_\perp$. This requirement applied to expansion (3.52) yields

$$\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{k}} = \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{k}} = 0. \tag{3.53}$$

So, polarization vectors are orthogonal to wave vector, which explains their name. By analogy to classical electrodynamics we conclude that there are two vectors orthogonal to the given $\vec{\mathbf{k}}$. Hence the index λ takes on two possible values $\lambda = 1,\,2$. Two real vectors $\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}$ correspond to two linear polarizations. When polarization is circular polarization vectors are complex. Moreover, it is convenient to assume that two polarization vectors are mutually orthogonal, that is

$$\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\mu} = \delta_{\lambda\mu}. \tag{3.54}$$

The boundary conditions imposed on the fields result in the requirements imposed upon functions $\vec{\mathbf{f}}_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}})$. These requirements may be phrased as periodic boundary conditions

$$\vec{\mathbf{f}}_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}}+\vec{\mathbf{e}}_i L) \;=\; \vec{\mathbf{f}}_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}}), \tag{3.55}$$ fq109

where L is the length of the edge of the cubic cavity and $\vec{\mathbf{e}}_i$ is a unit vector directed along one of the three orthogonal edges. Imposing this condition on the plane waves (fq97 3.49) we arrive at the quantization of the wave vector

$$\vec{\mathbf{k}} \;=\; \frac{2\pi}{L}\,\big(\, n_x\vec{\mathbf{e}}_x \;+\; n_y\vec{\mathbf{e}}_y \;+\; n_z\vec{\mathbf{e}}_z\,\big), \tag{3.56}$$ fq111

where n_x, n_y, n_z are triples of integers. Hence numbering of the plane wave modes by wave vector $\vec{\mathbf{k}}$ is fully equivalent to numbering by triples of integers. It is, however, important that the numbering of the modes, as discussed here, should not be mixed with photon numbers $n_{\vec{\mathbf{k}}\lambda}$ which are nonnegative integers and they number the states of the quantized field in the abstract Hilbert space of states of the type indicated in (fq83 3.42).

Finally we note that

$$\mathrm{rot}\,\vec{\mathbf{f}}_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}}) \;=\; i\,\left(\,\vec{\mathbf{k}}\times\vec{\mathbf{f}}_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}})\,\right). \tag{3.57}$$ fq113

which is necessary to express the magnetic induction according to Eq. (fq93m 3.47c).

3.4.3 Quantization in cubic box of volume V

Having discussed the main features of the plane wave representation of modes in the cubic cavity we can express the fields in this representation. Although we have already considered the vector potential (see (fq103 3.52) we collect all the results which follow from Eqs.(fq93 3.47) and from the above given discussion. Vector potential quantized in the cubic box of volume V is fq115

$$\vec{\mathbf{A}}_\perp(\vec{\mathbf{x}},t) = \sum_{\vec{\mathbf{k}}\lambda}\,\sqrt{\frac{\hbar}{2\epsilon_0\omega_k V}}\,\left[\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,a_{\vec{\mathbf{k}}\lambda}(t)\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;+\; \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\,a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right], \tag{3.58a}$$ fq1151

$$= \sum_{\vec{\mathbf{k}}\lambda}\,\frac{\mathcal{E}_k}{\omega_k}\,\left[\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,a_{\vec{\mathbf{k}}\lambda}(t)\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;+\; \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\,a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right]. \tag{3.58b}$$ fq1152

Transverse electric field (in Coulomb gauge) in the cubic box of volume V, fq117

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{x}},t) = i\,\sum_{\vec{\mathbf{k}}\lambda}\,\sqrt{\frac{\hbar\omega_k}{2\epsilon_0 V}}\,\left[\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,a_{\vec{\mathbf{k}}\lambda}(t)\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;-\; \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\,a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right], \tag{3.59a}$$ fq1171

$$= i\,\sum_{\vec{\mathbf{k}}\lambda}\,\mathcal{E}_k\,\left[\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,a_{\vec{\mathbf{k}}\lambda}(t)\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;-\; \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\,a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right]. \tag{3.59b}$$ fq1172

fq119 The corresponding magnetic field is of the form

$$\vec{\mathbf{B}}(\vec{\mathbf{x}},t) = i \sum_{\vec{\mathbf{k}}\lambda} \sqrt{\frac{\hbar}{2\epsilon_0\omega_k V}} \left[\left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right) a_{\vec{\mathbf{k}}\lambda}(t)\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} - \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\right) a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \right], \tag{3.60a}$$ fq1191

$$= i \sum_{\vec{\mathbf{k}}\lambda} \frac{\mathcal{E}_k}{\omega_k} \left[\left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right) a_{\vec{\mathbf{k}}\lambda}(t)\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} - \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\right) a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \right]. \tag{3.60b}$$ fq1192

In these equations we have introduced a useful and convenient notation

$$\mathcal{E}_k = \sqrt{\frac{\hbar\omega_k}{2\epsilon_0 V}}\,. \tag{3.61}$$ fq121

It is worth noting that operators of the electric field and magnetic induction are related as

$$\vec{\mathbf{B}} = \sum_{\vec{\mathbf{k}}\lambda} \frac{1}{\omega_k}\, \vec{\mathbf{k}}\times\vec{\mathbf{E}}_{\vec{\mathbf{k}}\lambda} \tag{3.62}$$ fq123

The Hamiltonian of the field in the plane wave representation has an obvious form

$$H_F = \sum_{\vec{\mathbf{k}}\lambda} \hbar\,\omega_k\, a^\dagger_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda}. \tag{3.63}$$ fq125

The eigenstates of this Hamiltonian are denoted similarly as in (3.42) fq83 the only difference being in numbering of the modes

$$|\,\{\, n_{\vec{\mathbf{k}}\lambda}\,\}\,\rangle = |\,\ldots,\, n_{\vec{\mathbf{k}}\lambda},\,\ldots\,\rangle = \bigotimes_{\vec{\mathbf{k}}\lambda} \frac{(\hat{a}^\dagger_{n_{\vec{\mathbf{k}}\lambda}})^{n_{\vec{\mathbf{k}}\lambda}}}{\sqrt{(n_{\vec{\mathbf{k}}\lambda})\,!}}\,|\,\Omega\,\rangle \tag{3.64}$$ fq127

For sake of completeness let us write the commutation relation for field operators. It obviously follows from (3.38) fq75 and now is of the form

$$\left[\, a_{\vec{\mathbf{k}}\lambda},\, a^\dagger_{\vec{\mathbf{k}}'\lambda'}\,\right] = \delta_{\vec{\mathbf{k}}\vec{\mathbf{k}}'}\,\delta_{\lambda\lambda'}, \tag{3.65}$$ fq129

where the first Kronecker delta is understood as a product of three deltas with indices following from the allowed values of the wave vector as in Eq.(3.56) fq111. The Hamiltonian (3.63) fq125 and commutation relations are sufficient to derive the Heisenberg equations of motion for field operators

$$\frac{d}{dt} a_{\vec{\mathbf{k}}\lambda} = -\frac{i}{\hbar}\left[\, a_{\vec{\mathbf{k}}\lambda},\, H_F\,\right] = -i\omega_k\, a_{\vec{\mathbf{k}}\lambda}. \tag{3.66}$$ fq131

This equation of motion obviously yields the solution

$$a_{\vec{\mathbf{k}}\lambda}(t) = a_{\vec{\mathbf{k}}\lambda}(t_0)\, e^{-i\omega_k(t-t_0)}. \tag{3.67}$$ fq133

Since annihilation and creation operators determine the dynamics (time evolution) of the fields, we see that after inserting (3.67) fq133 into expansions (3.58) fq115–(3.60) fq119 we obtain the fields as the combinations of plane waves.

3.4.4 Density of the modes

In many practical applications need to perform summations over allowed wave vectors and polarizations. We will consider this problem in more detail. Let us assume that we have to compute the sum

$$\sum_{\vec{\mathbf{k}}}\sum_{\lambda}\,(\dots), \tag{3.68}$$ fq135

of some function of summation variables. Summation is usually difficult, therefore we will show how to replace summation by integration.

In the $\vec{\mathbf{k}}$-space the allowed wave vectors are specified by points with integer coordinates (see (3.56)). The region of the volume of $(2\pi/L)^3$ around such a point is inaccessible for other wave vectors. Thus, the given volume determines the elementary cell in the $\vec{\mathbf{k}}$-space. Hence summation as in (3.68) corresponds to counting the number of points in $\vec{\mathbf{k}}$-space with weights specified by the summed function. The number of such points is equal to the volume in $\vec{\mathbf{k}}$ space divided by the volume of the elementary cell. Thus we can write fq137

$$\sum_{\vec{\mathbf{k}}}\sum_{\lambda}\,(\dots) = \sum_{\lambda}\,\frac{1}{(2\pi/L)^3}\int d\vec{\mathbf{k}}\,(\dots) \;=\; \sum_{\lambda}\,\frac{V}{(2\pi)^3}\int d\vec{\mathbf{k}}\,(\dots) \tag{3.69a}$$ fq137a

$$= \frac{V}{8\pi^3}\,\sum_{\lambda}\,\int_0^\infty k^2\,dk\int d\Omega_{\vec{\mathbf{k}}}\,(\dots) \tag{3.69b}$$ fq137b

where we expressed the last integral in spherical coordinates. We will apply this result to some practically important cases.

As a example, which can be easily adopted to practical problems, we consider the function $G_\lambda(\omega_k)$ which depends only on polarizations and the length of the wave vector $k = \omega_k/c$. Then in (3.69b) we can easily integrate over the angles. Changing the integration variable to ω_k we get

$$\sum_{\vec{\mathbf{k}},\lambda}\,G_\lambda(\omega_k) \quad\longrightarrow\quad \frac{V}{2\pi^2\,c^3}\,\sum_{\lambda}\,\int_0^\infty \omega_k^2\,d\omega_k\;G_\lambda(\omega_k) \tag{3.70}$$ fq139

As the second example, we go further and take the function $G(\omega_k)$ which depends only on the field frequency. The sum over polarizations in (3.70) can be performed and yield a factor 2 because there are two polarizations. Hence, we obtain

$$\sum_{\vec{\mathbf{k}},\lambda}\,G(\omega_k) \quad\longrightarrow\quad \frac{V}{\pi^2\,c^3}\,\sum_{\lambda}\,\int_0^\infty \omega_k^2\,d\omega_k\;G_\lambda(\omega_k), \tag{3.71}$$ fq141

which is sometimes written as

$$\sum_{\vec{\mathbf{k}},\lambda}\,G(\omega_k) \quad\longrightarrow\quad \int_0^\infty d\omega_k\;V\,\rho(\omega_k)\,G(\omega_k). \tag{3.72}$$ fq143

The introduced quantity $\rho(\omega_k)$ is given as

$$\rho(\omega_k) \;=\; \frac{\omega_k^2}{\pi^2\,c^3}, \tag{3.73}$$ fq145

an is called the density of the modes. It gives the number of modes of any polarization which lie within the frequency interval $(\omega_k,\ \omega_k + d\omega_k)$ per unit volume of the cavity. The notion of mode density is useful when we have to evaluate the integrals of the type given in (3.72).

3.4.5 Quantization in free space

Fields given above in terms of the plane waves in a cubic box by Eqs.(3.58)–(3.60), are in fact Fourier series. There is no difficulty in transforming Fourier series in the bounded region into Fourier integrals in the whole space. The quantity $(2\pi/L)^3 = 8\pi^3/V$ determines the elementary cell in the $\vec{\mathbf{k}}$-space (see the discussion in the previous section). This implies that the functions orthonormalized to Kronecker delta in the box by a constant $1/\sqrt{V}$ and summed over discrete $\vec{\mathbf{k}}$ will in the whole space be normalized by a factor $1/(2\pi)^{3/2}$ to Dirac delta and integrated over whole space of wave vectors. This procedure allows us to rewrite the above discrete expansions of the fields into Fourier integrals over whole $\vec{\mathbf{k}}$-space.
Vector potential quantized in free space with plane waves

$$\begin{aligned}\vec{\mathbf{A}}_\perp(\vec{\mathbf{x}},t) &= \sum_\lambda \int \frac{d^3k}{\sqrt{(2\pi)^3}}\ \sqrt{\frac{\hbar}{2\epsilon_0\omega_k}}\ \left[\ \vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\, a_{\vec{\mathbf{k}}\lambda}(t)\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ +\ \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\, a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ \right], \\ &= \sum_\lambda \int \frac{d^3k}{\sqrt{(2\pi)^3}}\ \frac{\mathcal{E}'_k}{\omega_k}\ \left[\ \vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\, a_{\vec{\mathbf{k}}\lambda}(t)\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ +\ \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\, a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ \right]. \qquad (3.74)\end{aligned}$$

fq147

Electric field (in Coulomb gauge) in this case is

$$\begin{aligned}\vec{\mathbf{E}}_\perp(\vec{\mathbf{x}},t) &= i\ \sum_\lambda \int \frac{d^3k}{\sqrt{(2\pi)^3}}\ \sqrt{\frac{\hbar\omega_k}{2\epsilon_0}}\ \left[\ \vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\, a_{\vec{\mathbf{k}}\lambda}(t)\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ -\ \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\, a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ \right], \\ &= i\ \sum_\lambda \int \frac{d^3k}{\sqrt{(2\pi)^3}}\ \mathcal{E}'_k\ \left[\ \vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\, a_{\vec{\mathbf{k}}\lambda}(t)\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ -\ \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\, a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ \right]. \qquad (3.75)\end{aligned}$$

fq149

Corresponding magnetic field

$$\begin{aligned}\vec{\mathbf{B}}(\vec{\mathbf{x}},t) &= i\ \sum_\lambda \int \frac{d^3k}{\sqrt{(2\pi)^3}}\ \sqrt{\frac{\hbar}{2\epsilon_0\omega_k}}\ \Big[\ \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right)\ a_{\vec{\mathbf{k}}\lambda}(t)\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \\ &\qquad - \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\right)\ a^\dagger_{\vec{\mathbf{k}}\lambda}(t)\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ \Big], \\ &= i\ \sum_\lambda \int \frac{d^3k}{\sqrt{(2\pi)^3}}\ \frac{\mathcal{E}'_k}{\omega_k}\ \Big[\ \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right)\ a_{\vec{\mathbf{k}}\lambda}(t) e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \\ &\qquad -\ \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\right)\ a^\dagger_{\vec{\mathbf{k}}\lambda}(t) e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\ \Big], \qquad (3.76)\end{aligned}$$

fq151

We have also introduced a useful notation

$$\mathcal{E}'_k\ =\ \sqrt{\frac{\hbar\omega_k}{2\epsilon_0}}\,. \qquad (3.77)$$

fq153

The relation between the electric field and magnetic induction (3.62) still holds, but the sum is replaced by the integral. Similarly the commutation relation for annihilation

and creation operators now reads

$$\left[\, a_{\vec{\mathbf{k}}\lambda},\; a^{\dagger}_{\vec{\mathbf{k}}'\lambda'} \,\right] \;=\; \delta(\vec{\mathbf{k}}-\vec{\mathbf{k}}')\,\delta_{\lambda\lambda'}, \tag{3.78}$$ fq155

The Hamiltonian of the field in the plane wave representation has now the integral form

$$H_{field} \;=\; \int d\vec{\mathbf{k}}\;\hbar\,\omega_k\, a^{\dagger}_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda}. \tag{3.79}$$ fq157

The eigenstates of this Hamiltonian are denoted as in (3.64) fq127 only the tensor product is now performed over the continuous variable.

3.5 Equations of motion – Maxwell's equations

We work in the Coulomb gauge, that is div $\vec{\mathbf{A}} = 0$. This ensures that two homogeneous Maxwell's equations (for vacuum, in absence of sources)

$$\operatorname{div}\vec{\mathbf{B}} = 0, \qquad\qquad \operatorname{div}\vec{\mathbf{E}} = 0, \tag{3.80}$$ fq159

are automatically satisfied, which is due to the definitions (3.3) fq05. It remains to check that two other Maxwell's equations are satisfied.

Let us first check that $\operatorname{rot}\vec{\mathbf{E}} = -\partial\vec{\mathbf{B}}/\partial t$. We first calculate rotation of the electric field. Taking the field as in (3.59b) fq1172, using relation (3.57) fq113 and its complex conjugate, we get

$$\operatorname{rot}\vec{\mathbf{E}}_{\perp}(\vec{\mathbf{x}},t) \;=\; -\sum_{\vec{\mathbf{k}}\lambda}\mathcal{E}_k\left[\left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right) a_{\vec{\mathbf{k}}\lambda}\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;+\; \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\right) a^{\dagger}_{\vec{\mathbf{k}}\lambda}\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\right]. \tag{3.81}$$ fq161

On the other hand, computing the time derivative of $\vec{\mathbf{B}}$ we take Eq.(3.60) fq119 and we see that the only time dependence in the right-hand side may enter via annihilation and creation operators. Then using Eq.(3.66) fq131 and its hermitian conjugate we obtain

$$\begin{aligned}\frac{\partial\vec{\mathbf{B}}}{\partial t} &= i\sum_{\vec{\mathbf{k}}\lambda}\frac{\mathcal{E}_k}{\omega_k}\left[\left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right)\left(-i\,\omega_k\, a_{\vec{\mathbf{k}}\lambda}\right) e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;-\; \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\right)\left(i\,\omega_k\, a^{\dagger}_{\vec{\mathbf{k}}\lambda}\right) e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\right], \\ &= \sum_{\vec{\mathbf{k}}\lambda}\mathcal{E}_k\left[\left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right) a_{\vec{\mathbf{k}}\lambda}\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;+\; \left(\vec{\mathbf{k}}\times\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\right) a^{\dagger}_{\vec{\mathbf{k}}\lambda}\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\right]. \end{aligned} \tag{3.82}$$ fq163

Comparing rhs of the last two equations we see that the Maxwell's equation $\operatorname{rot}\vec{\mathbf{E}}_{\perp} = -\partial\vec{\mathbf{B}}/\partial t$ is indeed satisfied.

Thus it remains to check the fourth Maxwell's equation, namely

$$\frac{\partial\vec{\mathbf{E}}_{\perp}}{\partial t} \;=\; c^2\operatorname{rot}\vec{\mathbf{B}} \tag{3.83}$$ fq165

We compute left-hand side by differentiating Eq.(3.59) fq117 over time and taking into account relations (3.66) fq131. We get, similarly as in (3.82) fq163:

$$\frac{\partial\vec{\mathbf{E}}_{\perp}(\vec{\mathbf{x}},t)}{\partial t} \;=\; c^2\sum_{\vec{\mathbf{k}}\lambda}\frac{\mathcal{E}_k}{\omega_k}\,k^2\left[\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\, a_{\vec{\mathbf{k}}\lambda}\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;+\; \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\, a^{\dagger}_{\vec{\mathbf{k}}\lambda}\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right], \tag{3.84}$$ fq167

where we have used the dispersion relation: $\omega_k = ck$. Now we proceed to compute the rotation of the magnetic induction.

$$\mathrm{rot}\,\vec{\mathbf{B}}(\vec{\mathbf{x}},t) \;=\; i\sum_{\vec{\mathbf{k}}\lambda}\frac{\mathcal{E}_k}{\omega_k}\,\mathrm{rot}\,\Big[\,\Big(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\Big)\,a_{\vec{\mathbf{k}}\lambda}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;-\; \Big(\vec{\mathbf{k}}\times\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\Big)\,a^{\dagger}_{\vec{\mathbf{k}}\lambda}\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\Big], \quad (3.85)$$ fq169

To find the rotation we need the expression $\mathrm{rot}\,\big[\Big(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\Big)\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\big]$. So we compute it.

$$\begin{aligned}
\mathrm{rot}\,\big[\Big(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\Big)\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\big]_a &= \varepsilon_{abc}\,\partial_b\,\big[\Big(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\Big)_c\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\big]\\
&= \varepsilon_{abc}\varepsilon_{cmn}\,\partial_b\,\big[k_m\,\big(\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\big)_n\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\big]\\
&= \big(\delta_{am}\,\delta_{bn}-\delta_{an}\,\delta_{bm}\big)\,i\,k_m\big(\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\big)_n\,k_b\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\\
&= i\,\Big[k_a\,\Big(\vec{\mathbf{k}}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\Big) \;-\; \big(\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\big)_a\,\Big(\vec{\mathbf{k}}\cdot\vec{\mathbf{k}}\Big)\Big]]e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}. \qquad (3.86)
\end{aligned}$$ fq171

Since polarization vectors and wave vector are orthogonal, the first term vanishes, and we finally obtain

$$\mathrm{rot}\,\big[\Big(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\Big)\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\big]_a \;= -i\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,k^2\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \qquad (3.87)$$ fq173

We use the obtained relation and its complex conjugate in (3.85), this yields rotation of the magnetic induction

$$\mathrm{rot}\;\vec{\mathbf{B}}(\vec{\mathbf{x}},t) \;=\; \sum_{\vec{\mathbf{k}}\lambda}\frac{\mathcal{E}_k}{\omega_k}\,k^2\,\Big[\,\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\,a_{\vec{\mathbf{k}}\lambda}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;+\; \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\,a^{\dagger}_{\vec{\mathbf{k}}\lambda}\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\Big] \qquad (3.88)$$ fq175

Comparing Eqs.(3.84) and the last one we see that the Maxwell's equation (3.83) is indeed satisfied.

We conclude this section by stating that the Maxwell's equations are satisfied by the quantized field (in the cubic cavity). Checking that this is so also in a general case is much more tedious, but nevertheless can be done along the same lines. On the other hand Maxwell's equations are equivalent to Heisenberg equations of motion for field operators. This follows, since we used (3.66) in the derivation, and the latter equations are just the Heisenberg ones for annihilation and creation operators.

* *

Chapter 4

States of quantized electromagnetic fields

c:fs

Quantization of the electromagnetic field has led us to the so-called Fock space (fq127 3.64), that is to the states

$$|\{ n_{\vec{\mathbf{k}}\lambda} \}\rangle = | \ldots, n_{\vec{\mathbf{k}}\lambda}, \ldots \rangle = \bigotimes_{\vec{\mathbf{k}}\lambda} \frac{(\hat{a}^\dagger_{n_{\vec{\mathbf{k}}\lambda}})^{n_{\vec{\mathbf{k}}\lambda}}}{\sqrt{(n_{\vec{\mathbf{k}}\lambda})!}} |\Omega\rangle \tag{4.1}$$ f1s01

where $|\Omega\rangle$ is a vacuum state specified by a sequence of zeroes – no photons in any of the allowed modes, which are numbered by the wave vector $\vec{\mathbf{k}}$ and polarization index $\lambda = 1, 2$. Each of such states is specified by a sequence of nonnegative integers. Obviously, these photon number states are the eigenstates of the Hamiltonian H_F given in (fq125 3.63).

4.1 Introduction and general discussion

4.1.1 Vacuum state

It is natural to consider the vacuum state $|\Omega\rangle$ as the first one. Since vacuum state can be defined by the relation $a_{\vec{\mathbf{k}}\lambda}|\Omega\rangle = 0$ or $\langle\Omega|a^\dagger_{\vec{\mathbf{k}}\lambda} = 0$, we easily see that the vacuum expectation values of the vector potential $\vec{\mathbf{A}}\perp$ (fq115 3.58), electric field $\vec{\mathbf{E}}_\perp$ (fq117 3.59) and magnetic field $\vec{\mathbf{B}}$ (fq119 3.60) all vanish

$$\langle\Omega|\vec{\mathbf{A}}_\perp|\Omega\rangle = 0, \qquad \langle\Omega|\vec{\mathbf{E}}_\perp|\Omega\rangle = 0, \qquad \langle\Omega|\vec{\mathbf{B}}|\Omega\rangle = 0. \tag{4.2}$$ f1s04

On the other hand, expectation values of the intensities, that is of the squares of the fields do not vanish in the vacuum state. Let us compute the expectation value of the square of the electric field (which is a Hermitian operator). Using (fq117 3.59) we get

$$\langle\Omega|\vec{\mathbf{E}}^2_\perp|\Omega\rangle = -\sum_{\vec{\mathbf{k}}\lambda}\sum_{\vec{\mathbf{k}}'\lambda'} \frac{\hbar\sqrt{\omega_k\omega_{k'}}}{2\epsilon_0 V} \langle\Omega| \Big(\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\, \hat{a}_{\vec{\mathbf{k}}\lambda}\, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} - \vec{\mathbf{e}}^*_{\vec{\mathbf{k}}\lambda}\, \hat{a}^\dagger_{\vec{\mathbf{k}}\lambda}\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \Big)$$
$$\Big(\vec{\mathbf{e}}_{\vec{\mathbf{k}}'\lambda'}\, \hat{a}_{\vec{\mathbf{k}}'\lambda'}\, e^{i\vec{\mathbf{k}}'\cdot\vec{\mathbf{x}}} - \vec{\mathbf{e}}^*_{\vec{\mathbf{k}}'\lambda'}\, \hat{a}^\dagger_{\vec{\mathbf{k}}'\lambda'}\, e^{-i\vec{\mathbf{k}}'\cdot\vec{\mathbf{x}}} \Big) |\Omega\rangle. \tag{4.3}$$ f1s5a

We stress that the fields $\vec{\mathbf{E}}_\perp$ are both taken at the same space-time point $(\vec{\mathbf{x}}, t)$. By straightforward multiplication we get

$$\begin{aligned}\langle\,\Omega\,|\,\vec{\mathbf{E}}_\perp^2\,|\,\Omega\,\rangle \;=\; -\sum_{\vec{\mathbf{k}}\lambda}\sum_{\vec{\mathbf{k}}'\lambda'}\frac{\hbar\sqrt{\omega_k\omega_{k'}}}{2\epsilon_0 V}\,\langle\,\Omega\,|\,\Big\{\;&\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}'\lambda'}\,\hat{a}_{\vec{\mathbf{k}}\lambda}\,\hat{a}_{\vec{\mathbf{k}}'\lambda'}\,e^{i(\vec{\mathbf{k}}+\vec{\mathbf{k}}')\cdot\vec{\mathbf{x}}}\\ &-\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}'\lambda'}\,\hat{a}_{\vec{\mathbf{k}}\lambda}\,\hat{a}^\dagger_{\vec{\mathbf{k}}'\lambda'}\,e^{i(\vec{\mathbf{k}}-\vec{\mathbf{k}}')\cdot\vec{\mathbf{x}}}\\ &-\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}'\lambda'}\,\hat{a}^\dagger_{\vec{\mathbf{k}}\lambda}\,\hat{a}_{\vec{\mathbf{k}}'\lambda'}\,e^{-i(\vec{\mathbf{k}}-\vec{\mathbf{k}}')\cdot\vec{\mathbf{x}}}\\ &+\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}'\lambda'}\,\hat{a}^\dagger_{\vec{\mathbf{k}}\lambda}\,\hat{a}^\dagger_{\vec{\mathbf{k}}'\lambda'}\,e^{-i(\vec{\mathbf{k}}+\vec{\mathbf{k}}')\cdot\vec{\mathbf{x}}}\Big\}\,|\,\Omega\,\rangle. \qquad (4.4)\end{aligned}$$ f1s5b

The first term vanishes, since each of the annihilation operators acting on $|\,\Omega\,\rangle$ yields zero. The same applies to the last (fourth) term (only it acts on the right, that is on $\langle\,\Omega\,|$). So the nonzero contribution is at most due to two terms only, and we get

$$\begin{aligned}\langle\,\Omega\,|\,\vec{\mathbf{E}}_\perp^2\,|\,\Omega\,\rangle \;=\; \sum_{\vec{\mathbf{k}}\lambda}\sum_{\vec{\mathbf{k}}'\lambda'}\frac{\hbar\sqrt{\omega_k\omega_{k'}}}{2\epsilon_0 V}\,\langle\,\Omega\,|\,\Big\{\;&\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}'\lambda'}\,\hat{a}_{\vec{\mathbf{k}}\lambda}\,\hat{a}^\dagger_{\vec{\mathbf{k}}'\lambda'}\,e^{i(\vec{\mathbf{k}}-\vec{\mathbf{k}}')\cdot\vec{\mathbf{x}}}\\ &+\vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}'\lambda'}\,\hat{a}^\dagger_{\vec{\mathbf{k}}\lambda}\,\hat{a}_{\vec{\mathbf{k}}'\lambda'}\,e^{-i(\vec{\mathbf{k}}-\vec{\mathbf{k}}')\cdot\vec{\mathbf{x}}}\Big\}\,|\,\Omega\,\rangle. \qquad (4.5)\end{aligned}$$ f1s5c

The diagonal terms behave differently than off-diagonal. Let us discuss the latter ones first. If $\vec{\mathbf{k}} \neq \vec{\mathbf{k}}'$ and/or $\lambda \neq \lambda'$ then operators $\hat{a}_{\vec{\mathbf{k}}\lambda}$ and $\hat{a}^\dagger_{\vec{\mathbf{k}}'\lambda'}$ commute. So we can move annihilation operators to the right and then these operators act on vacuum state giving zeroes. The conclusion is that all off-diagonal terms vanish, do not contribute. Non-zero contribution may arise only due to diagonal terms with $\vec{\mathbf{k}} = \vec{\mathbf{k}}'$ and $\lambda = \lambda'$. The double sum reduces to a single one. Thus (4.5) reduces to

$$\langle\,\Omega\,|\,\vec{\mathbf{E}}_\perp^2\,|\,\Omega\,\rangle \;=\; \sum_{\vec{\mathbf{k}}\lambda}\frac{\hbar\omega_k}{2\epsilon_0 V}\,\langle\,\Omega\,|\,\Big\{\;a_{\vec{\mathbf{k}}\lambda}a^\dagger_{\vec{\mathbf{k}}\lambda}\;+\;a^\dagger_{\vec{\mathbf{k}}\lambda}a_{\vec{\mathbf{k}}\lambda}\Big\}\,|\,\Omega\,\rangle, \qquad (4.6)$$ f1s5d

because exponential factors give unity and so do the products of polarization vectors (see (3.54)). Due to canonical commutation relation we finally arrive at an expression

$$\langle\,\Omega\,|\,\vec{\mathbf{E}}_\perp^2\,|\,\Omega\,\rangle \;=\; \sum_{\vec{\mathbf{k}}\lambda}\frac{\hbar\omega_k}{2\epsilon_0 V}\,\langle\,\Omega\,|\,\Big\{2a^\dagger_{\vec{\mathbf{k}}\lambda}a_{\vec{\mathbf{k}}\lambda}\;+\;1\Big\}\,|\,\Omega\,\rangle,\;\;=\;\sum_{\vec{\mathbf{k}}\lambda}\frac{\hbar\omega_k}{2\epsilon_0 V}. \qquad (4.7)$$ f1s5f

Very similar calculation can be performed for the magnetic field $\vec{\mathbf{B}}$ specified in (3.60). The only difference consists in different vectorial factors. The argument about annihilation and creation operators in diagonal and off-diagonal terms remains unchanged. The sum reduces to a single one and we have to consider the vector products. It is easy to show that

$$(\vec{\mathbf{k}}\times\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda})^2 \;=\; \vec{\mathbf{k}}^2\;\vec{\mathbf{e}}^{\,2}_{\vec{\mathbf{k}}\lambda} - (\vec{\mathbf{k}}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda})^2 \;=\; \vec{\mathbf{k}}^2, \qquad (4.8)$$ f1s6a

where the second term vanishes due to transversality of the field (3.53), so the vectorial products reduces to $\vec{\mathbf{k}}^2$. Therefore, the expectation value of the square of the magnetic field follows in exactly the same manner as that for electric field, yielding

$$\langle\,\Omega\,|\,\vec{\mathbf{B}}^2\,|\,\Omega\,\rangle \;=\; \sum_{\vec{\mathbf{k}}\lambda}\frac{\hbar\vec{\mathbf{k}}^2}{2\epsilon_0\omega_k V} \;\;=\;\sum_{\vec{\mathbf{k}}\lambda}\frac{\hbar\omega_k}{2\epsilon_0 V c^2}, \qquad (4.9)$$ f1s6b

because (see (3.50)) we have the dispersion relation $\omega_k = |\vec{\mathbf{k}}|\, c$. Due to dispersion relation, both quantities $\langle\, \Omega \,|\, \vec{\mathbf{E}}_\perp^2 \,|\, \Omega \,\rangle$ and $\langle\, \Omega \,|\, \vec{\mathbf{B}}^2 \,|\, \Omega \,\rangle$, in principle, diverge with growing $\vec{\mathbf{k}}$.

In our considerations we use nonrelativistic approach, so we do not allow for creation or destruction of material particles. Hence the energy range in which we work must be restricted to energies less than $m_e c^2$, where m_e is the electron rest mass. Or, in other words, nonrelativistic approach becomes invalid for frequencies approaching $\omega_{_M} = m_e c^2/\hbar$. Hence we can limit the energies by introducing the frequency cut-off equal to $\omega_{_M}$. Adopting such a limit we see that our expressions (4.7) and (4.9) contain summations over all modes but concern the functions of frequency only. Thus we can use the summation prescription (3.72) and we can expressed the obtained expectation values as

$$\langle\, \Omega \,|\, \vec{\mathbf{E}}_\perp^2 \,|\, \Omega \,\rangle \;=\; c^2 \,\langle\, \Omega \,|\, \vec{\mathbf{B}}^2 \,|\, \Omega \,\rangle \;=\; \int_0^{\omega_{_M}} d\omega \;\frac{\omega^2}{\pi^2 c^3}\;\frac{\hbar\omega}{2\epsilon_0}. \tag{4.10}$$ f1s7

Hence, the these expectation values diverge as $\omega_{_M}^4$. Since the averages (4.2) vanish, the corresponding variances are equal to the expectation values (4.10), so the variances are also divergent as $\omega_{_M}^4$. This is typical (purely quantum) problem with vacuum fields. The procedure of renormalization is aimed at removal of the divergencies, but it is a subject which we will not consider here.

4.1.2 Photon number states

The states (4.1) introduced previously are called photon number states. So they are the eigenstates of the hamiltonian (3.63) with eigenvalues $E_{\vec{\mathbf{k}}\lambda} = \sum_{\vec{\mathbf{k}}\lambda} \hbar\omega_k n_{\vec{\mathbf{k}}\lambda}$. It is easy to argue that when the field is in the photon number state the expectation values of the field operators (3.58)–(3.60) are

$$\langle\, \{n_{\vec{\mathbf{k}}\lambda}\} \,|\, \vec{\mathbf{A}} \,|\, \{n_{\vec{\mathbf{k}}\lambda}\} \,\rangle \;=\; \langle\, \{n_{\vec{\mathbf{k}}\lambda}\} \,|\, \vec{\mathbf{E}}_\perp \,|\, \{n_{\vec{\mathbf{k}}\lambda}\} \,\rangle \;=\; \langle\, \{n_{\vec{\mathbf{k}}\lambda}\} \,|\, \vec{\mathbf{B}} \,|\, \{n_{\vec{\mathbf{k}}\lambda}\} \,\rangle \;=\; 0, \tag{4.11}$$ f1s11

which follows directly from the fact that $\hat{a}_{\vec{\mathbf{k}}\lambda}$ lowers and $a^\dagger_{\vec{\mathbf{k}}\lambda}$ raises the number of photons, while states with different photon numbers (different eigenstates of $H_{_F}$) are orthogonal.

The expectation values of the squares of the fields can be computed in an exactly the same manner as for vacuum state. Computation for the average of $\vec{\mathbf{E}}_\perp^2$ in the vacuum state was, up to the first part of eq.(4.7), done in a quite a general manner. Thus, it is sufficient to replace $|\, \Omega \,\rangle$ by $|\, \{n_{\vec{\mathbf{k}}\lambda}\} \,\rangle$, and we get

$$\begin{aligned}\langle\, \{n_{\vec{\mathbf{k}}\lambda}\} \,|\, \vec{\mathbf{E}}_\perp^2 \,|\, \{n_{\vec{\mathbf{k}}\lambda}\} \,\rangle &= \sum_{\vec{\mathbf{k}}\lambda} \;\frac{\hbar\omega_k}{2\epsilon_0 V}\; \langle\, \{n_{\vec{\mathbf{k}}\lambda}\} \,|\, \Big\{ 2a^\dagger_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda} \;+\; 1 \Big\} \,|\, \{n_{\vec{\mathbf{k}}\lambda}\} \,\rangle, \\ &= \sum_{\vec{\mathbf{k}}\lambda} \;\frac{\hbar\omega_k}{2\epsilon_0 V}\; (2n_{\vec{\mathbf{k}}\lambda} + 1). \end{aligned} \tag{4.12}$$ f1s12

We note that terms such as $a_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda}$ do not contribute in this case due to orthonormality of the states with unequal photon numbers. Obviously the expression for the expectation value of $\vec{\mathbf{B}}^2$ is the same as (4.12) only divided by an additional factor c^2. We shall return to the discussion of this results in a more specific case of a single mode field.

At present we will add only several comments. The variances of the fields follow immediately from two previous formulas. We obtain

$$\sigma^2(\vec{\mathbf{E}}_\perp) \;=\; \sum_{\vec{\mathbf{k}}\lambda} \frac{\hbar\omega_k}{2\epsilon_0 V}\,(2n_{\vec{\mathbf{k}}\lambda}+1) \;=\; c^2\,\sigma^2(\vec{\mathbf{B}}) \tag{4.13}$$ f1s14

Certainly, we encounter here the same problems with divergencies, so again we can consider the cut-off frequency ω_M. Finally, we note that photon number states (eigenstates of H_F) are stationary ones. Therefore, all expectation values are time independent. This is strictly nonclassical, because in the classical picture the fields are quantities oscillating in time. We can view the photon number states as states of well-defined amplitude of the oscillations, but with completely undetermined phase, hence the fields average out to zero as in (4.11). f1s11

4.1.3 Single mode field

It is possible to consider a multimode field, just as we have done in the previous section, that is a field in which many modes specified by $(\vec{\mathbf{k}},\lambda)$ are occupied – many numbers $n_{\vec{\mathbf{k}},\lambda}$ are nonzero. However, the field may be viewed as a Fourier series, or linear combination of many modes. Thus, it is frequently sufficient to consider only one (single) mode, while the generalizations to many modes usually poses no difficulties.

For these reason, and also for reason of simplicity, we will now consider only a single mode of the quantized electromagnetic field. Hence, we drop the indices denoting the modes and from (3.58)–(3.60) we have the fields given by single terms, as fq115 fq119 f2s01

$$\vec{\mathbf{A}}_\perp(\vec{\mathbf{x}},t) = \sqrt{\frac{\hbar}{2\epsilon_0\omega V}}\;\vec{\mathbf{e}}\left[\,\hat{a}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;+\; \hat{a}^\dagger\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right], \tag{4.14a}$$ f2s01a

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{x}},t) = i\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\;\vec{\mathbf{e}}\left[\,\hat{a}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;-\; \hat{a}^\dagger\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right], \tag{4.14b}$$ f2s01b

$$\vec{\mathbf{B}}(\vec{\mathbf{x}},t) = i\sqrt{\frac{\hbar}{2\epsilon_0\omega V}}\;(\vec{\mathbf{k}}\times\vec{\mathbf{e}})\left[\,\hat{a}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;-\; \hat{a}^\dagger\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\right], \tag{4.14c}$$ f2s01c

where we assumed the polarization vector $\vec{\mathbf{e}}$ to be real.

The physical state of the field is specified by the n-photon state $|\,n\,\rangle$. We note that the vacuum state $|\,\Omega\,\rangle$ corresponds to $n=0$. The results of previous section can be specified to fit the present needs. In particular, the expectation values for the field follow from (4.11) and in this special case they are f1s11

$$\langle\,n\,|\,\vec{\mathbf{A}}_\perp\,|\,n\,\rangle \;=\; \langle\,n\,|\,\vec{\mathbf{E}}_\perp\,|\,n\,\rangle \;=\; \langle\,n\,|\,\vec{\mathbf{B}}\,|\,n\,\rangle \;=\; 0, \tag{4.15}$$ f2s02

where $n=0$, corresponding to vacuum, is also allowed. Similarly, for the expectation value of the square of the field, from (4.12) we get f1s12

$$\langle\,n\,|\,\vec{\mathbf{E}}_\perp^2\,|\,n\,\rangle \;=\; \frac{\hbar\omega}{2\epsilon_0 V}\,(2n\;+\;1) \tag{4.16}$$ f2s03

This is not unexpected. The expression $\epsilon_0\langle\,\vec{\mathbf{E}}^2\,\rangle/2$ gives half of the energy density of the field. Since we use oscillator analogy, we see that result (4.16) is indeed proportional to f2s03

energy density. However, for the field in the n-state the expectation value of the field amplitude is zero (see (4.15)). This may be explained by saying that photons can have any phases, so that the field averages out to zero. Energy is phase independent, hence the non-zero result (4.16).

Before proceeding, let us recall the identifications (3.30), namely

$$q \;=\; \sqrt{\frac{\hbar}{2\omega}}\,\left(\,\hat{a}\;+\;\hat{a}^\dagger\,\right), \qquad\qquad p \;=\; -\,i\,\sqrt{\frac{\hbar\,\omega}{2}}\,\left(\,\hat{a}\;-\;\hat{a}^\dagger\,\right), \tag{4.17}$$

which immediately yield expectation values in n-state

$$\langle\, q\,\rangle_n \;=\; \langle\, n\,|\,q\,|\,n\,\rangle \;=\; 0, \qquad\qquad \langle\, p\,\rangle_n \;=\; \langle\, n\,|\,p\,|\,n\,\rangle \;=\; 0. \tag{4.18}$$

The expectation values of the squares are also easy to compute, and we get

$$\langle\, q^2\,\rangle_n = \langle\, n\,|\,q^2\,|\,n\,\rangle \;=\; \frac{\hbar}{2\omega}\,\langle\, n\,|\,\left(\hat{a}+\hat{a}^\dagger\right)^2\,|\,n\,\rangle \;=\; \frac{\hbar}{2\omega}\,(2n+1) \tag{4.19a}$$

$$\langle\, p^2\,\rangle_n = \langle\, n\,|\,p^2\,|\,n\,\rangle \;=\; -\,\frac{\hbar\omega}{2}\,\langle\, n\,|\,\left(\hat{a}-\hat{a}^\dagger\right)^2\,|\,n\,\rangle \;=\; \frac{\hbar\omega}{2}\,(2n+1) \tag{4.19b}$$

The quantum averages (4.18) vanish, so the above expectations are equal to variances, eg. $\sigma_n^2(q) = \langle\, q^2\,\rangle_n$, and similarly for p. Therefore the product of variances becomes

$$\sigma_n^2(q)\,\sigma_n^2(p) \;=\; \frac{\hbar^2}{4}\,(2n+1)^2 \;\geq\; \frac{\hbar^2}{4} \tag{4.20}$$

Since $[\,q,\;p\,] = i\hbar$, the last inequality follows from Heisenberg uncertainty relation for noncommuting observables. We see that even for the vacuum state ($n = 0$) the product of variances satisfies the uncertainty principle, which for $n \geq 1$ is satisfied as a "real–sharp" inequality.

Therefore, an important question arises: can we construct fields such, that the uncertainty principle is minimized ?

4.2 Coherent states (single mode)

Coherent states are the states which answer to the given question. We shall introduce these states in a formal manner and we will investigate their properties.

The coherent state $|\,z\,\rangle$ is defined as the normalized eigenstate of the annihilation operator

$$\hat{a}|\,z\,\rangle \;=\; z|\,z\,\rangle, \quad z\in\mathbb{C}, \qquad\qquad \langle\, z\,|\,z\,\rangle \;=\; 1. \tag{4.21}$$

Annihilation operator is not hermitian, so we do not *a priori* know whether states $|\,z\,\rangle$ and $|\,\xi\,\rangle$ are orthogonal.

4.2.1 Expansion in n-photon states

Fock states, that is n-photon states, are complete and orthonormal (they are eigenstates of hermitian operator $\hat{n} = \hat{a}^\dagger\hat{a}$). Thus, any state can be expanded as

$$|\,z\,\rangle \;=\; \sum_{n=0}^{\infty}|\,n\,\rangle\langle\, n\,|\,z\,\rangle \;=\; \sum_{n=0}^{\infty}|\,n\,\rangle\,C_n(z). \tag{4.22}$$

$C_n(z)$ are probability amplitudes, that for the field in coherent state $|\,z\,\rangle$ we will find it in the n-photon state. Applying the annihilation operator to both sides we get

$$\hat{a}\,|\,z\,\rangle \;=\; \sum_{n=0}^{\infty}\sqrt{n}\;|\,n-1\,\rangle\,C_n(z) \;=\; \sum_{n=0}^{\infty}\sqrt{n+1}\;|\,n\,\rangle\,C_{n+1}(z), \tag{4.23}$$ f2s12

where in the second equality we have renumbered the series. On the other hand, from (4.22) f2s11 we obtain

$$\hat{a}\,|\,z\,\rangle \;=\; z\,|\,z\,\rangle \;=\; \sum_{n=0}^{\infty} z\,|\,n\,\rangle\,C_n(z). \tag{4.24}$$ f2s13

Comparing rhs of two last formulas we arrive at the recurrence relation

$$C_{n+1}(z) \;=\; \frac{z}{\sqrt{n+1}}\,C_n(z), \tag{4.25}$$ f2s14

which easily gives the probability amplitude

$$C_n(z) \;=\; \frac{z^n}{\sqrt{n!}}\,C_0(z), \tag{4.26}$$ f2s15

so it remains to compute $C_0(z)$. This is done by invoking the normalization requirement. From expansion (4.22) f2s11 after insertion of (4.26) f2s15 we have

$$\begin{aligned} 1 \;&=\; \langle\,z\,|\,z\,\rangle = |C_0(z)|^2\sum_{m,n=0}^{\infty}\frac{(z^*)^m z^n}{\sqrt{n!\,m!}}\,\langle\,m\,|\,n\,\rangle \\ &= |C_0(z)|^2\sum_{n=0}^{\infty}\frac{|z|^{2n}}{n!} \;=\; |C_0(z)|^2\;e^{|z|^2}, \end{aligned} \tag{4.27}$$ f2s16

where we used orthonormality of the n-states. Adopting zero phase we get $C_0(z) = \exp(-|z|^2/2)$. Hence, the final form of the expansion of the coherent state $|\,z\,\rangle$ in the n-states becomes

$$|\,z\,\rangle \;=\; \exp(-|z|^2/2)\;\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,|\,n\,\rangle. \tag{4.28}$$ f2s17

We note that the vacuum state $|\,\Omega\,\rangle$ is the coherent state corresponding to $z = 0$. The expansion coefficients give probability

$$P_n(z) \;=\; |C_n|^2 \;=\; \exp(-|z|^2)\,\frac{|z|^{2n}}{n!}, \tag{4.29}$$ f2s18

which is the Poisson distribution with mean $\langle\,n\,\rangle_z = |z|^2$. Indeed, it is straightforward to check that the average number of photons for the field in the coherent state $|\,z\,\rangle$ is given as

$$\langle\,n\,\rangle_z \;=\; \langle\,z\,|\,\hat{a}^\dagger\hat{a}\,|\,z\,\rangle \;=\; \|\,\hat{a}|\,z\,\rangle\,\|^2 \;=\; |z|^2, \tag{4.30}$$ f2s19

as it follows from the definition (4.21) f2s10.

4.2.2 Scalar product $\langle\, z \,|\, \xi \,\rangle$

Employing expansions (4.28) for two coherent states we can write

$$\langle\, z \,|\, \xi \,\rangle \;=\; \exp\left(-\frac{|z|^2}{2}-\frac{|\xi|^2}{2}\right)\sum_{m,n=0}^{\infty}\frac{(z^*)^n\xi^m}{\sqrt{m!\,n!}}\,\langle\, n \,|\, m \,\rangle, \tag{4.31}$$

f2s20a

and due to orthonormality of n-states we get

$$\langle\, z \,|\, \xi \,\rangle \;=\; \exp\left(-\frac{|z|^2}{2}-\frac{|\xi|^2}{2}+z^*\xi\right). \tag{4.32}$$

f2s20b

The obtained relation immediately entails

$$|\langle\, z \,|\, \xi \,\rangle|^2 \;=\; \exp\left(-|z|^2-|\xi|^2+z^*\xi+z\xi^*\right) \;=\; \exp\left(-|z-\xi|^2\right). \tag{4.33}$$

f2s21

The bigger the difference between two complex numbers z and ξ, two coherent states become "more orthogonal".

4.2.3 Completeness of coherent states

Complex numbers which parameterize coherent states span a two-dimensional space with continuous variable. Thus it seems natural to investigate the operator

$$\begin{aligned}\int d^2z\;|\, z \,\rangle\langle\, z \,| &= \int d^2z\;\; e^{-|z|^2}\sum_{m,n=0}^{\infty}\frac{(z^*)^n z^m}{\sqrt{m!\,n!}}\;|\, m \,\rangle\langle\, n \,| \\ &= \sum_{m,n=0}^{\infty}\frac{|\, m \,\rangle\langle\, n \,|}{\sqrt{m!\,n!}}\int d^2z\;\; e^{-|z|^2}\,(z^*)^n z^m\end{aligned} \tag{4.34}$$

f2s22

Taking the polar coordinates in the complex plane, we transform the integral and we obtain

$$\begin{aligned}\int d^2z\;\; e^{-|z|^2}\,(z^*)^n z^m &= \int_0^{\infty} dr\;\; r^{m+n+1}\,e^{-r^2}\int_0^{2\pi} d\varphi\; e^{i(m-n)\varphi} \\ &= 2\pi\,\delta_{mn}\int_0^{\infty} dr\;\; r^{m+n+1}\,e^{-r^2} \;=\; \pi\,\delta_{mn}\,n!\end{aligned} \tag{4.35}$$

f2s23

Using this result in the operator (4.34) we express it as

$$\int d^2z\;|\, z \,\rangle\langle\, z \,| \;=\; \pi\sum_{n=0}^{\infty}\;|\, n \,\rangle\langle\, n \,| \;=\; \pi\hat{\mathbf{1}}. \tag{4.36}$$

f2s24

Hence, we arrived at the completeness relation for coherent states, which can be written as

$$\frac{1}{\pi}\int d^2z\;|\, z \,\rangle\langle\, z \,| \;=\; \hat{\mathbf{1}}. \tag{4.37}$$

f2s25

Since coherent states are not orthogonal (see (4.32)) but complete, it is possible to expand one coherent state $|\, \alpha \,\rangle$ in terms of all other ones. This means, that the coherent states

constitute, the so called, overcomplete set. The obtained relation allows us to write for an arbitrary (single mode) state $|\,\psi\,\rangle$ of the radiation field

$$|\,\psi\,\rangle \;=\; \frac{1}{\pi}\int d^2z\;|\,z\,\rangle\langle\,z\,|\,\psi\,\rangle. \tag{4.38}$$ f2s25b

It seems tempting to call $\langle\,z\,|\,\psi\,\rangle$ the wave function of state $|\,\psi\,\rangle$ in the coherent state representation. This, is, however, incorrect, because $\langle\,z\,|\,\psi\,\rangle$ is a function of two real variables which have the sense of phase space variables, so can be interpreted (considered) as position and momentum.

4.2.4 Minimalization of uncertainty

In Eqs.(4.19) f2s06 we have computed the expectation values of operators q and p for the field in the n-photon state. Here, we shall repeat these calculations for the field in the coherent state $|\,z\,\rangle$.

f2s33 First we compute the corresponding expectation values

$$\langle\,q\,\rangle_z = \langle\,z\,|\,\sqrt{\frac{\hbar}{2\omega}}\,\left(\,\hat{a}\;+\;\hat{a}^\dagger\,\right)\,|\,z\,\rangle \;=\; \sqrt{\frac{\hbar}{2\omega}}\;(z^*+z) \tag{4.39a}$$ f2s33a

$$\langle\,p\,\rangle_z = \langle\,z\,|\,i\,\sqrt{\frac{\hbar\omega}{2}}\,\left(\,\hat{a}^\dagger\;-\;\hat{a}\,\right)\,|\,z\,\rangle \;=\; i\,\sqrt{\frac{\hbar\omega}{2}}\,(z^*-z)\,. \tag{4.39b}$$ f2s33b

These relations follow from definition of the coherent state (4.21) f2s10 and its hermitian conjugate: $\langle\,z\,|\hat{a}^\dagger = z^*\langle\,z\,|$. Next we proceed to find the expectation values of the squares q^2 and p^2. In the calculation we use the canonical commutation relation for annihilation and

f2s35 creation operators and we obtain

$$\langle\,q^2\,\rangle_z = \langle\,z\,|\,\frac{\hbar}{2\omega}\,\left(\,\hat{a}\;+\;\hat{a}^\dagger\,\right)^2\,|\,z\,\rangle \;=\; \frac{\hbar}{2\omega}\,\left[(z^*)^2+2|z|^2+z^2+1\,\right] \tag{4.40a}$$ f2s35a

$$\langle\,p^2\,\rangle_z = -\,\langle\,z\,|\,\frac{\hbar\omega}{2}\,\left(\,\hat{a}^\dagger\;-\;\hat{a}\,\right)^2\,|\,z\,\rangle \;=\; -\;\frac{\hbar\omega}{2}\,\left[(z^*)^2-2|z|^2+z^2-1\,\right] \tag{4.40b}$$ f2s35b

f2s37 Variances follow immediately, we easily get the following expressions

$$\sigma_z^2(q) \;=\; \langle\,z\,|\,q^2\,|\,z\,\rangle - \langle\,z\,|\,q\,|\,z\,\rangle^2 = \frac{\hbar}{2\omega} \tag{4.41a}$$ f2s37a

$$\sigma_z^2(p) \;=\; \langle\,z\,|\,p^2\,|\,z\,\rangle - \langle\,z\,|\,p\,|\,z\,\rangle^2 = \frac{\hbar\omega}{2}. \tag{4.41b}$$ f2s37b

Hence, the product of the variances, for the field in the coherent state $|\,z\,\rangle$ is given as

$$\sigma_z^2(q)\sigma_z^2(p) \;=\; \frac{\hbar^2}{4} \;\geq\; \frac{\hbar^2}{4}, \tag{4.42}$$ f2s39

so indeed the uncertainty relation is satisfied, but it is minimized, the product of variances attains the minimum allowed value. Thus, we can say that coherent states minimize the uncertainty, and as such can be considered to be as close to classical states as it is allowed by the principles of quantum mechanics. From general course of quantum mechanics we, for example, know how to construct the minimum uncertainty wave packet. Replacing the averages of q and p by the expectation values in the coherent state, we may construct the coherent state wave packet.

4.2.5 Comments on electric field

The electric field for one mode is given by Eq.(4.14b). Its expectation value in the coherent state reads

$$\langle z|\vec{\mathbf{E}}_\perp|z\rangle = i\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\,\vec{\mathbf{e}}\left(z\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} - z^*\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\right). \tag{4.43}$$

We already know that this field corresponds to the state with minimum uncertainty and as we see it, is of the form of classical plane wave. This is another argument, why the coherent states are considered to be the closest to the classical ones.

Let us analyze the variance of the photon number for the field in the coherent state. We have the obvious relations (in the second one we use commutation relation)

$$\langle n\rangle_z = \langle z|\hat{a}^\dagger\hat{a}|z\rangle = |z|^2 \tag{4.44a}$$

$$\langle n^2\rangle_z = \langle z|\left(\hat{a}^\dagger\hat{a}\right)^2|z\rangle = \langle z|\hat{a}^\dagger(\hat{a}^\dagger\hat{a}+1)\hat{a}|z\rangle = |z|^4+|z|^2. \tag{4.44b}$$

Thus, the variance of the photon number in this case is given as

$$\sigma_z^2(n) = \langle n^2\rangle_z - \langle n\rangle_z^2 = |z|^2 = \langle n\rangle_z. \tag{4.45}$$

Relative fluctuations of the mean photon number can thus be estimated as

$$\frac{\sqrt{\sigma_z^2(n)}}{\langle n\rangle_z} = \frac{1}{\sqrt{\langle n\rangle_z}}, \tag{4.46}$$

so it becomes very small when the field is strong (with large mean photon number $\langle n\rangle_z = |z|^2$). So, if the mode contains (on average) many photons, the fluctuations of $\langle n\rangle_z$ are small and the field approaches the classical one.

We continue our discussion of the field in the coherent state and we compute the variance of the electric field intensity. The average is already given in Eq.(4.43) so we proceed to find the average of the square

$$\begin{aligned}\langle z|\vec{\mathbf{E}}_\perp^2|z\rangle &= \frac{\hbar\omega}{2\epsilon_0 V}\langle z|\left(\hat{a}^\dagger\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} - \hat{a}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\right)\left(\hat{a}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} - \hat{a}^\dagger\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\right)|z\rangle \\ &= \frac{\hbar\omega}{2\epsilon_0 V}\left(2|z|^2+1 - (z^*)^2\,e^{-2i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} - z^2\,e^{2i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\right).\end{aligned} \tag{4.47}$$

Calculation of the variance is now easy, and we get

$$\langle z|\vec{\mathbf{E}}_\perp^2|z\rangle - \langle z|\vec{\mathbf{E}}_\perp|z\rangle^2 = \frac{\hbar\omega}{2\epsilon_0 V} \xrightarrow[\hbar\to 0]{} 0, \tag{4.48}$$

because classical limit corresponds to $\hbar\to 0$. This limit for the variance is independent of the field intensity (its energy), in contrast to the n-photon states (see Eqs.(4.16) and (4.15)). This is an additional argument explaining why coherent states of the field are closely related to classical ones.

4.2.6 Time evolution of the coherent state

We still consider one mode field, hence its Hamiltonian is simply $H_F = \hbar\omega\,\hat{a}^\dagger\hat{a}$. Let us assume that the mode was initially in the coherent state

$$|\,\psi(t_0)\,\rangle \;=\; |\,z\,\rangle. \tag{4.49}$$ f2s51

We want to find what happens with the mode when time $t > t_0$. Since Hamiltonian is explicitly time independent, we can invoke general rules of quantum mechanics to write

$$|\,\psi(t)\,\rangle \;=\; \exp\left(-\frac{iH_F}{\hbar}(t-t_0)\right)|\,\psi(t_0)\,\rangle \;=\; \exp\left(-i\omega\hat{a}^\dagger\hat{a}(t-t_0)\right)|\,z\,\rangle. \tag{4.50}$$ f2s53

Expanding the coherent state $|\,z\,\rangle$ in n-photon states, as in (4.28) f2s17 we obtain

$$|\,\psi(t)\,\rangle \;=\; \exp(-|z|^2/2)\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,e^{-i\omega n(t-t_0)}\,|\,n\,\rangle. \tag{4.51}$$ f2s54

Additional phase factor $e^{-i\omega(t-t_0)}$ does not change the modulus of number z, thus we can write rhs of (4.51) f2s54 as

$$|\,\psi(t)\,\rangle \;=\; |\,z(t)\,\rangle \;=\; |\,\left(z\,e^{-i\omega(t-t_0)}\right)\rangle, \tag{4.52}$$ f2s55

which still is a coherent state only with $\xi = e^{-i\omega(t-t_0)}z$, that is with time dependent phase. So, free evolution of the coherent state produces a new coherent state, or we may say equivalently, that an evolving coherent state remains coherent. Let us also note that this result may be written as

$$|\,\psi(t)\,\rangle \;=\; |\,z(t)\,\rangle \;=\; D\left(z\,e^{-i\omega(t-t_0)}\right)|\,\Omega\,\rangle, \tag{4.53}$$ f2s55x

which agrees with the property (B.43) z2dsim of the displacement operator.

For some further discussion, let us denote $z(t_0) = x_0 + iy_0$. Thus, the time evolution of z can be written as

$$z(t) = x_0\cos\omega(t-t_0) + y_0\sin\omega(t-t_0) - ix_0\sin\omega(t-t_0) + iy_0\cos\omega(t-t_0) \tag{4.54}$$ f2s56

Then, the time dependent expectation values of phase space variables are

$$\begin{aligned}\langle\,q(t)\,\rangle &= \langle\,z(t)\,|\,\sqrt{\frac{\hbar}{2\omega}}\;\left(\hat{a}+\hat{a}^\dagger\right)\,|\,z(t)\,\rangle\\ &= \sqrt{\frac{\hbar}{2\omega}}\;\left(z(t)+z^*(t)\right) \;=\; \sqrt{\frac{\hbar}{2\omega}}\;2\,\mathrm{Re}[z(t)]\\ &= \sqrt{\frac{2\hbar}{\omega}}\;\left[x_0\cos\omega(t-t_0)+y_0\sin\omega(t-t_0)\right].\end{aligned} \tag{4.55}$$ f2s57

And similarly, we obtain

$$\begin{aligned}\langle\,p(t)\,\rangle &= -i\,\langle\,z(t)\,|\,\sqrt{\frac{\hbar\omega}{2}}\;\left(\hat{a}-\hat{a}^\dagger\right)\,|\,z(t)\,\rangle\\ &= -i\,\sqrt{\frac{\hbar\omega}{2}}\;\left(z(t)-z^*(t)\right) \;=\; \sqrt{\frac{\hbar\omega}{2}}\;2\,\mathrm{Im}[z(t)]\\ &= \sqrt{2\hbar\omega}\;\left[-x_0\sin\omega(t-t_0)+y_0\cos\omega(t-t_0)\right].\end{aligned} \tag{4.56}$$ f2s58

These relations reproduce the evolution of classical harmonic oscillator. We conclude that a coherent state during its time (free) evolution remains coherent and follows the trajectory of the classical orbit in the phase space. The uncertainties (variances) $\sigma_z(q)$ and $\sigma_z(p)$ remain constant and minimal.

4.2.7 Coherent state as a displaced vacuum

Let us combine expression (4.28) with that for the n state, that is with (3.36). As a result we can write

$$|\,z\,\rangle \;=\; \exp\left(-\frac{|z|^2}{2}\right)\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|\,\Omega\,\rangle \;=\; \exp\left(-\frac{|z|^2}{2}\right)\exp\left(z\hat{a}^\dagger\right)\,|\,\Omega\,\rangle \quad (4.57)$$ f2s26

Since there holds the relation $\hat{a}|\,\Omega\,\rangle = 0$, then it is obvious that $e^{-z^*\hat{a}}|\,\Omega\,\rangle = |\,\Omega\,\rangle$. Therefore, we can recast the above relation as

$$|\,z\,\rangle \;=\; \exp\left(-\frac{|z|^2}{2}\right)\exp\left(z\hat{a}^\dagger\right)\,\exp\left(-z^*\hat{a}\right)\,|\,\Omega\,\rangle. \quad (4.58)$$ f2s27

Using relation (B.27b), ie.: $e^{\alpha\hat{a}+\beta\hat{a}^\dagger} = e^{\beta\hat{a}^\dagger}\,e^{\alpha\hat{a}}\,e^{\alpha\beta/2}$ with $\alpha = -z^*$ and $\beta = z$ we rewrite the above formula as

$$|\,z\,\rangle \;=\; \exp\left(z\hat{a}^\dagger - z^*\hat{a}\right)\,|\,\Omega\,\rangle \;=\; D(z)|\,\Omega\,\rangle, \quad (4.59)$$ f2s28

where we have introduced an operator, which we will call the displacement operator

$$D(z) \;=\; \exp\left(z\hat{a}^\dagger - z^*\hat{a}\right). \quad (4.60)$$ f2s29

The displacement operator is unitary, indeed we have

$$D^\dagger(z) \;=\; \exp\left(z^*\hat{a} - z\hat{a}^\dagger\right) \;=\; \exp\left[-(z\hat{a}^\dagger - z^*\hat{a}^\dagger)\right] \;=\; D(-z), \quad (4.61)$$ f2s30a

and it is evident that

$$D^\dagger(z) \;=\; D(-z) \;=\; D^{-1}(z), \quad (4.62)$$ f2s30b

which proves that it is unitary, while the operator acting on the vacuum in (4.57) does not possess such a property. Unitarity is the reason why we have introduced $D(z)$.

Let us also recall relation (B.37), that is $e^{-\alpha\hat{a}-\beta\hat{a}^\dagger}\,\hat{a}\,e^{\alpha\hat{a}+\beta\hat{a}^\dagger} = \hat{a} + \beta$, which allows us to write

$$D^\dagger(z)\,\hat{a}\,D(z) \;=\; e^{z^*\hat{a}-z\hat{a}^\dagger}\,\hat{a}\,e^{z\hat{a}^\dagger-z^*\hat{a}} \;=\; \hat{a} \;+\; z, \quad (4.63)$$ f2s31

which explains the name "displacement" operator. This is also the reason why we call the coherent state (see (4.59)) "the displaced vacuum" state.

It may be worth discussing some analogy with quantum mechanical harmonic oscillator. The hamiltonian of the oscillator is quadratic in momentum and position. If we add an additional potential energy term (for example coupling of the charged oscillator with an external, uniform electric field) linear in position, it is then easy to show that the

wave functions and energies will be displaced. This follows by expressing the hamiltonian in a canonical form: $ax^2 + bx = a(x + b/2a)^2 - b^2/4a$. Similar considerations could also be done for linear shift in momentum. This is so, because position and momentum of the oscillator both enter the hamiltonian quadratically (they are canonically equivalent). The given arguments suggest that a displaced state of the oscillator is generated by an operator proportional to position (or momentum), that is by a combination of annihilation and creation operators. Requirement of unitarity then leads to the displacement operator $D(z)$ as given in (4.60). So we see, that the discussed analogy could be used to define a coherent state via the relation (4.59), which could be then used to prove other properties of coherent states, including the fact that $|\, z\,\rangle$ is an eigenvector of the annihilation operator. Moreover, this analogy gives additional clarification to the notion of coherent state as a displaced vacuum state.

4.3 Squeezed states (single mode)

4.3.1 Introduction and basic definition

We know that a quantized mode of the radiation field can be expressed via fields (4.14), that is via annihilation and creation operators. We will concentrate our attention on the electric field,

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{x}}, t) \;=\; i\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\;\vec{\mathbf{e}}\,\Big[\,\hat{a}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} \;-\; \hat{a}^\dagger\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}\,\Big]. \tag{4.64}$$ f3s01

Discussing the field oscillators and coherent states we have used the phase space operators q and p (position and momentum operators of the oscillator with unit mass). We will now introduce two operators

$$X = \frac{1}{\sqrt{2}}\,(\hat{a} + \hat{a}^\dagger) \qquad\qquad Y = \frac{-i}{\sqrt{2}}\,(\hat{a} - \hat{a}^\dagger), \tag{4.65}$$ f3s02

which, by comparison with (4.17) may be viewed as dimensionless (rescaled) position and momentum. We shall discuss the importance of the absence of dimensionality later. At present we note that both operators X and Y are hermitian, and as such, can be considered observables. The relations (4.65) imply the inverse ones

$$\hat{a} = \frac{1}{\sqrt{2}}\,(X + i\,Y) \qquad\qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\,(X - i\,Y), \tag{4.66}$$ f3s03

in the essentially the same manner as it was done for harmonic oscillator. Moreover, we note that operators X and Y satisfy an obvious commutation relation

$$[X,\, Y] \;=\; i, \tag{4.67}$$ f3s04

which follows immediately from the properties of annihilation and creation operators.

To clarify the physical meaning of the operators X and Y, let us consider the electric field (4.64). We recall that in the Heisenberg picture $\hat{a}(t) = \hat{a}e^{-i\omega t}$ (as in (3.67)), so we can write

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{x}}, t) \;=\; i\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\;\vec{\mathbf{e}}\,\big[\,\hat{a}\,e^{i\phi} \;-\; \hat{a}^\dagger\,e^{-i\phi}\,\big], \tag{4.68}$$ f3s05

where, for brevity, we have denoted $\phi = \vec{\mathbf{k}} \cdot \vec{\mathbf{r}} - \omega t$. Introducing relations (f3s03 4.66), after simple manipulations we get

$$\vec{\mathbf{E}}_\perp(\vec{\mathbf{x}}, t) \;=\; -\sqrt{2}\,\sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}\;\vec{\mathbf{e}}\,[\,X\sin\phi \;+\; Y\cos\phi\,]\,. \tag{4.69}$$ f3s06

Hence, X and Y are amplitudes of the two quadratures of the electric field (f3s01 4.64) having a phase difference of $\pi/2$.

The commutation relation (f3s04 4.67) implies that the variances of observables X and Y satisfy the uncertainty relation

$$\sigma^2(X)\,\sigma^2(Y) \geq \frac{1}{4}. \tag{4.70}$$ f3s07

f3s08 Before continuing our discussion, it may be worth recalling that the variances of quadratures are:

- for n − photon state (see(f2s06 4.19)) : $\sigma_n^2(X) = \sigma_n^2(Y) = \frac{1}{2}\,(2n+1)$ (4.71a) f3s08a
- for coherent state (see(f2s37 4.41)) : $\sigma_z^2(X) = \sigma_z^2(Y) = \frac{1}{2}$ (4.71b) f3s08b

These relations show that we reach the minimum uncertainty (the product of variances equal to 1/4) for the vacuum state $|\,\Omega\,\rangle = |\,n=0\,\rangle$ and for a coherent state $|\,z\,\rangle$. For future reference, we also recall that according to Eq.(f2s05 4.18), for n-photon state we have the expectation values

$$\langle\,X\,\rangle_n \;=\; \langle\,n\,|\,X\,|\,n\,\rangle \;=\; 0, \qquad\qquad \langle\,Y\,\rangle_n \;=\; \langle\,n\,|\,Y\,|\,n\,\rangle \;=\; 0. \tag{4.72}$$ f3s09a

f3s09b For the coherent state, these expectations become (see (f2s33 4.39)

$$\langle\,X\,\rangle_z = \langle\,z\,|\,X\,|\,z\,\rangle \;=\; \frac{1}{\sqrt{2}}\,(z+z^*) \;=\; \sqrt{2}\;\mathrm{Re}(z), \tag{4.73a}$$ f3so9ba

$$\langle\,Y\,\rangle_z = \langle\,z\,|\,Y\,|\,z\,\rangle \;=\; \frac{-i}{\sqrt{2}}\,(z-z^*) \;=\; \sqrt{2}\;\mathrm{Im}(z), \tag{4.73b}$$ f3s09bb

We are now in position to define a squeezed state of the radiation field as such, for which one of the variances of quadrature operators goes below the vacuum limit 1/2. That is:

Definition: State $|\,\psi\,\rangle$ of the radiation field is a squeezed state if either $\sigma^2(X) < 1/2$ or $\sigma^2(Y) < 1/2$. The product of the variances, however, must still satisfy the uncertainty relation (f3s07 4.70).

Sometimes an additional requirement is imposed, namely, that state $|\,\psi\,\rangle$ is also a minimum uncertainty state, but this is not necessary. We shall call state $|\,\psi\,\rangle$ a *squeezed state* when one of the quadratures has less fluctuations than in vacuum or coherent state. The squeezed state can be called ideal if it is also a state with minimum uncertainty (when in (f3s07 4.70) we have equality).

The fact that both quadratures have the same dimension is essential, because then scaling the dimensions does not change the ratio of the variances. The feature of quantum fluctuations below vacuum value is most important and it implies the quantum-mechanical nature of squeezed states.

4.3.2 Operator approach

Squeeze operator. Introduction

The wave function of the ground state of the harmonic oscillator is (see (10.57)):

$$\varphi_0(q) \;=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega q^2}{2\hbar}\right), \tag{4.74}$$

so it becomes narrower when ω gets larger. The width of this function is governed by the strength of the potential energy which is quadratic in position. Frequency can be enlarged by the additional term in the hamiltonian which must be quadratic in position. Hence, a transformation generated by q^2 is expected to narrow the oscillator's wave function. This suggests that an operator quadratic in annihilation and creation operators should "narrow", or squeeze the states of the radiation field. This reasoning is similar to that concerning the displacement operator leading to coherent states.

Following this argument, we postulate that an operator

$$S(\xi) \;=\; \exp\left[\frac{1}{2}\,\xi^*\hat{a}^2 \;-\; \frac{1}{2}\,\xi\left(\hat{a}^\dagger\right)^2\right], \qquad \text{with} \quad \xi \;=\; \rho\, e^{i\theta} \in \mathbb{C}, \tag{4.75}$$

generates states which can be justified to be called squeezed states of the radiation field. The simplest candidate for a squeezed state would then be

$$|\,0,\xi\,\rangle \;=\; S(\xi)\,|\,\Omega\,\rangle, \tag{4.76}$$

where $|\,\Omega\,\rangle = |\,n=0\,\rangle$ is a usual vacuum state. Obviously, we have to prove that the state (4.76) indeed is a squeezed state, according to the above given definition. Before we do so, we will study some basic properties of squeeze operator (4.75) which is also investigated in the Appendix B. We have shown that $S(\xi)$ is unitary and that it transforms the annihilation and creation operators as

$$S^\dagger(\xi)\,\hat{a}\,S(\xi) = \hat{a}\cosh(\rho) \;-\; \hat{a}^\dagger\, e^{i\theta}\sinh(\rho), \tag{4.77a}$$
$$S^\dagger(\xi)\,\hat{a}^\dagger\,S(\xi) = \hat{a}^\dagger\cosh(\rho) \;-\; \hat{a}\, e^{-i\theta}\sinh(\rho). \tag{4.77b}$$

Since squeezing of the states is defined by quadrature operators, we should devote some time to study them together with operator $S(\xi)$. But before we do so, let us note that relations (4.77) immediately imply that

$$\begin{aligned}\langle\,0,\xi\,|\,\hat{a}\,|\,0,\xi\,\rangle &= \langle\,\Omega\,|\,S^\dagger(\xi)\,\hat{a}S(\xi)\,|\,\Omega\,\rangle \\ &= \langle\,\Omega\,|\,\left(\hat{a}\cosh(\rho) - \hat{a}^\dagger\, e^{i\theta}\sinh(\rho)\right)\,|\,\Omega\,\rangle \;=\; 0, \qquad (4.78a)\\ \langle\,0,\xi\,|\,\hat{a}^\dagger\,|\,0,\xi\,\rangle &= \langle\,\Omega\,|\,S^\dagger(\xi)\,\hat{a}^\dagger S(\xi)\,|\,\Omega\,\rangle \\ &= \langle\,\Omega\,|\,\left(\hat{a}^\dagger\cosh(\rho) - \hat{a}\, e^{-i\theta}\sinh(\rho)\right)\,|\,\Omega\,\rangle \;=\; 0, \qquad (4.78b)\end{aligned}$$

due to the fact that annihilation (creation) operator acting on vacuum state $|\,\Omega\,\rangle$ ($\langle\,\Omega\,|$) produces zero.

Similarity relations for quadratures

To investigate the expectation values of quadrature operators in state $|\,0,\xi\,\rangle$ we obviously need expressions of the type of $S^\dagger(\xi)XS(\xi)$. Hence, we proceed to find such expressions.

From the definition (f3s02 4.65) of the quadratures and from (f3s14 4.77) we have

$$S^\dagger(\xi)\,XS(\xi) = \frac{1}{\sqrt{2}}\left[\,\hat{a}\cosh(\rho) - \hat{a}^\dagger\, e^{i\theta}\sinh(\rho) + \hat{a}^\dagger\cosh(\rho) - \hat{a}\, e^{-i\theta}\sinh(\rho)\,\right]$$
$$= X\cosh(\rho) - \frac{1}{\sqrt{2}}\left(\,\hat{a}^\dagger\, e^{i\theta} + \hat{a}\, e^{-i\theta}\,\right)\,\sinh(\rho). \qquad (4.79)\quad \texttt{f3s15a}$$

Expressing the term in brackets by (f3s03 4.66) we get

$$\hat{a}^\dagger\, e^{i\theta} + \hat{a}\, e^{-i\theta} \;=\; \sqrt{2}\,(X\cos\theta + Y\sin\theta)\,. \qquad (4.80)\quad \texttt{f3s15b}$$

Combining the two last equations yields

$$S^\dagger(\xi)\,XS(\xi) \;=\; X\,(\cosh(\rho) - \cos\theta\sinh(\rho)) - Y\sin\theta\sinh(\rho). \qquad (4.81)\quad \texttt{f3s15c}$$

In fully analogous manner we easily derive the similarity relation for the second quadrature operator

$$S^\dagger(\xi)\,YS(\xi) \;=\; Y\,(\cosh(\rho) + \cos\theta\sinh(\rho)) - X\sin\theta\sinh(\rho). \qquad (4.82)\quad \texttt{f3s15f}$$

These relations, though correct are neither illuminating nor convenient. Nevertheless, we f3s17 can find the expectation values of the quadratures for the field in the state (f3s13 4.76):

$$\langle\, X\,\rangle = \langle\, 0,\xi\,|\,X\,|\,0,\xi\,\rangle \;=\; \langle\,\Omega\,|\,S^\dagger(\xi)\,XS(\xi)\,|\,\Omega\,\rangle \;=\; 0, \qquad (4.83a)\quad \texttt{f3s17a}$$
$$\langle\, Y\,\rangle = \langle\, 0,\xi\,|\,Y\,|\,0,\xi\,\rangle \;=\; \langle\,\Omega\,|\,S^\dagger(\xi)\,YS(\xi)\,|\,\Omega\,\rangle \;=\; 0. \qquad (4.83b)\quad \texttt{f3s17b}$$

This is so, because operator $S^\dagger(\xi)\,XS(\xi)$ is expressed by (f3s15c 4.81), i.e., by a combination of $\hat{a}$ and $\hat{a}^\dagger$. The expectation values of the latter vanish for the field in the vacuum state. Hence our result (f3s17 4.83). We can also refer to Eqs.(f3s14x 4.78), quadratures are combinations of $\hat{a}$ and $\hat{a}^\dagger$, so mentioned equations imply the obtained ones.

Computation of the expectation values of the squares of the quadratures is greatly inconvenient. It appears that to consider the quadratures further it is useful to introduce some additional transformations.

Rotated operators

To simplify the above obtained relations it is convenient to introduce new operators

$$\hat{b} = \hat{a}\, e^{-i\theta/2}, \qquad\qquad \hat{b}^\dagger = \hat{a}^\dagger\, e^{i\theta/2}, \qquad (4.84)\quad \texttt{f3s19}$$

which, obviously, satisfy the commutation rule:

$$\left[\,\hat{b},\,\hat{b}^\dagger\,\right] \;=\; 1, \qquad (4.85)\quad \texttt{f3s20}$$

and which means that they are also annihilation and creation operators. Analyzing the similarity relation (4.77), we almost automatically obtain

$$S^\dagger(\xi)\,\hat{b}\,S(\xi) = \hat{b}\cosh(\rho) \;-\; \hat{b}^\dagger\sinh(\rho), \tag{4.86a}$$

$$S^\dagger(\xi)\,\hat{b}^\dagger\,S(\xi) = \hat{b}^\dagger\cosh(\rho) \;-\; \hat{b}\sinh(\rho). \tag{4.86b}$$

Since $\hat{b}$ and $\hat{b}^\dagger$ are annihilation and creation operators we can construct new (hermitian) quadrature operators in an exactly the same manner as previously. Namely, we introduce

$$\tilde{X} \;=\; \frac{1}{\sqrt{2}}\left(\hat{b} \;+\; \hat{b}^\dagger\right), \qquad \tilde{Y} \;=\; \frac{-i}{\sqrt{2}}\left(\hat{b} \;-\; \hat{b}^\dagger\right), \tag{4.87}$$

so the inverse relations read

$$\hat{b} \;=\; \frac{1}{\sqrt{2}}\left(\tilde{X} \;+\; i\tilde{Y}\right), \qquad \hat{b}^\dagger \;=\; \frac{1}{\sqrt{2}}\left(\tilde{X} \;-\; i\tilde{Y}\right). \tag{4.88}$$

Moreover, we note that new quadratures satisfy the commutation relation

$$\left[\tilde{X},\,\tilde{Y}\right] \;=\; i, \tag{4.89}$$

which is the same one as for old quadratures (4.67). This implies that new quadratures also satisfy the same uncertainty relation

$$\sigma^2(\tilde{X})\,\sigma^2(\tilde{Y}) \geq \frac{1}{4}, \tag{4.90}$$

where the variances are taken in the arbitrary state of the field. This suggests that we can look for squeezed state in terms of new quadratures. Before we do so, let us look at the properties of new quadratures.

First we seek the connection between old and new quadratures. We insert operators $\hat{b}$, $\hat{b}^\dagger$ given according to (4.84) into Eqs.(4.87), secondly we express old annihilation and creation operators by old quadratures as in (4.65). Simple manipulation yields

$$\tilde{X} = X\cos(\theta/2) + Y\sin(\theta/2), \tag{4.91a}$$

$$\tilde{Y} = -X\sin(\theta/2) + Y\cos(\theta/2), \tag{4.91b}$$

which is a simple rotation by an angle $\theta/2$. Rotation is an orthogonal transformation, so automatically unitary. Hence, it is not surprising that new quadratures satisfy commutation relation (4.89), the same as old quadratures. Moreover, rotational character of transformation (4.91) enables us to write an inverse one

$$X = \tilde{X}\cos(\theta/2) - \tilde{Y}\sin(\theta/2) \tag{4.92a}$$

$$Y = \tilde{X}\sin(\theta/2) + \tilde{Y}\cos(\theta/2), \tag{4.92b}$$

which is a rotation by a negative angle $-\theta/2$.

Finally, having specified new quadrature operators, we look for the similarity relations. We apply operator $S^\dagger(\xi)$ on the left and $S(\xi)$ on the right of $\tilde{X}$ and $\tilde{Y}$. Then

we use equations (4.87). Applying similarity relations (4.86) and using the properties of f3s29 hyperbolic functions, we arrive at

$$S^\dagger(\xi)\,\tilde{X}\,S(\xi) = \frac{1}{\sqrt{2}}\left(\hat{b}+\hat{b}^\dagger\right)(\cosh\rho-\sinh\rho) \;=\; \tilde{X}\,e^{-\rho} \tag{4.93a}$$ f3s29a

$$S^\dagger(\xi)\,\tilde{Y}\,S(\xi) = \frac{-i}{\sqrt{2}}\left(\hat{b}-\hat{b}^\dagger\right)(\cosh\rho+\sinh\rho) \;=\; \tilde{Y}\,e^{\rho} \tag{4.93b}$$ f3s29b

It is possible to cross-check the consistency of the theory, for example by obtaining equations (4.81) and (4.82) from relations (4.93) by using suitable correspondence between new and old operators.

Moreover, having specified new quadrature operators we look for their expectation f3s30 values in n-photon and coherent states. Thus, from (4.91) and (4.72) we easily obtain

$$\langle\,\tilde{X}\,\rangle_n = \langle\,n\,|\,\tilde{X}\,|\,n\,\rangle \;=\; \langle\,n\,|\,(X\cos(\theta/2)+Y\sin(\theta/2))\,|\,n\,\rangle \;=\; 0, \tag{4.94a}$$ f3s30a

$$\langle\,\tilde{Y}\,\rangle_n = \langle\,n\,|\,\tilde{Y}\,|\,n\,\rangle \;=\; \langle\,n\,|\,(-X\sin(\theta/2)+Y\cos(\theta/2))\,|\,n\,\rangle \;=\; 0. \tag{4.94b}$$ f3s30b

f3s30x Similarly, for the field in the coherent state $|\,z\,\rangle$, using (4.73) we obtain

$$\begin{aligned}\langle\,\tilde{X}\,\rangle_z &= \langle\,z\,|\,\tilde{X}\,|\,z\,\rangle \;=\; \langle\,z\,|\,(X\cos(\theta/2)+Y\sin(\theta/2))\,|\,z\,\rangle\\ &= \sqrt{2}\,(\cos(\theta/2)\mathrm{Re}(z)+\sin(\theta/2)\mathrm{Im}(z))\\ &= \sqrt{2}\;\mathrm{Re}\left(z\,e^{-i\theta/2}\right)\end{aligned} \tag{4.95a}$$ f3s30xa

$$\begin{aligned}\langle\,\tilde{Y}\,\rangle_z &= \langle\,z\,|\,\tilde{Y}\,|\,z\,\rangle \;=\; \langle\,z\,|\,(-X\sin(\theta/2)+Y\cos(\theta/2))\,|\,z\,\rangle\\ &= \sqrt{2}\,(-\,\sin(\theta/2)\mathrm{Re}(z)+\cos(\theta/2)\mathrm{Im}(z))\\ &= \sqrt{2}\;\mathrm{Im}\left(z\,e^{-i\theta/2}\right)\end{aligned} \tag{4.95b}$$ f3s30xb

Having specified some auxiliary quantities, we proceed to investigate the single mode squeezed state (4.76).

4.3.3 Squeezed vacuum states

Calculation of expectation values for quadratures

As we already mentioned the state (4.76), that is $|\,0,\xi\,\rangle \;=\; S(\xi)\,|\,\Omega\,\rangle$ is suspected to be a squeezed state of the electromagnetic single mode field. We suggested the construction of this state by reasoning stemming from harmonic oscillator, expecting that squeezing occurs due to displacement quadratic in annihilation and creation operators. We recall that the state $|\,\psi\,\rangle$ is called squeezed if the variance of one of the quadratures goes below $1/2$ – its vacuum value. So we have to check whether the discussed state $|\,0,\xi\,\rangle$ satisfies this definition. We need to find the variances of the quadratures, and in Eqs.(4.81) and (4.82) we found that old quadratures are inconvenient. Therefore, we will consider the expectation values and variances of new quadratures $\tilde{X}$ and $\tilde{Y}$.

First we compute simple averages – expectation values. From similarities (4.93) we obtain

$$\langle\,\tilde{X}\,\rangle \;=\; \langle\,0,\xi\,|\,\tilde{X}\,|\,0,\xi\,\rangle \;=\; \langle\,\Omega\,|\,S^\dagger(\xi)\tilde{X}S(\xi)\,|\,\Omega\,\rangle \;=\; \langle\,\Omega\,|\,\tilde{X}\,|\,\Omega\,\rangle\,e^{-\rho}, \tag{4.96}$$ f3s32a

and similarly for the second quadrature $\tilde{Y}$. Next, we express new quadratures by the old ones, as in (4.91) and since the averages of old quadratures vanish in vacuum state, [see (4.72)], we finally obtain

$$\langle \tilde{X} \rangle \;=\; \langle 0,\xi \,|\, \tilde{X} \,|\, 0,\xi \rangle \;=\; 0, \qquad\qquad \langle \tilde{Y} \rangle \;=\; \langle 0,\xi \,|\, \tilde{Y} \,|\, 0,\xi \rangle \;=\; 0, \tag{4.97}$$ f3s33

Computation of the expectation values of the squares of the quadratures is a bit lengthy, but rather straightforward. We illustrate the procedure by considering $\tilde{X}^2$. By definition, in state $|\, 0,\xi \,\rangle$ we have

$$\langle \tilde{X}^2 \rangle \;=\; \langle 0,\xi \,|\, \tilde{X}^2 \,|\, 0,\xi \rangle \;=\; \langle \Omega \,|\, S^\dagger(\xi)\tilde{X}S(\xi)\;\; S^\dagger(\xi)\tilde{X}S(\xi) \,|\, \Omega \rangle, \tag{4.98}$$ f3s34a

due to unitarity of $S(\xi)$.Next, from (4.93) we get

$$\langle \tilde{X}^2 \rangle \;=\; \langle \Omega \,|\, \tilde{X}^2 \,|\, \Omega \rangle \, e^{-2\rho}, \tag{4.99}$$ f3s34b

Expressing new quadratures by the old ones, according to (4.91) (remembering that quadratures do not commute) we have

$$\begin{aligned} \langle \tilde{X}^2 \rangle \;=\; e^{-2\rho} \big[\langle \Omega \,|\, X^2 \,|\, \Omega \rangle \cos^2(\theta/2) \;+\; \langle \Omega \,|\, Y^2 \,|\, \Omega \rangle \sin^2(\theta/2) \\ +\; \langle \Omega \,|\, (XY+YX) \,|\, \Omega \rangle \sin(\theta/2)\cos(\theta/2) \big]. \end{aligned} \tag{4.100}$$ f3s34c

The first two matrix elements correspond to vacuum expectations, each of which due to (4.71a) gives 1/2. Thus,

$$\langle \tilde{X}^2 \rangle \;=\; e^{-2\rho} \left[\frac{1}{2} \;+\; \langle \Omega \,|\, (XY+YX) \,|\, \Omega \rangle \sin(\theta/2)\cos(\theta/2) \right]. \tag{4.101}$$ f3s34x

The remaining matrix element can be simplified with the aid of the commutation relation (4.89), which yields

$$\begin{aligned} \langle \tilde{X}^2 \rangle \;=\; e^{-2\rho} \Big[\frac{1}{2} \;+\; i\, \sin(\theta/2)\cos(\theta/2) \\ +\; 2\, \langle \Omega \,|\, YX \,|\, \Omega \rangle \sin(\theta/2)\cos(\theta/2) \Big]. \end{aligned} \tag{4.102}$$ f3s36a

So we have to calculate the matrix element $\langle \Omega \,|\, YX \,|\, \Omega \rangle$. We invoke definitions (4.65) and we write

$$\begin{aligned} \langle \Omega \,|\, YX \,|\, \Omega \rangle &= -\frac{i}{2} \, \langle \Omega \,|\, (\hat{a}-\hat{a}^\dagger)(\hat{a}+\hat{a}^\dagger) \,|\, \Omega \rangle \\ &= -\frac{i}{2} \, \langle \Omega \,|\, \left[\hat{a}^2 + \big(1+\hat{a}^\dagger\hat{a}\big) - \hat{a}^\dagger\hat{a} - (\hat{a}^\dagger)^2 \right] \,|\, \Omega \rangle, \end{aligned} \tag{4.103}$$ f3s36b

where in the second term we used the commutation relation for $\hat{a}$ and $\hat{a}^\dagger$. We easily see that operator terms do not contribute, and only term with unity survives, so we have

$$\langle \Omega \,|\, YX \,|\, \Omega \rangle \;=\; -\frac{i}{2} \, \langle \Omega \,|\, 1 \,|\, \Omega \rangle \;=\; -\frac{i}{2}. \tag{4.104}$$ f3s36bx

Finally, we see that two last terms in (4.101) cancel out and we have for the expectation value of the square of the first quadrature

$$\langle \tilde{X}^2 \rangle \;=\; \langle 0,\xi\,|\,\tilde{X}^2\,|\,0,\xi\rangle \;=\; \langle \Omega\,|\,S^\dagger(\xi)\,\tilde{X}^2 S(\xi)\,|\,\Omega\rangle \;=\; \frac{1}{2}\,e^{-2\rho}. \tag{4.105}$$

Calculation of the expectation value for $\tilde{Y}^2$ goes along exactly the same lines, so we give the final result, which is of the form

$$\langle \tilde{Y}^2 \rangle \;=\; \langle 0,\xi\,|\,\tilde{Y}^2\,|\,0,\xi\rangle \;=\; \langle \Omega\,|\,S^\dagger(\xi)\,\tilde{Y}^2 S(\xi)\,|\,\Omega\rangle \;=\; \frac{1}{2}\,e^{2\rho}. \tag{4.106}$$

Thus, summarizing our results we can say that for the state of the radiation field which is generated by the operator $S(\xi)$

$$|\,0,\xi\rangle \;=\; S(\xi)\,|\,\Omega\rangle \tag{4.107}$$

the expectation values of quadratures vanish (see Eqs.(4.97)), while the expectation values of the squares of quadratures are given by (4.105) and (4.106). This means that the corresponding variances are

$$\sigma^2(\tilde{X}) \;=\; \frac{1}{2}\,e^{-2\rho}, \qquad\qquad \sigma^2(\tilde{Y}) \;=\; \frac{1}{2}\,e^{2\rho}, \tag{4.108}$$

so that the product of variance follows as

$$\sigma^2(\tilde{X})\,\sigma^2(\tilde{Y}) \;=\; \frac{1}{4}. \tag{4.109}$$

We see that the uncertainty relation (4.90) is minimalized and variance of quadrature $\tilde{X}$ is reduced with respect to its vacuum value, while the variance of $\tilde{Y}$ is correspondingly enhanced.

Squeezed vacuum states

The state $|\,0,\xi\rangle = S(\xi)\,|\,\Omega\rangle$ is a minimum uncertainty state, for which variance of one quadrature is enhanced, while variance of the second one is reduced below the so-called vacuum limit (equal to 1/2). By definition, this state is a squeezed state, which we can call a vacuum squeezed state. We also note, that the expectation values of the quadratures themselves give zero (see (4.97), which is characteristic for a vacuum state. As a consequence, since the field $\vec{\mathbf{E}}_\perp(\vec{\mathbf{x}},t)$ is linear in quadratures (see (4.69)), relations (4.97) imply that the expectation value of the field in the squeezed vacuum state vanishes

$$\langle \vec{\mathbf{E}}_\perp \rangle = \langle 0,\xi\,|\,\vec{\mathbf{E}}_\perp\,|\,0,\xi\rangle = \langle \Omega\,|\,S^\dagger(\xi)\,\vec{\mathbf{E}}_\perp\,S(\xi)\,|\,\Omega\rangle = 0, \tag{4.110}$$

similarly as in the n-photon state, but differently from a coherent state.

Next, let us compute the expectation value of the number of photons in the squeezed vacuum state. We then have

$$\begin{aligned}\langle \hat{a}^\dagger\hat{a}\rangle = \langle 0,\xi\,|\,\hat{a}^\dagger\hat{a}\,|\,0,\xi\rangle \;&=\; \langle \Omega\,|\,S^\dagger(\xi)\,\hat{a}^\dagger\hat{a}\,S(\xi)\,|\,\Omega\rangle \\ &= \langle \Omega\,|\,S^\dagger(\xi)\,\hat{a}^\dagger\,S(\xi)S^\dagger\hat{a}\,S(\xi)\,|\,\Omega\rangle.\end{aligned} \tag{4.111}$$

Using similarity relations (f3s14 4.77) we further get

$$\langle\, \hat{a}^\dagger\hat{a}\,\rangle \;=\; \langle\,\Omega\,|\,\big(\hat{a}^\dagger\hat{a}\cosh^2(\rho) - (\hat{a}^\dagger)^2\, e^{i\theta}\,\sinh(\rho)\cosh(\rho) \\ -\hat{a}^2\, e^{-i\theta}\,\sinh(\rho)\cosh(\rho) + \hat{a}\hat{a}^\dagger\sinh^2(\rho)\big)\,|\,\Omega\,\rangle. \qquad (4.112)$$ 3sqnf2

It is obvious that three first terms do no contribute (give zeroes), while due to commutation rule, the term $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1$ contributes unity, so we have

$$\langle\, \hat{a}^\dagger\hat{a}\,\rangle \;=\; \langle\, 0,\xi\,|\,\hat{a}^\dagger\hat{a}\,|\,0,\xi\,\rangle \;=\; \sinh^2(\rho). \qquad (4.113)$$ 3sqnf3

So, the squeezed vacuum state has nonzero expectation value of photon number. The averages of the quadratures, however, remain zero, as it is in a "normal vacuum". This explains why we keep the word "vacuum", calling the state $|\,0,\xi\,\rangle$ – squeezed vacuum. The states $|\,0,\xi\,\rangle$ are made out of "real vacuum", but may be arbitrarily intense.

Time evolution of squeezed vacuum state

The squeezed vacuum state $|\,0,\xi\,\rangle$ evolves freely according to usual rules of quantum mechanics, that is

$$|\,\psi_{sq}(t)\,\rangle \;=\; \exp\left[-\frac{i}{\hbar}H_F t\right]|\,0,\xi\,\rangle \;=\; e^{-i\omega\hat{a}^\dagger\hat{a}t}S(\xi)|\,\Omega\,\rangle. \qquad (4.114)$$ 3sqe1

Obviously we can write

$$|\,\psi_{sq}(t)\,\rangle = e^{-i\omega\hat{a}^\dagger\hat{a}t}S(\xi)e^{i\omega\hat{a}^\dagger\hat{a}t}\; e^{-i\omega\hat{a}^\dagger\hat{a}t}|\,\Omega\,\rangle \\ = S\left(\xi e^{-2i\omega t}\right)|\,\Omega\,\rangle \;=\; |\,0,\,\xi e^{-2i\omega t}\,\rangle, \qquad (4.115)$$ 3sqe2

where in the second line we have used similarity relation(z2squ10 B.54) from the appendix, while in the last step we applied a definition of the squeezed vacuum state with time-shifted (time-dependent) argument. Since the number $\xi = \rho\, e^{i\theta}$, we may say that the angle θ is a time dependent function with

$$\theta(t) \;=\; \theta_0 - 2\omega t, \qquad (4.116)$$ 3sqth|

which corresponds to a clockwise rotation with angular frequency 2ω, We shall return to the discussion of this point in more geometric context in next sections.

4.3.4 Fluctuations of photon number in squeezed vacuum state

To investigate the fluctuations of photon number we need the variance of photon number and thus we need $\langle\,(\hat{a}^\dagger\hat{a})^2\,\rangle = \langle\, n^2\,\rangle$

$$\langle\, n^2\,\rangle \;=\; \langle\, 0,\xi\,|\,(\hat{a}^\dagger\hat{a})^2\,|\,0,\xi\,\rangle \;=\; \langle\,\Omega\,|\,S^\dagger(\xi)\,\hat{a}^\dagger\hat{a}\,S(\xi)\;S^\dagger(\xi)\,\hat{a}^\dagger\hat{a}\,S(\xi)\,|\,\Omega\,\rangle. \qquad (4.117)$$ 3fpn1

We can use the operator appearing in (3sqnf2 4.112), so we can write

$$\langle\, n^2\,\rangle \;=\; \langle\,\Omega\,|\,\big[\hat{a}^\dagger\hat{a}\cosh^2(\rho) - (\hat{a}^\dagger)^2\, e^{i\theta}\,\sinh(\rho)\cosh(\rho) \\ -\hat{a}^2\, e^{-i\theta}\,\sinh(\rho)\cosh(\rho) + \hat{a}\hat{a}^\dagger\sinh^2(\rho)\big] \\ \big[\hat{a}^\dagger\hat{a}\cosh^2(\rho) - (\hat{a}^\dagger)^2\, e^{i\theta}\,\sinh(\rho)\cosh(\rho) \\ -\hat{a}^2\, e^{-i\theta}\,\sinh(\rho)\cosh(\rho) + \hat{a}\hat{a}^\dagger\sinh^2(\rho)\big]\,|\,\Omega\,\rangle. \qquad (4.118)$$ 3fpn2

In general, multiplication gives sixteen terms, but those which contain unequal numbers of $\hat{a}$ and $\hat{a}^\dagger$ do not contribute. Moreover, the terms having $\hat{a}$ as the rightmost operator also vanish. So, out of sixteen terms, the nonzero ones may arise only from three terms. We thus have

$$\begin{aligned}\langle\, n^2\,\rangle \;&=\; \cosh^2(\rho)\sinh^2(\rho)\,\langle\,\Omega\,|\,\hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger\,|\,\Omega\,\rangle \\ &+\; \cosh^2(\rho)\sinh^2(\rho)\,\langle\,\Omega\,|\,\hat{a}^2(\hat{a}^\dagger)^2\,|\,\Omega\,\rangle \\ &+\; \sinh^4(\rho)\,\langle\,\Omega\,|\,\hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger\,|\,\Omega\,\rangle. \end{aligned} \tag{4.119}$$ 3fpn3

Calculations of the remaining three matrix elements is very simple if we take into account the canonical commutation relation $\hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a}$ and the fact that $\hat{a}|\,\Omega\,\rangle = 0$. We just 3fpn4 state the results

$$\langle\,\Omega\,|\,\hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger\,|\,\Omega\,\rangle = 0, \tag{4.120a}$$ 3fpn4a

$$\langle\,\Omega\,|\,\hat{a}^2(\hat{a}^\dagger)^2\,|\,\Omega\,\rangle = 2, \tag{4.120b}$$ 3fpn4b

$$\langle\,\Omega\,|\,\hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger\,|\,\Omega\,\rangle = 1. \tag{4.120c}$$ 3fpn4c

Inserting results (3fpn4 4.120) into (3fpn3 4.119) we obtain

$$\begin{aligned}\langle\, n^2\,\rangle = \langle\,(\hat{a}^\dagger\hat{a})^2\,\rangle \;&=\; 2\,\cosh^2(\rho)\sinh^2(\rho) \;+\; \sinh^4(\rho) \\ &= \sinh^4(\rho) \;+\; \frac{1}{2}\,\sinh^2(2\rho). \end{aligned} \tag{4.121}$$ 3fpn5

The variance of the photon number in the vacuum squeezed state follows from (3fpn5 4.121) and (3sqnf3 4.113). It is

$$\sigma^2(n) = \langle\, n^2\,\rangle - \langle\, n\,\rangle^2 = \frac{1}{2}\,\sinh^2(2\rho). \tag{4.122}$$ 3fpn6

Let us now discuss relative fluctuations, as we did it for the field in the coherent state as in (f2s43 4.46). In the present case of squeezed vacuum we have

$$\frac{\sqrt{\sigma^2(n)}}{\langle\, n\,\rangle} = \frac{\sinh(2\rho)}{\sqrt{2}\,\sinh^2(\rho)} = \sqrt{2}\;\frac{\cosh(\rho)}{\sinh(\rho)}. \tag{4.123}$$ 3fpn7

Since $\sqrt{\langle\, n\,\rangle} = \sinh(\rho)$ according to (3sqnf3 4.113), we can write the relative fluctuations as

$$\frac{\sqrt{\sigma^2(n)}}{\langle\, n\,\rangle} = \sqrt{2}\;\frac{\cosh(\rho)}{\sqrt{\langle\, n\,\rangle}} > \frac{1}{\sqrt{\langle\, n\,\rangle}}. \tag{4.124}$$ 3fpn8

Comparing this result with (f2s43 4.46) we can say that relative photon number fluctuations in vacuum squeezed state are larger than in the coherent state, because $\cosh(\rho) \geq 1$.

4.3.5 Similarity relations for operators $\hat{a}^2$, $(\hat{a}^\dagger)^2$, $\hat{a}^\dagger\hat{a}$

In the main text (see (f3s14 4.77)) and in the appendix (z2squ9 B.53) we have already used the following x2sac similarity relations for annihilation and creation operators

$$S^\dagger(\xi)\,\hat{a}\,S(\xi) = \hat{a}\cosh(\rho) \;-\; \hat{a}^\dagger\,e^{i\theta}\sinh(\rho), \tag{4.125a}$$ x2saca

$$S^\dagger(\xi)\,\hat{a}^\dagger\,S(\xi) = \hat{a}^\dagger\cosh(\rho) \;-\; \hat{a}\,e^{-i\theta}\sinh(\rho). \tag{4.125b}$$ x2sacc

Since operator $S(\xi)$ is a unitary one, it is straightforward to utilize these formulas to compute other similarity relations. Therefore, we will only give the results, without a detailed derivation, which in fact, reduces to performing some operator multiplication. We also note that, when necessary, we use the canonical commutation relation $\hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a}$. The similarities which we will employ in further developments are as follows.

For the square of the annihilation operator

$$\begin{aligned} S^\dagger(\xi)\,\hat{a}^2\,S(\xi) &= S^\dagger(\xi)\,\hat{a}\,S(\xi)\;\; S^\dagger(\xi)\,\hat{a}\,S(\xi) \\ &= \hat{a}^2\cosh^2(\rho) \;-\; (2\hat{a}^\dagger\hat{a}+1)\,e^{i\theta}\sinh(\rho)\cosh(\rho) \\ &\qquad +\; (\hat{a}^\dagger)^2\,e^{2i\theta}\sinh^2(\rho). \end{aligned} \tag{4.126}$$

x2saa

Analogous similarity relation for the square of the creation operator follows by hermitian conjugation and yields

$$\begin{aligned} S^\dagger(\xi)\,(\hat{a}^\dagger)^2\,S(\xi) &= S^\dagger(\xi)\,\hat{a}^\dagger\,S(\xi)\;\; S^\dagger(\xi)\,\hat{a}^\dagger\,S(\xi) \\ &= (\hat{a}^\dagger)^2\cosh^2(\rho) \;-\; (2\hat{a}^\dagger\hat{a}+1)\,e^{-i\theta}\sinh(\rho)\cosh(\rho) \\ &\qquad +\; (\hat{a})^2\,e^{-2i\theta}\sinh^2(\rho). \end{aligned} \tag{4.127}$$

x2scc

Finally, for photon number operator we get

$$\begin{aligned} S^\dagger(\xi)\,\hat{a}^\dagger\hat{a}\,S(\xi) &= S^\dagger(\xi)\,\hat{a}^\dagger\,S(\xi)\;\; S^\dagger(\xi)\,\hat{a}\,S(\xi) \\ &= \hat{a}^\dagger\hat{a}\cosh^2(\rho) \;+\; (\hat{a}^\dagger\hat{a}+1)\sinh^2(\rho) \\ &\qquad -\; [\hat{a}^2\,e^{-i\theta} + (\hat{a}^\dagger)^2\,e^{i\theta}]\sinh(\rho)\cosh(\rho). \end{aligned} \tag{4.128}$$

x2sca

We shall need these relation in our next steps.

4.3.6 Expectation value for $\vec{\mathbf{E}}_\perp^2$ in squeezed vacuum state

Using notation introduced earlier in (4.68) we investigate the expectation value of the square of the electric field which is in the squeezed vacuum state. Thus, we write

$$\begin{aligned} \langle\,\vec{\mathbf{E}}_\perp^2\,\rangle &= \langle\,0,\xi\,|\,\vec{\mathbf{E}}_\perp^2\,|\,0,\xi\,\rangle \\ &= -\,\frac{\hbar\omega}{2\epsilon_0 V}\,\langle\,\big(\,\hat{a}\,e^{i\phi} - \hat{a}^\dagger\,e^{-i\phi}\,\big)^2\,\rangle \\ &= \frac{\hbar\omega}{2\epsilon_0 V}\,\langle\,\big(\,2\hat{a}^\dagger\hat{a} + 1 - \hat{a}^2\,e^{2i\phi} - (\hat{a}^\dagger)^2\,e^{-2i\phi}\,\big)\,\rangle \end{aligned} \tag{4.129}$$

x2ee1

from the definition (4.76) of the squeezed vacuum state we have

$$\begin{aligned} \langle\,\vec{\mathbf{E}}_\perp^2\,\rangle \;=\; \frac{\hbar\omega}{2\epsilon_0 V}\,\big\{ & 1 + 2\langle\,\Omega\,|\,S^\dagger(\xi)\,\hat{a}^\dagger\hat{a}\,S(\xi)\,|\,\Omega\,\rangle \\ & - \langle\,\Omega\,|\,S^\dagger(\xi)\,\hat{a}^2\,S(\xi)\,|\,\Omega\,\rangle\,e^{2i\phi} \\ & - \langle\,\Omega\,|\,S^\dagger(\xi)\,(\hat{a}^\dagger)^2\,S(\xi)\,|\,\Omega\,\rangle\,e^{-2i\phi}\big\}\,. \end{aligned} \tag{4.130}$$

x2ee2

We have to consider each of the three matrix elements using similarity relations (4.126)–(4.128). For the term involving the photon number operator we get

$$\begin{aligned}\langle\,\Omega\,|\,S^{\dagger}(\xi)\,\hat{a}^{\dagger}\hat{a}\,S(\xi)\,|\,\Omega\,\rangle &= \langle\,\Omega\,|\,\big\{\hat{a}^{\dagger}\hat{a}\cosh^2(\rho)\;+\;(\hat{a}^{\dagger}\hat{a}+1)\sinh^2(\rho)\\ &\qquad -\;[\hat{a}^2\,e^{-i\theta}+(\hat{a})^2\,e^{i\theta}]\sinh(\rho)\cosh(\rho)\big\}\,|\,\Omega\,\rangle\\ &= \sinh^2(\rho). \qquad (4.131)\end{aligned}$$

x2elm1

The next term includes the square of the annihilation operator. For this term we get

$$\begin{aligned}\langle\,\Omega\,|\,S^{\dagger}(\xi)\,\hat{a}^2\,S(\xi)\,|\,\Omega\,\rangle &= \langle\,\Omega\,|\,\big\{\hat{a}^2\cosh^2(\rho)\;-\;(2\hat{a}^{\dagger}\hat{a}+1)\,e^{i\theta}\sinh(\rho)\cosh(\rho)\\ &\qquad +\;(\hat{a}^{\dagger})^2\,e^{2i\theta}\sinh^2(\rho)\big\}\,|\,\Omega\,\rangle\\ &= -\,e^{i\theta}\sinh(\rho)\cosh(\rho). \qquad (4.132)\end{aligned}$$

x2elm2

The last term with the square of creation operator follows by hermitian conjugation of the previous one

$$\langle\,\Omega\,|\,S^{\dagger}(\xi)\,(\hat{a}^{\dagger})^2\,S(\xi)\,|\,\Omega\,\rangle = -\,e^{-i\theta}\sinh(\rho)\cosh(\rho). \qquad (4.133)$$

x2elm3

Inserting the obtained matrix elements into Eq.(4.130) we express the expectation value of the square of the field as

$$\begin{aligned}\langle\,\vec{\mathbf{E}}_{\perp}^2\,\rangle &= \frac{\hbar\omega}{2\epsilon_0 V}\big\{1+2\sinh^2(\rho)\\ &\qquad +\,e^{i\theta}\sinh(\rho)\cosh(\rho)\,e^{2i\phi}\;+\;e^{-i\theta}\sinh(\rho)\cosh(\rho)\,e^{-2i\phi}\big\}\\ &= \frac{\hbar\omega}{2\epsilon_0 V}\big\{1+2\sinh^2(\rho)\;+\;2\sinh(\rho)\cosh(\rho)\cos(\theta+2\phi)\big\}. \qquad (4.134)\end{aligned}$$

x2ee3

Due to well-known properties of the hyperbolic functions we have $2\sinh(\rho)\cosh(\rho) = \sinh(2\rho)$ and $1+2\sinh^2(\rho) = \cosh(2\rho)$. Therefore we obtain

$$\begin{aligned}\langle\,\vec{\mathbf{E}}_{\perp}^2(\vec{\mathbf{x}},t)\,\rangle &= \frac{\hbar\omega}{2\epsilon_0 V}\left[\cosh(2\rho)\;+\;\sinh(2\rho)\cos(\theta+2\phi)\right].\\ &= \frac{\hbar\omega}{2\epsilon_0 V}\left[\,e^{-2\rho}\;+\;\sinh(2\rho)\,(1+\cos(\theta+2\phi))\right]. \qquad (4.135)\end{aligned}$$

x2ee4

First of all, we note that in the absence of squeezing, that is when $\rho = 0$, formula (4.135) exactly reproduces the expectation value (4.7) which is characteristic for the pure vacuum state $|\,\Omega\,\rangle$. Next, we recall that $\phi = \vec{\mathbf{k}}\cdot\vec{\mathbf{x}} - \omega t$. Therefore, we conclude that there exist such space-time points in which the cosine in (4.135) equals minus unity. Then, we have

$$\langle\,\vec{\mathbf{E}}_{\perp}^2\,\rangle \;=\; \frac{\hbar\omega}{2\epsilon_0 V}\left[\cosh(2\rho)\;-\;\sinh(2\rho)\right] \;=\; \frac{\hbar\omega}{2\epsilon_0 V}\,e^{-2\rho}. \qquad (4.136)$$

x2ee5

This relation may be interpreted as showing that in certain regions of space-time the field is squeezed, while in some other ones it is not necessarily the case. We will not present a detailed investigation of the temporal and/or spatial dependencies of squeezing. It suffices to realize, that squeezing may occur only in some regions of space-time, not necessarily everywhere.

4.4 Squeezed coherent states

4.4.1 Introductory remarks

We have already investigated the squeezed vacuum states (4.76) defined as $|\,0,\xi\,\rangle = S(\xi)|\,\Omega\,\rangle$. We also know that a displacement operator $D(z) = \exp(z\hat{a}^\dagger - z^*\hat{a})$ when applied to the vacuum state $|\,\Omega\,\rangle$ produces a coherent state $|\,z\,\rangle = D(z)|\,\Omega\,\rangle$. Thus we see that we have two alternatives to construct new quantum-mechanical states of the radiation field, namely

$$|\,\alpha,\xi\,\rangle = D(\alpha)S(\xi)|\,\Omega\,\rangle, \tag{4.137a}$$

$$|\,z,\xi\,\rangle = S(\xi)D(z)|\,\Omega\,\rangle. \tag{4.137b}$$

The question is whether these two possible definitions are equivalent or not. To answer this question we refer to Appendix. In eq.(B.57) we have shown that

$$D(\alpha)\,S(\xi) \;=\; S(\xi)\,D(z), \tag{4.138}$$

where $\xi = \rho\,e^{i\theta}$ as previously, while α and z are complex numbers connected by the relations

$$z = \alpha\cosh(\rho) + \alpha^* e^{i\theta}\sinh(\rho) \tag{4.139a}$$

$$\alpha = z\cosh(\rho) - z^* e^{i\theta}\sinh(\rho), \tag{4.139b}$$

which can be written equivalently, as

$$\mathrm{Re}\left(z\,e^{-i\theta/2}\right) = e^{\rho}\,\mathrm{Re}\left(\alpha\,e^{-i\theta/2}\right), \tag{4.140a}$$

$$\mathrm{Im}\left(z\,e^{-i\theta/2}\right) = e^{-\rho}\,\mathrm{Im}\left(\alpha\,e^{-i\theta/2}\right). \tag{4.140b}$$

These relations allow discussion of two possible definitions of the coherent squeezed states (4.137). Therefore we conclude that the states (4.137a) and (4.137b) are the same, provided relations (4.139) or, equivalently, (4.140) are met.

We can say that squeezing of vacuum (done by $S(\xi)$) followed by displacement (performed by $D(\alpha)$) leads to a squeezed coherent state $|\,\alpha,\xi\,\rangle = D(\alpha)S(\xi)|\,\Omega\,\rangle$. This has the same effect as a displacement (by $D(z)$) of the vacuum state followed by squeezing $S(\xi)$, provided the parameters α and z are connected by relations (4.139) or (4.140). So we can consider either the state $|\,\alpha,\xi\,\rangle$, or the $|\,z,\xi\,\rangle$. Due to relations (4.139)– (4.140) we can easily transform results concerning $|\,\alpha,\xi\,\rangle$ into those corresponding to $|\,z,\xi\,\rangle$ or vice versa. The choice between the two states is rather a matter of convenience, and less of physics.

We note, that we have used the name "squeezed coherent state" not really knowing whether the discussed states are indeed squeezed or not. Hence we proceed to investigate the properties of these states and to validate the name associated with them.

4.4.2 Expectation values for $|\,z,\xi\,\rangle$

Here, we choose to investigate the expectation values for various operators, for the case when the radiation field is in the state

$$|\,z,\xi\,\rangle \;=\; S(\xi)D(z)|\,\Omega\,\rangle \;=\; S(\xi)|\,z\,\rangle. \tag{4.141}$$

According to our discussion above, we shall then transform our results to describe the other state: $|\,\alpha,\xi\,\rangle = D(\alpha)S(\xi)|\,\Omega\,\rangle$. The subsequent calculations are rather straightforward, so we only indicate main steps.

First, we compute the expectation value of the annihilation operator.

$$\langle\,\hat{a}\,\rangle \;=\; \langle\,z,\xi\,|\,\hat{a}\,|\,z,\xi\,\rangle \;=\; \langle\,\Omega\,|\,D^\dagger(z)S^\dagger(\xi)\hat{a}S(\xi)D(z)\,|\,\Omega\,\rangle \;=\; \langle\,z\,|\,S^\dagger(\xi)\hat{a}S(\xi)\,|\,z\,\rangle. \quad (4.142)$$ 3scea1

By similarity relation (f3s14a 4.77a) we get

$$\langle\,\hat{a}\,\rangle \;=\; \langle\,z\,|\,\left(\hat{a}\cosh(\rho) - \hat{a}^\dagger\, e^{i\theta}\sinh(\rho)\right)\,|\,z\,\rangle \;=\; z\cosh(\rho) - z^*\, e^{i\theta}\sinh(\rho). \quad (4.143)$$ 3scea2

As the second expectation value, we consider the one for photon number operator. Thus, we calculate as follows

$$\begin{aligned}\langle\,\hat{a}^\dagger\hat{a}\,\rangle &= \langle\,z,\xi\,|\,\hat{a}^\dagger\hat{a}\,|\,z,\xi\,\rangle \\ &= \langle\,\Omega\,|\,D^\dagger(z)S^\dagger(\xi)\;\hat{a}^\dagger\hat{a}\;S(\xi)D(z)\,|\,\Omega\,\rangle \\ &= \langle\,z\,|\,S^\dagger(\xi)\;\hat{a}^\dagger\;S(\xi)\;S^\dagger(\xi)\;\hat{a}\;S(\xi)\,|\,z\,\rangle \\ &= \langle\,z\,|\,\left(\hat{a}^\dagger\cosh(\rho) - \hat{a}\,e^{-i\theta}\sinh(\rho)\right)\left(\hat{a}\cosh(\rho) - \hat{a}^\dagger\,e^{i\theta}\sinh(\rho)\right)\,|\,z\,\rangle, \quad (4.144)\end{aligned}$$ 3scfn1

where we used the similarity relations (f3s14 4.77). Performing the multiplications and using the commutation relation for annihilation and creation operators, we get

$$\begin{aligned}\langle\,\hat{a}^\dagger\hat{a}\,\rangle \;&=\; \langle\,z\,|\,\Big[\,\hat{a}^\dagger\hat{a}\cosh^2(\rho) \;+\; \left(\hat{a}^\dagger\hat{a}+1\right)\sinh^2(\rho) \\ &\qquad -\hat{a}^2\,e^{-i\theta}\sinh(\rho)\cosh(\rho) - (\hat{a}^\dagger)^2\,e^{i\theta}\sinh(\rho)\cosh(\rho)\,\Big]\,|\,z\,\rangle \\ &=\; |z|^2\left(\cosh^2(\rho)+\sinh^2(\rho)\right) \;+\; \sinh^2(\rho) \\ &\qquad -\; z^2\,e^{-i\theta}\sinh(\rho)\cosh(\rho) \;-\; (z^*)^2\,e^{i\theta}\sinh(\rho)\cosh(\rho) \\ &=\; \left(z\cosh(\rho) \;-\; z^*\,e^{i\theta}\sinh(\rho)\right)\left(z^*\cosh(\rho) \;-\; z\,e^{-i\theta}\sinh(\rho)\right) \;+\; \sinh^2(\rho) \\ &=\; \left|z\cosh(\rho) \;-\; z^*\,e^{i\theta}\sinh(\rho)\right|^2 \;+\; \sinh^2(\rho) \quad (4.145)\end{aligned}$$ 3scfn2

We calculate the expectation value of the quadrature operator $\tilde{X}$ as the third one. In the similar manner we obtain

$$\begin{aligned}\langle\,\tilde{X}\,\rangle &= \langle\,z,\xi\,|\,\tilde{X}\,|\,z,\xi\,\rangle \\ &= \langle\,\Omega\,|\,D^\dagger(z)S^\dagger(\xi)\;\tilde{X}\;S(\xi)D(z)\,|\,\Omega\,\rangle \\ &= \langle\,z\,|\,\tilde{X}\,e^{-\rho}\,|\,z\,\rangle, \quad (4.146)\end{aligned}$$ 3scx1

where we used similarity relation (f3s29a 4.93a). Employing also the connection between old and new quadratures (f3s26a 4.91a) we have

$$\langle\,\tilde{X}\,\rangle \;=\; e^{-\rho}\,\langle\,z\,|\,\left(X\cos(\theta/2) \;+\; Y\sin(\theta/2)\right)\,|\,z\,\rangle. \quad (4.147)$$ 3scx2

Next, taking into account expectation values (f3s09b 4.73) taken in the coherent state $|\,z\,\rangle$ we get

$$\begin{aligned}\langle\,\tilde{X}\,\rangle &= e^{-\rho}\,\sqrt{2}\;\left[\,\mathrm{Re}(z)\cos(\theta/2) \;+\; \mathrm{Im}(z)\sin(\theta/2)\right] \\ &= e^{-\rho}\,\sqrt{2}\,\mathrm{Re}\left(z\,e^{-i\theta/2}\right) \quad (4.148)\end{aligned}$$ 3scx3

The fourth expectation value to consider is the one for the second quadrature. In this case we can calculate along the same lines as for $\tilde{X}$, but we will present a little different approach. At first, we start as for $\tilde{X}$, and using (4.93b) we get

$$\begin{aligned}\langle \tilde{Y} \rangle &= \langle z,\xi \,|\, \tilde{Y} \,|\, z,\xi \rangle \;=\; \langle \Omega \,|\, D^\dagger(z) S^\dagger(\xi)\, \tilde{Y}\, S(\xi) D(z) \,|\, \Omega \rangle \\ &= \langle z \,|\, \tilde{Y}\, e^{\rho} \,|\, z \rangle, \end{aligned} \tag{4.149}$$

3scy1

Next, we express the quadrature $\tilde{Y}$ via operators $\hat{b}$ and $\hat{b}^\dagger$ according to (4.87), then we use (4.83) to arrive at the expression with old annihilation and creation operators. This yields

$$\begin{aligned}\langle \tilde{Y} \rangle &= e^{\rho} \,\langle z \,|\, \frac{-i}{\sqrt{2}} \left(\hat{b} - \hat{b}^\dagger \right) \,|\, z \rangle \\ &= \frac{-i}{\sqrt{2}}\, e^{\rho} \,\langle z \,|\, \hat{a}\, e^{-i\theta/2} - \hat{a}^\dagger\, e^{i\theta/2} \,|\, z \rangle, \end{aligned} \tag{4.150}$$

3scy2

Then, by simple properties of usual coherent states we obtain

$$\begin{aligned}\langle \tilde{Y} \rangle &= e^{\rho}\, \frac{-i}{\sqrt{2}} \left(z\, e^{-i\theta/2} - z^*\, e^{i\theta/2} \right) \\ &= e^{\rho}\, \sqrt{2}\, \mathrm{Im}\left(z\, e^{-i\theta/2} \right) \end{aligned} \tag{4.151}$$

3scy3

In order to estimate the uncertainties we need also the expectation values of the squares of the quadratures. So we compute them. First we consider $\tilde{X}^2$, obtaining

$$\begin{aligned}\langle \tilde{X}^2 \rangle &= \langle z,\xi \,|\, \tilde{X}^2 \,|\, z,\xi \rangle \;=\; \langle \Omega \,|\, D^\dagger(z) S^\dagger(\xi)\, \tilde{X}^2\, S(\xi) D(z) \,|\, \Omega \rangle \\ &= \langle z \,|\, S^\dagger(\xi)\, \tilde{X}\, S(\xi)\; S^\dagger(\xi)\, \tilde{X}\, S(\xi) \,|\, z \rangle \;=\; e^{-2\rho} \,\langle z \,|\, \tilde{X}^2 \,|\, z \rangle, \end{aligned} \tag{4.152}$$

3scxx1

where we used similarity (4.93a). Expressing the quadrature via $\hat{b}$ and $\hat{b}^\dagger$ we get

$$\begin{aligned}\langle \tilde{X}^2 \rangle &= \frac{1}{2}\, e^{-\rho} \,\langle z \,|\, \left(\hat{b} \;+\; \hat{b}^\dagger \right)^2 \,|\, z \rangle \\ &= \frac{1}{2}\, e^{-\rho} \,\langle z \,|\, \left(\hat{b}^2 \;+\; (\hat{b}^\dagger)^2 \;+\; 2\hat{b}^\dagger \hat{b} \;+\; 1 \right) \,|\, z \rangle \end{aligned} \tag{4.153}$$

3scxx2

where we used the commutation relation (4.85). Going to old annihilation and creation operators as in (4.83) we get

$$\begin{aligned}\langle \tilde{X}^2 \rangle &= \frac{1}{2}\, e^{-2\rho} \,\langle z \,|\, \left(\hat{a}^2\, e^{-i\theta} \;+\; (\hat{a}^\dagger)^2\, e^{i\theta} \;+\; 2\, \hat{a}^\dagger \hat{a} \;+\; 1 \right) \,|\, z \rangle \\ &= \frac{1}{2}\, e^{-2\rho} \,\left(z^2\, e^{-i\theta} \;+\; (z^*)^2\, e^{i\theta} \;+\; 2|z|^2 \;+\; 1 \right) \\ &= \frac{1}{2}\, e^{-2\rho} \,\left[\left(z\, e^{-i\theta/2} \;+\; (z^*)\, e^{i\theta/2} \right)^2 \;+\; 1 \right] \\ &= \frac{1}{2}\, e^{-2\rho} \,\left[1 \;+\; 4\, \left(\mathrm{Re}(z\, e^{-i\theta/2}) \right)^2 \right]. \end{aligned} \tag{4.154}$$

3scxx3

Finally, we need the expectation value of the second quadrature. Since the calculation goes along exactly the same lines as for $\tilde{X}^2$ we now give only the final result

$$\begin{aligned}\langle \tilde{Y}^2 \rangle &= \langle z,\xi \,|\, \tilde{Y}^2 \,|\, z,\xi \rangle \;=\; \langle \Omega \,|\, D^\dagger(z) S^\dagger(\xi)\, \tilde{Y}^2\, S(\xi) D(z) \,|\, \Omega \rangle \\ &= \frac{1}{2}\, e^{2\rho} \,\left[1 \;+\; 4\, \left(\mathrm{Im}(z\, e^{-i\theta/2}) \right)^2 \right]. \end{aligned} \tag{4.155}$$

3scyy1

Having computed the necessary expectation values we are in position to write down the corresponding variances. From (4.148) and (4.154) for the first quadrature, from (4.151) and (4.155) for the second one we get the variances

3scv

$$\sigma^2(\tilde{X}) = \langle\, \tilde{X}^2 \,\rangle \;-\; \langle\, \tilde{X} \,\rangle^2 \;=\; e^{-2\rho}/2, \tag{4.156a}$$ 3scvx

$$\sigma^2(\tilde{Y}) = \langle\, \tilde{Y}^2 \,\rangle \;-\; \langle\, \tilde{Y} \,\rangle^2 \;=\; e^{2\rho}/2. \tag{4.156b}$$ 3scvy

To summarize, we have considered states of the radiation field which arise by first displacing and then squeezing of the vacuum state $|\, z, \xi \,\rangle = S(\xi)D(z)|\, \Omega \,\rangle$. We may also view this state as squeezing of the coherent state $|\, z, \xi \,\rangle = S(\xi)|\, z \,\rangle$. The expectation values of the quadratures (4.148) and (4.151) can be written as

$$\langle\, \tilde{X} \,\rangle \;=\; \sqrt{2}\ \mathrm{Re}\left(e^{-\rho}\, z\, e^{-i\theta/2}\right), \qquad \langle\, \tilde{Y} \,\rangle \;=\; \sqrt{2}\ \mathrm{Im}\left(e^{\rho}\, z\, e^{-i\theta/2}\right). \tag{4.157}$$ 3scq

Comparing these results with Eqs.(4.95) we can say that they indeed correspond to some specific coherent state. Moreover, we see that the considered state is a minimum uncertainty state, since the product of variances equals 1/4. On the other hand, one of the variances is reduced below 1/2 – the vacuum limit, and the second is correspondingly enhanced. Thus, we see that we indeed can call the state $|\, z, \xi \,\rangle = S(\xi)D(z)|\, \Omega \,\rangle$ a coherent squeezed state.

4.4.3 Expectation values for $|\, \alpha, \xi \,\rangle$

Now, we proceed to investigate the similar expectation values, but for the state of the radiation field defined as

$$|\, \alpha, \xi \,\rangle \;=\; D(\alpha)S(\xi)|\, \Omega \,\rangle, \tag{4.158}$$ 3sqal

which is first squeezed and then displaced. Due to relations (4.139) and (4.140) we have an easy connection between two types of squeezed coherent states. So in principle we can just rewrite previous results with suitable replacements of z by α, as indicated in (4.139) and (4.140).

However, the direct computation may be of interest. The reason is as follows. Calculation with $|\, z, \xi \,\rangle = S(\xi)D(z)|\, \Omega \,\rangle = S(\xi)|\, z \,\rangle$, was simplified since in fact we have dealt with the coherent state $|\, z \,\rangle$. We only had to consider similarity transformations induced by squeeze operator. In the present case we also need the similarities induced by a displacement operator $D(\alpha)$. Therefore, we first consider such similarities.

3dad

First we recall already used similarity relations

$$D^\dagger(\alpha)\, \hat{a}\, D(\alpha) = \hat{a} + \alpha \tag{4.159a}$$ 3dada

$$D^\dagger(\alpha)\, \hat{a}^\dagger\, D(\alpha) = \hat{a}^\dagger + \alpha^*. \tag{4.159b}$$ 3dadc

Other similarity relations for combinations of annihilation and creation operators follow from the two given above. For example, we evidently have for the photon number operator

$$D^\dagger(\alpha)\, \hat{a}^\dagger\hat{a}\, D(\alpha) \;=\; \hat{a}^\dagger\hat{a} + \alpha\hat{a}^\dagger + \alpha^*\hat{a} + |\alpha|^2. \tag{4.160}$$ 3daad

Since old quadratures X and Y are combinations of $\hat{a}$ and $\hat{a}^\dagger$ (f3s02 4.65) we easily find that

$$D^\dagger(\alpha)\, X\, D(\alpha) = \frac{1}{\sqrt{2}}\, D^\dagger(\alpha)(\hat{a}+\hat{a}^\dagger)D(\alpha) \;=\; \frac{1}{\sqrt{2}}\left(\hat{a}+\alpha+\hat{a}^\dagger+\alpha^*\right)$$
$$= X + \sqrt{2}\ \mathrm{Re}(\alpha). \qquad (4.161)$$ 3dxd

In completely analogous manner we get

$$D^\dagger(\alpha)\, Y\, D(\alpha) \;=\; Y + \sqrt{2}\ \mathrm{Im}(\alpha). \qquad (4.162)$$ 3dyd

3dxyd Since new quadratures are linear combinations of the old ones (f3s26 4.91) we obtain

$$D^\dagger(\alpha)\, \tilde{X}\, D(\alpha) = \tilde{X} + \sqrt{2}\ \mathrm{Re}\left(\alpha\, e^{-i\theta/2}\right), \qquad (4.163a)$$ 3dxydx
$$D^\dagger(\alpha)\, \tilde{Y}\, D(\alpha) = \tilde{Y} + \sqrt{2}\ \mathrm{Im}\left(\alpha\, e^{-i\theta/2}\right). \qquad (4.163b)$$ 3dxydy

Having collected auxiliary relations we can proceed to calculations of various expectation values for the state $|\,\alpha,\xi\,\rangle = D(\alpha)S(\xi)|\,\Omega\,\rangle$. As previously, we start with the annihilation operator. Using similarity relation (3dada 4.159a) we simply get

$$\langle\,\hat{a}\,\rangle = \langle\,\alpha,\xi\,|\,\hat{a}\,|\,\alpha,\xi\,\rangle \;=\; \langle\,\Omega\,|\,S^\dagger(\xi)D^\dagger(\alpha)\,\hat{a}\,D(\alpha)S(\xi)\,|\,\Omega\,\rangle$$
$$= \langle\,\Omega\,|\,S^\dagger(\xi)(\hat{a}+\alpha)S(\xi)\,|\,\Omega\,\rangle \;=\; \alpha + \langle\,\Omega\,|\,S^\dagger(\xi)\,\hat{a}\,S(\xi)\,|\,\Omega\,\rangle \;=\; \alpha. \qquad (4.164)$$ 3aaav

The remaining matrix element vanished due to (f3s14x 4.78) – it reproduces the corresponding expectation value for the squeezed vacuum. If we take into account the relation (3zaa 4.139b) then we see that (3aaav 4.164) reproduces exactly (3scea2 4.143), as it should.

The next expectation value concerns photon number operator. Employing (3daad 4.160) we get

$$\langle\,\hat{a}^\dagger\hat{a}\,\rangle = \langle\,\alpha,\xi\,|\,\hat{a}^\dagger\hat{a}\,|\,\alpha,\xi\,\rangle \;=\; \langle\,\Omega\,|\,S^\dagger(\xi)D^\dagger(\alpha)\,\hat{a}^\dagger\hat{a}\,D(\alpha)S(\xi)\,|\,\Omega\,\rangle$$
$$= \langle\,\Omega\,|\,S^\dagger(\xi)\left(\hat{a}^\dagger\hat{a}+\alpha\hat{a}^\dagger+\alpha^*\hat{a}+|\alpha|^2\right)S(\xi)\,|\,\Omega\,\rangle$$
$$= |\alpha|^2 + \langle\,\Omega\,|\,S^\dagger(\xi)\,\hat{a}^\dagger\hat{a}\,S(\xi)\,|\,\Omega\,\rangle \qquad (4.165)$$ 3safn

because terms linear in annihilation and creation operators do not contribute, as it was the case with squeezed vacuum state [see (f3s14x 4.78). The last term is the same as for squeezed vacuum, hence from (3sqnf3 4.113) we get

$$\langle\,\hat{a}^\dagger\hat{a}\,\rangle \;=\; |\alpha|^2 + \langle\,0,\xi\,|\,\hat{a}^\dagger\hat{a}\,|\,0,\xi\,\rangle \;=\; |\alpha|^2 + \sinh^2(\rho). \qquad (4.166)$$ 3safn1

Noting that (3zaa 4.139b) holds, we see that the above relation exactly reproduces (3scfn2 4.145), as it should.

To study squeezed states we must investigate the expectation values of quadratures. So we proceed to do that. The expectation value of the first of the new quadratures is found by using similarity relation (3dxydx 4.163a) and it is

$$\langle\,\tilde{X}\,\rangle = \langle\,\alpha,\xi\,|\,\tilde{X}\,|\,\alpha,\xi\,\rangle \;=\; \langle\,\Omega\,|\,S^\dagger(\xi)D^\dagger(\alpha)\,\tilde{X}\,D(\alpha)S(\xi)\,|\,\Omega\,\rangle$$
$$= \langle\,\Omega\,|\,S^\dagger(\xi)\left(\tilde{X}+\sqrt{2}\ \mathrm{Re}(\alpha\, e^{-i\theta/2})\right)S(\xi)\,|\,\Omega\,\rangle$$
$$= \sqrt{2}\ \mathrm{Re}(\alpha\, e^{-i\theta/2}) \;+\; \langle\,\Omega\,|\,S^\dagger(\xi)\,\tilde{X}\,S(\xi)\,|\,\Omega\,\rangle$$
$$= \sqrt{2}\ \mathrm{Re}(\alpha\, e^{-i\theta/2}), \qquad (4.167)$$ 3sxt1

where the last result follows from (4.94a) or from (4.97) for the squeezed vacuum state. Due to connection (4.140a) we see that the obtained formula (4.167) reproduces (4.148).

In the exactly the same manner we obtain the expectation value of the second quadrature. The result is

$$\langle \tilde{Y} \rangle = \langle \alpha, \xi | \tilde{Y} | \alpha, \xi \rangle = \sqrt{2}\, \mathrm{Im}(\alpha\, e^{-i\theta/2}), \tag{4.168}$$ 3syt1

which in turn, reproduces (4.151) when we take into account (4.140b). Comparing the obtained expectation values with (4.95) we see that we indeed have the expectations for a coherent state.

To estimate the variances we also need the expectation values of the squares of the quadratures. Hence, using the square of the similarity (4.163a) we get

$$\begin{aligned}\langle \tilde{X}^2 \rangle = \langle \alpha, \xi | \tilde{X}^2 | \alpha, \xi \rangle &= \langle \Omega | S^\dagger(\xi) D^\dagger(\alpha)\, \tilde{X}^2\, D(\alpha) S(\xi) | \Omega \rangle \\ &= \langle \Omega | S^\dagger(\xi) \left(\tilde{X} + \sqrt{2}\, \mathrm{Re}(\alpha\, e^{-i\theta/2}) \right)^2 S(\xi) | \Omega \rangle \\ &= 2 \left[\mathrm{Re}(\alpha\, e^{-i\theta/2}) \right]^2 + \langle \Omega | S^\dagger(\xi)\, \tilde{X}^2\, S(\xi) | \Omega \rangle, \end{aligned} \tag{4.169}$$ 3sxxt1

because due to (4.97), the term linear in $\tilde{X}$ does not contribute. The remaining matrix element is identical to the one for squeezed vacuum (4.105), so we obtain

$$\langle \tilde{X}^2 \rangle = \langle \alpha, \xi | \tilde{X}^2 | \alpha, \xi \rangle = \frac{1}{2}\, e^{-2\rho} + 2 \left[\mathrm{Re}(\alpha\, e^{-i\theta/2}) \right]^2, \tag{4.170}$$ 3sxxt2

which, together with (4.140a) is clearly identical to (4.154), as it is expected to be. Computation of the expectation value of $\tilde{Y}^2$ is evidently similar and it yields

$$\langle \tilde{Y}^2 \rangle = \langle \alpha, \xi | \tilde{Y}^2 | \alpha, \xi \rangle = \frac{1}{2}\, e^{2\rho} + 2 \left[\mathrm{Im}(\alpha\, e^{-i\theta/2}) \right]^2, \tag{4.171}$$ 3syyt2

which coincides with (4.155), when we replace α by z according to (4.140b).

Corresponding variances follow immediately from Eqs.(4.170), (4.167), (4.171) and (4.168). We easily obtain 3scvv

$$\sigma^2(\tilde{X}) = \langle \tilde{X}^2 \rangle - \langle \tilde{X} \rangle^2 = \frac{1}{2}\, e^{-2\rho}, \tag{4.172a}$$ 3scvvx

$$\sigma^2(\tilde{Y}) = \langle \tilde{Y}^2 \rangle - \langle \tilde{Y} \rangle^2 = \frac{1}{2}\, e^{2\rho}, \tag{4.172b}$$ 3scvvy

We conclude that we can in fact repeat the comments given after Eqs.(4.157). Both states $|\, z, \xi \rangle = S(\xi) D(z) |\, \Omega \rangle$ and $|\, \alpha, \xi \rangle = D(\alpha) S(\xi) |\, \Omega \rangle$ are indeed squeezed states and since the expectation values of quadratures correspond to coherent state, they can be called coherent squeezed states.

4.5 Squeezed photon number states

4.5.1 New role of squeezed vacuum state

The vacuum state $|\, \Omega \rangle$ is an eigenstate of the annihilation operator belonging to the eigenvalue zero. On the other hand, the squeeze operator $S(\xi)$ is a unitary one. Therefore we can write

$$0 = \hat{a} |\, \Omega \rangle = \hat{a} S^\dagger(\xi) S(\xi) |\, \Omega \rangle = \hat{a} S^\dagger(\xi) |\, 0, \xi \rangle, \tag{4.173}$$ 3sqn1

where $|\,0,\xi\,\rangle$ is the squeezed vacuum state defined in (4.76). The obvious conclusion from this relation is

$$S(\xi)\hat{a}S^{\dagger}(\xi)|\,0,\xi\,\rangle = 0. \tag{4.174}$$ 3sqn2

The operators on the left do not have a typical form of the similarity relation, so we may ask a question: what kind of an operator is the one appearing in the lhs of (4.174). The answer is simple, if we notice that $S(\xi)$ is unitary and $S^{\dagger}(\xi) = S^{-1}(\xi) = S(-\xi)$. Thus, we can define the operator

$$\hat{c} = S(\xi)\hat{a}S^{\dagger}(\xi) = S^{\dagger}(-\xi)\hat{a}S(-\xi). \tag{4.175}$$ 3cdef

Recalling similarity relation (4.77a) we note that $-\xi = -\rho\, e^{i\theta}$ and that sinh is an odd function. Therefore we get 3cc

$$\hat{c} = S^{\dagger}(-\xi)\hat{a}S^{\dagger}(-\xi) \;=\; \hat{a}\cosh(\rho) + \hat{a}^{\dagger}\, e^{i\theta}\sinh(\rho), \tag{4.176a}$$ 3cca

$$\hat{c}^{\dagger} = S^{\dagger}(-\xi)\hat{a}^{\dagger}S^{\dagger}(-\xi) \;=\; \hat{a}^{\dagger}\cosh(\rho) + \hat{a}\, e^{-i\theta}\sinh(\rho), \tag{4.176b}$$ 3ccc

Definition of $\hat{c}$ operators allows us to check the commutation relation

$$\begin{aligned}\left[\,\hat{c},\;\hat{c}^{\dagger}\,\right] &= \left[\hat{a}\cosh(\rho) + \hat{a}^{\dagger}\, e^{i\theta}\sinh(\rho),\;\hat{a}^{\dagger}\cosh(\rho) + \hat{a}\, e^{-i\theta}\sinh(\rho)\,\right] \\ &= \cosh^2(\rho) - \sinh^2(\rho) \;=\; 1,\end{aligned} \tag{4.177}$$ 3ccom

which shows that operators $\hat{c}$ and $\hat{c}^{\dagger}$ are also annihilation and creation operators. Thus relation (4.174) is equivalent to

$$\hat{c}|\,0,\xi\,\rangle = 0. \tag{4.178}$$ 3sqnv

We can interpret this expression as follows. The vacuum squeezed state $|\,0,\xi\,\rangle$ plays the role of the vacuum state for the annihilation operator $\hat{c}$. This clearly suggest the following definition of the new states of a single mode electromagnetic field

$$|\,n,\xi\,\rangle \;=\; \frac{(\hat{c}^{\dagger})^n}{\sqrt{n!}}\;|\,0,\xi\,\rangle, \tag{4.179}$$ 3sndef

and tempts us to call these states – squeezed photon number states. This, however, requires some discussion, we have to see if these states have the necessary properties. Obviously they are number states for operators $\hat{c}$ and $\hat{c}^{\dagger}$, so we can write 3scan

$$\hat{c}\,|\,n,\xi\,\rangle = \sqrt{n}\;|\,n-1,\xi\,\rangle \tag{4.180a}$$ 3scana

$$\hat{c}^{\dagger}\,|\,n,\xi\,\rangle = \sqrt{n+1}\;|\,n+1,\xi\,\rangle \tag{4.180b}$$ 3scanc

$$\hat{c}^{\dagger}\hat{c}\,|\,n,\xi\,\rangle = n\,|\,n,\xi\,\rangle \tag{4.180c}$$ 3scann

So our next steps should be aimed at investigation of the properties of the newly introduced quantum states of the field.

4.5.2 Squeezed photon number states

Firstly, we study the definition (3sndef 4.179). Expressing $\hat{c}^\dagger$ according to the hermitian conjugate of (3cdef 4.175) and using the definition of the vacuum squeezed state we get

$$|\,n,\xi\,\rangle = \frac{(\hat{c}^\dagger)^n}{\sqrt{n!}}\,|\,0,\xi\,\rangle \;=\; \frac{\left[S(\xi)\,\hat{a}^\dagger\,S^\dagger(\xi)\right]^n}{\sqrt{n!}}\,S(\xi)\,|\,\Omega\,\rangle$$
$$= \frac{1}{\sqrt{n!}}\,S(\xi)\,(\hat{a}^\dagger)^n\,S^\dagger(\xi)S(\xi)\,|\,\Omega\,\rangle \;=\; S(\xi)\,\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|\,\Omega\,\rangle \;=\; S(\xi)|\,n\,\rangle, \qquad (4.181)$$ 3sqn3

which, at least partly, justifies the name "squeezed photon number state". Nevertheless, it remains to check whether this state is indeed squeezed, in the sense defined earlier. To do so we need to study the variances of quadratures of the field.

So we investigate the expectation values of the new quadratures $\tilde{X}$ and $\tilde{Y}$. The simple averages follow from (3sqn3 4.181) and from (f3s17 4.83) 3snq

$$\langle\,\tilde{X}\,\rangle = \langle\,n,\xi\,|\,\tilde{X}\,|\,n,\xi\,\rangle = \langle\,n\,|\,S^\dagger(\xi)\,\tilde{X}\,S(\xi)\,|\,n\,\rangle = 0, \qquad (4.182a)$$ 3snqx
$$\langle\,\tilde{Y}\,\rangle = \langle\,n,\xi\,|\,\tilde{Y}\,|\,n,\xi\,\rangle = \langle\,n\,|\,S^\dagger(\xi)\,\tilde{Y}\,S(\xi)\,|\,n\,\rangle = 0. \qquad (4.182b)$$ 3snqy

The expectation values of the quadratures vanish, as it is the case for a usual photon number state $|\,n\,\rangle$. So we proceed to compute the expectation values of the squares of the quadratures. We start with the $\tilde{X}$ quadrature

$$\langle\,\tilde{X}^2\,\rangle \;=\; \langle\,n,\xi\,|\,\tilde{X}^2\,|\,n,\xi\,\rangle = \langle\,n\,|\,S^\dagger(\xi)\tilde{X}^2S(\xi)\,|\,n\,\rangle = \langle\,n\,|\,\Big(S^\dagger(\xi)\,\tilde{X}\,S(\xi)\Big)^2\,|\,n\,\rangle \qquad (4.183)$$ 3snxx1

In this case we have to be more careful, since we deal with product of operators. We shall proceed similarly as in (3scxx1 4.152)-(3scxx3 4.154). The present case differs from the previous one only by the presence of photon number states instead of coherent ones. So we can write

$$\langle\,\tilde{X}^2\,\rangle \;=\; \frac{1}{2}\,e^{-2\rho}\,\langle\,n\,|\,\left(\hat{a}^2\,e^{-i\theta} \;+\; (\hat{a}^\dagger)^2\,e^{i\theta} \;+\; 2\,\hat{a}^\dagger\hat{a} \;+\; 1\right)\,|\,n\,\rangle. \qquad (4.184)$$ 3snxx2

The two first terms do not contribute, hence we have

$$\langle\,\tilde{X}^2\,\rangle \;=\; \frac{1}{2}\,e^{-2\rho}\;(2n+1)\,. \qquad (4.185)$$ 3snxx3

Clearly, the similar calculation for the second quadrature yields

$$\langle\,\tilde{Y}^2\,\rangle \;=\; \langle\,n,\xi\,|\,\tilde{Y}^2\,|\,n,\xi\,\rangle \;=\; \frac{1}{2}\,e^{2\rho}\;(2n+1)\,. \qquad (4.186)$$ 3snyy3

The averages (3sng 4.182) and the expectation values of the squares of quadratures allow us to write the corresponding variances

$$\sigma^2(\tilde{X}) \;=\; \frac{1}{2}\,e^{-2\rho}\,(2n+1), \qquad\qquad \sigma^2(\tilde{Y}) \;=\; \frac{1}{2}\,e^{2\rho}\,(2n+1). \qquad (4.187)$$ 3snvar

The product of these variances is

$$\sigma^2(\tilde{X})\,\sigma^2(\tilde{Y}) \;=\; \frac{1}{4}\,(2n+1)^2 \geq \frac{1}{4}, \qquad (4.188)$$ 3snun

which is characteristic for the photon number states. State $|\,n,\xi\,\rangle$ is not minimalizing the uncertainty relation. Nevertheless, for given (but arbitrary) n we can choose the real number ρ in such a way that one of the variances will attain a value less than $1/2$, that is below the magnitude which is characteristic for the vacuum state. Thus, we see that the name *squeezed number state*, for the state $|\,n,\xi\,\rangle$, may be considered justified.

4.6 Expansion of squeezed vacuum state into n-photon states

Considering the coherent states, we have expanded the coherent state $|\, z \,\rangle$ into n-photon ones in Eq.(4.28). We now intend to find a similar expansion for the squeezed vacuum state, that is we look for series

$$|\, 0, \xi \,\rangle \;=\; \sum_{n=0}^{\infty} A_n(\xi)\, |\, n \,\rangle. \tag{4.189}$$ 3svn1

Finding this expansion means finding the explicit expression for coefficients $A_n(\xi)$. In order to do so, we recall that the squeezed vacuum state $|\, 0, \xi \,\rangle$ is a vacuum for the operator $\hat{c}$ as in (4.178), with annihilation operator $\hat{c}$ related to "usual" ones by (4.176a). Now, we apply operator $\hat{c}$ to both sides of (4.189) obtaining

$$0 \;=\; \sum_{n=0}^{\infty} A_n(\xi)\, \hat{c}\, |\, n \,\rangle. \tag{4.190}$$ 3svn2

Expressing operator $\hat{c}$ via (4.176a) we get

$$0 \;=\; \cosh(\rho) \sum_{n=0}^{\infty} A_n(\xi)\, \hat{a}\, |\, n \,\rangle \;+\; e^{i\theta} \sinh(\rho) \sum_{n=0}^{\infty} A_n(\xi)\, \hat{a}^{\dagger}\, |\, n \,\rangle. \tag{4.191}$$ 3svn3

We know how operators $\hat{a}$ and $\hat{a}^{\dagger}$ act on n-photon states. We also note that the term $n = 0$ in the first sum vanishes, hence we have

$$0 \;=\; \cosh(\rho) \sum_{n=1}^{\infty} A_n(\xi) \sqrt{n}\; |\, n-1 \,\rangle \;+\; e^{i\theta} \sinh(\rho) \sum_{n=0}^{\infty} A_n(\xi) \sqrt{n+1}\; |\, n+1 \,\rangle. \tag{4.192}$$ 3svn4

In the first sum we change the summation index $n \to m = n - 1$, with $m = 0, 1, 2, \ldots$, and we take the term $m = 0$ out of the sum. In the second sum we also introduce a new summation index $n \to m = n + 1$, with $m = 1, 2, 3, \ldots$. Then from (4.192) we get

$$\begin{aligned} 0 = \cosh(\rho) A_1(\xi)\, |\, 0 \,\rangle \;+\; & \cosh(\rho) \sum_{m=1}^{\infty} A_{m+1}(\xi) \sqrt{m+1}\; |\, m \,\rangle \\ & +\; e^{i\theta} \sinh(\rho) \sum_{m=1}^{\infty} A_{m-1}(\xi) \sqrt{n}\; |\, m \,\rangle. \end{aligned} \tag{4.193}$$ 3svn5

This relation obviously implies that

$$A_1 \;\equiv\; 0. \tag{4.194}$$ 3svn6

Moreover, the kets $|\, n \,\rangle$ are the basis of the space of state vectors of the field. Thus, all the coefficients must be equal to zero. Therefore, we arrive at the relation

$$\cosh(\rho) \sqrt{m+1}\; A_{m+1}(\xi) \;=\; -\, e^{i\theta} \sinh(\rho) \sqrt{m}\; A_{m-1}(\xi), \tag{4.195}$$ 3svn7

which is equivalent to the recurrence relation

$$A_{m+1}(\xi) \;=\; -\; e^{i\theta}\tanh(\rho)\,\sqrt{\frac{m}{m+1}}\;A_{m-1}(\xi), \qquad \text{for} \quad m=1,2,3,\ldots \tag{4.196}$$ 3svn8

This recurrence is valid for $m>1$, so we conclude that A_0 is the first unknown coefficient. Since $A_1=0$, we see that only coefficients with even index are nonzero. In other words, all coefficients with odd index are equal to zero.

Putting $m=2k+1$ in recurrence relation (3svn8 4.196) we rewrite it as

$$A_{2k+2}(\xi) \;=\; -\; e^{i\theta}\tanh(\rho)\,\sqrt{\frac{2k+1}{2k+2}}\;A_{2k}(\xi), \qquad \text{for} \quad k=0,1,2,\ldots \tag{4.197}$$ 3svn9

Writing down several first coefficients, we can easily generalize the recurrence relation, which enables us to write

$$A_{2k}(\xi) \;=\; (-1)^k\,e^{ik\theta}\tanh^k(\rho)\,\sqrt{\frac{(2k-1)!!}{(2k)!!}}\;A_0(\xi), \qquad \text{for} \quad k=1,2,3,\ldots \tag{4.198}$$ 3svn10

It is straightforward to check (by induction) that the expression (3svn10 4.198) agrees with the recurrence relation (3svn8 4.196). The coefficient $A_0(\xi)$ is unknown, and must be determined from the requirement of normalization of the vacuum squeezed state $|\,0,\xi\,\rangle$. Before we do so, let us consider the term with factorials. It is evident that

$$(2k)!! \;=\; 2^k k!, \qquad \text{and} \qquad (2k)! \;=\; (2k)!!(2k-1)!!, \tag{4.199}$$ 3svn11

Which implies that

$$\frac{(2k-1)!!}{(2k)!!} \;=\; \frac{(2k)!}{[(2k)!!]^2} \;=\; \frac{(2k)!}{(2^k k!)^2}, \tag{4.200}$$ 3svn12

which, after inserting into (3svn10 4.198) gives

$$A_{2k}(\xi) \;=\; (-1)^k\,\frac{e^{ik\theta}}{k!}\left(\frac{\tanh(\rho)}{2}\right)^k\;\sqrt{(2k)!}\;A_0(\xi), \qquad \text{for} \quad k=1,2,3,\ldots \tag{4.201}$$ 3svn13

We use the obtained coefficients in the expansion (3svn1 4.189), we also account for the fact that odd terms are absent, and we have

$$|\,0,\xi\,\rangle \;=\; A_0(\xi)\;\sum_{k=0}^{\infty}\;(-1)^k\,\frac{e^{ik\theta}}{k!}\left(\frac{\tanh(\rho)}{2}\right)^k\;\sqrt{(2k)!}\;|\,2k\,\rangle. \tag{4.202}$$ 3svn14

It remains to find the coefficient $A_0(\xi)$ from the normalization requirement. Since the n-photon states are orthonormal, we easily obtain

$$1 \;=\; \langle\,0,\xi\,|\,0,\xi\,\rangle \;=\; |A_0(\xi)|^2\;\sum_{k=0}^{\infty}\;\frac{(2k)!}{(k!)^2}\left(\frac{\tanh(\rho)}{2}\right)^{2k}. \tag{4.203}$$ 3svn15

So it is necessary to perform the remaining summation. This not an easy task. To do so, we first note that from the definition of Hermite polynomials we have for ones of even order

$$H_{2k}(x) \;=\; (2k)! \sum_{m=0}^{k} \; (-1)^m \; \frac{(2x)^{2k-2m}}{m!\,(2k-2m)!}, \tag{4.204}$$ 3herm1

so, for $x = 0$ only the term with $m = k$ does not vanish. Hence, we have

$$H_{2k}(x=0) \;=\; (2k)! \; \frac{(-1)^k}{k!}. \tag{4.205}$$ 3herm2

This allows us to reexpress the terms under summation in (4.203), which is therefore rewritten as

$$1 \;=\; |A_0(\xi)|^2 \; \sum_{k=0}^{\infty} \; \frac{1}{(k!)} \left(- \; \frac{\tanh^2(\rho)}{4} \right)^k \; H_{2k}(x=0). \tag{4.206}$$ 3svn16

Since $\tanh^2(\rho) < 1$, the sum rule (C.1) applies. The summation is, thus, performed and we arrive at the formula

$$1 \;=\; |A_0(\xi)|^2 \; \frac{1}{\sqrt{1-\tanh^2(\rho)}} \;=\; |A_0(\xi)|^2 \cosh(\rho), \tag{4.207}$$ 3svn17

because $\cosh(\rho)$ is always positive. Denoting an arbitrary phase by φ, we express the last expansion coefficient as

$$A_0(\xi) \;=\; \frac{e^{i\varphi}}{\sqrt{\cosh(\rho)}}. \tag{4.208}$$ 3svn18

We adopt the overall phase $\varphi = 0$, then we insert A_0 into expansion (4.202) and we get

$$|\,0,\xi\,\rangle \;=\; \frac{1}{\sqrt{\cosh(\rho)}} \; \sum_{k=0}^{\infty} \; (-1)^k \; \frac{e^{ik\theta}}{k!} \left(\frac{\tanh(\rho)}{2} \right)^k \; \sqrt{(2k)!} \; |\,2k\,\rangle. \tag{4.209}$$ 3svn19

If we employ the expression (4.205) we can transform the obtained formula into

$$|\,0,\xi\,\rangle \;=\; \sum_{k=0}^{\infty} \; \frac{(-1)^k \, e^{ik\theta}}{\sqrt{k!\,\cosh(\rho)}} \left(\frac{\tanh(\rho)}{2} \right)^k \; \sqrt{(-1)^k H_{2k}(0)} \; |\,2k\,\rangle. \tag{4.210}$$ 3svn20

Combining the powers of (-1) into exponential phase we have

$$|\,0,\xi\,\rangle \;=\; \sum_{k=0}^{\infty} \; \frac{e^{ik(\theta+3\pi/2)}}{\sqrt{\Gamma(k+1)\,\cosh(\rho)}} \left(\frac{\tanh(\rho)}{2} \right)^k \; \sqrt{H_{2k}(0)} \; |\,2k\,\rangle. \tag{4.211}$$ 3svn21

At this point we can generalize this result by noting that Hermite polynomials of odd order taken at $x = 0$ are equal to zero, i.e., $H_{2k+1}(x = 0) = 0$. Therefore, we can include the odd terms in the sum (4.211) and we can write

$$|\,0,\xi\,\rangle \;=\; \sum_{n=0}^{\infty} \; \frac{e^{i(\theta+3\pi/2)n/2}}{\sqrt{\Gamma(n/2+1)\,\cosh(\rho)}} \left(\frac{\tanh(\rho)}{2} \right)^{n/2} \; \sqrt{H_n(0)} \; |\,n\,\rangle, \tag{4.212}$$ 3svn22

where the odd terms (with odd n) give the zero contribution, while the even terms (in which $n = 2k$) reproduce the sum (4.211). The obtained expression is the sought expansion of the vacuum squeezed state in the n-photon states. The coefficients of the expansion are the probability amplitudes. Therefore, we can say that

$$P_n(\xi) \;=\; \left|\frac{1}{2}\,\tanh(\rho)\right|^n \frac{|H_n(0)|}{\Gamma(n/2+1)\,\cosh(\rho)}, \tag{4.213}$$

is the probability that for the field in the vacuum squeezed state $|\,0,\xi\,\rangle$ we find n photons. We note that this probability is zero for n odd, while for n even, that is for $n = 2k$ it reads

$$P_{2k}(\xi) \;=\; \left|\frac{1}{2}\,\tanh(\rho)\right|^{2k} \frac{|H_{2k}(0)|}{\Gamma(k+1)\,\cosh(\rho)} \;=\; \left|\frac{1}{2}\,\tanh(\rho)\right|^{2k} \frac{1}{\cosh(\rho)}\,\frac{(2k)!}{(k!)^2}, \tag{4.214}$$

where we used relation (4.205). The squeezed vacuum state $|\,0,\xi\,\rangle = S(\xi)|\,\Omega\,\rangle$, and P_n is the probability that for the field in this state, we find n photons. The fact that $P_{2k+1}(\xi) \equiv 0$ seems not to be very surprising. Operator $S(\xi) = \exp[\xi^*\hat{a}^2/2 - \xi(\hat{a}^\dagger)^2/2)]$, while operators $\hat{a}^2$ and $(co)^2$ correspond either to destruction or to creation of two photons. Hence $S(\xi)|\,\Omega\,\rangle$ is composed of n-photon states in which photons are created (or annihilated) in pairs. Therefore, only $P_{2k})(\xi)$ may be expected to be nonzero.

4.7 Equivalence of coherent squeezed states $|\,z,\xi\,\rangle$ and $|\,\alpha,\xi\,\rangle$

Let us consider the coherent squeezed state (4.137b): $|\,z,\xi\,\rangle = S(\xi)D(z)|\,\Omega\,\rangle = S(\xi)|\,0,\xi\,\rangle$, and expand the coherent state $|\,z\,\rangle$ into photon number states according to (4.28). Then we get

$$\begin{aligned}
|\,z,\xi\,\rangle &= S(\xi)\exp\left(-\tfrac{1}{2}|z|^2\right)\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,|\,n\,\rangle \\
&= \exp\left(-\tfrac{1}{2}|z|^2\right)\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,S(\xi)\,|\,n\,\rangle \\
&= \exp\left(-\tfrac{1}{2}|z|^2\right)\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,|\,n,\xi\,\rangle,
\end{aligned} \tag{4.215}$$

where we used the definition (4.181) of the squeezed photon number states. Next we employ (4.179) to write

$$\begin{aligned}
|\,z,\xi\,\rangle &= \exp\left(-\tfrac{1}{2}|z|^2\right)\sum_{n=0}^{\infty}\frac{z^n\,(\hat{c}^\dagger)^2}{n!}\,|\,0,\xi\,\rangle, \\
&= \exp\left(-\tfrac{1}{2}|z|^2\right)\,e^{z\hat{c}^\dagger}\,|\,0,\xi\,\rangle.
\end{aligned} \tag{4.216}$$

The state $|\,0,\xi\,\rangle$ is an eigenstate of the annihilation operator $\hat{c}$. Thus The above formula is equivalent to

$$|\,z,\xi\,\rangle \;=\; \exp\left(-\tfrac{1}{2}|z|^2\right)\,e^{z\hat{c}^\dagger}\,e^{-z^*\hat{c}}\,|\,0,\xi\,\rangle. \tag{4.217}$$

Operators $\hat{c}^\dagger$ and $\hat{c}$ are creation and annihilation operators, thus relation (B.27b) (with $\alpha = -z^*$ and $\beta = z$) applies, and we get

$$\exp\left(-\tfrac{1}{2}|z|^2\right)\, e^{z\hat{c}^\dagger}\, e^{-z^*\hat{c}} \;=\; \exp\left(z\hat{c}^\dagger - z^*\hat{c}\right). \tag{4.218}$$

We combine two last equations, and we obtain

$$|\, z,\xi\,\rangle \;=\; \exp\left(z\hat{c}^\dagger - z^*\hat{c}\right)\, |\, 0,\xi\,\rangle \;=\; \exp\left(z\hat{c}^\dagger - z^*\hat{c}\right) S(\xi)|\,\Omega\,\rangle. \tag{4.219}$$

Next we need to consider the exponent in the leftmost operator. Due to relations (4.176)

$$\begin{aligned} z\hat{c}^\dagger - z^*\hat{c} &= z\left(\hat{a}^\dagger\cosh(\rho) + \hat{a}\, e^{-i\theta}\sinh(\rho)\right) \;-\; z^*\left(\hat{a}\cosh(\rho) + \hat{a}^\dagger\, e^{i\theta}\sinh(\rho)\right) \\ &= \alpha\,\hat{a}^\dagger - \alpha * *\,\hat{a}, \end{aligned} \tag{4.220}$$

where we have denoted $\alpha = z\cosh(\rho) - z^*\, e^{i\theta}\sinh(\rho)$. Introducing this new variable into Eq.(4.219) we have

$$|\, z,\xi\,\rangle \;=\; \exp\left(\alpha\hat{a}^\dagger - \alpha^*\hat{a}\right) S(\xi)|\,\Omega\,\rangle. \tag{4.221}$$

Recognizing the displacement operator we summarize our calculations by

$$|\, z,\xi\,\rangle \;=\; S(\xi)D(z)|\,\Omega\,\rangle \;=\; D(\alpha)S(\xi)|\,\Omega\,\rangle \;=\; |\,\alpha,\xi\,\rangle \tag{4.222}$$

provided the complex numbers z and α are connected by the relation

$$\alpha = z\cosh(\rho) - z^*\, e^{i\theta}\sinh(\rho). \tag{4.223}$$

This result is in full agreement with the discussion of two possible squeezed coherent states. This fact elucidates the sense of the squeezed photon number states. They have the same relation to squeezed coherent states as the corresponding usual number states to usual coherent ones. Obviously, the derivation presented here could have been done in the reversed direction, leading to the same final conclusion.

* *

Chapter 5

Atom–field interaction. Dipole approach

c:af

5.1 Hamiltonian of the system

In this chapter we consider an atom interacting with electromagnetic field. Therefore, we must construct the corresponding hamiltonian. It consists of three terms

$$H = H_A \otimes \hat{\mathbf{1}}_F + \hat{\mathbf{1}}_A \otimes H_F + H_{AF}, \tag{5.1}$$ i1

where H_A is the atomic hamiltonian, H_F corresponds to the field hamiltonian, while H_{AF} describes the interaction between two parts of the system under consideration.

5.1.1 Atomic hamiltonian

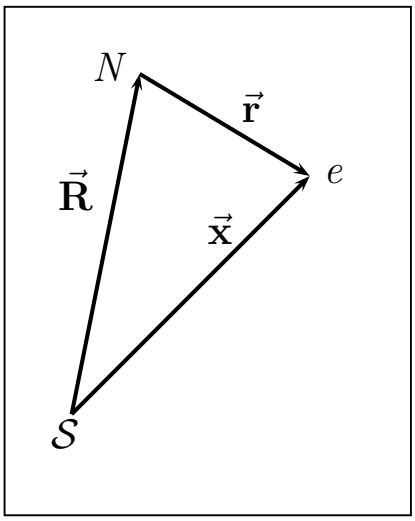

Fig. 5.1: Positions of atomic nucleus and its electron in arbitrary coordinate frame.

f:i1

We consider a simple one-electron atom. The center of an atom (its nucleus) is positioned at the point denoted by the vector $\vec{\mathbf{R}}$. The electron, with respect to the nucleus has radius vector $\vec{\mathbf{r}}$, while with respect to the point $\mathcal{S}$ – the center of the coordinate system, electron's position is given by a vector $\vec{\mathbf{x}}$. The atom as a single whole may perform a uniform motion. Such a case of a moving atom, if time permits, will be considered later (in next chapters). Then its position $\vec{\mathbf{R}}$ will be a time-dependent function varying (usually linearly) with time. Transforming our description to the center-of-mass frame we can separate the kinetic energy of an atom as a whole from its internal degrees of freedom. The latter ones are then given in the relative coordinates. Then, atomic kinetic energy is just a constant in the hamiltonian and as such can be neglected. So, we consider the electron motion in the center-of-mass frame. We denote by m the electron's reduced mass, which is very close to the well-known electron mass (the nucleus is much heavier than the electron). We assume that in the center-of-mass frame the Hamilto-

nian H_A of the atom may be diagonalized, that is the necessary stationary Schrödinger equation can be solved. We denote the eigenstates of H_A by $|\,a\,\rangle$ and the corresponding energies by $\hbar\omega_a$. Therefore, the standard hamiltonian of a free atom can be written as

$$H_A = \frac{\vec{\mathbf{p}}^2}{2m} + V(r) = \hbar \sum_a \omega_a |\,a\,\rangle\langle\,a\,|. \tag{5.2}$$ i2a

By definition states $|\,a\,\rangle$ are the eigenstates of the atomic hamiltonian:

$$H_A|\,a\,\rangle = \hbar\omega_a\,|\,a\,\rangle, \tag{5.3}$$ i2b

and are orthonormal and complete:

$$\langle\,a\,|\,b\,\rangle = \delta_{ab}, \qquad \text{and} \qquad \sum_a |\,a\,\rangle\langle\,a\,| = 1. \tag{5.4}$$ i2c

The set of vectors $\{|\,a\,\rangle\}$ is numbered by index a which may consists of several quantum numbers (as it is the case for the hydrogen-like atom). Eigenfrequencies ω_a are allowed to be degenerate, that is, it may happen that $\omega_a = \omega_b$ for different indices a and b.

5.1.2 Field hamiltonian

As we know from previous considerations, the hamiltonian of the quantized electromagnetic field is od the form

$$H_F = \sum_{\vec{\mathbf{k}}\lambda} \hbar\omega_k a^\dagger_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda}, \tag{5.5}$$ i5

where $a^\dagger_{\vec{\mathbf{k}}\lambda}$ and akl are annihilation and creation operators corresponding to the field mode specified by wave vector $\vec{\mathbf{k}}$ and polarization λ. The states of the field belong to the Fock space and are of the form

$$|\,\psi_F\,\rangle = \otimes_{\vec{\mathbf{k}},\lambda} |\,n_{\vec{\mathbf{k}},\lambda}\,\rangle, \tag{5.6}$$ i6

where numbers $n_{\vec{\mathbf{k}},\lambda}$ are nonnegative integers. We also recall that the wave vector $\vec{\mathbf{k}}$ and the frequency satisfy the dispersion relation

$$\omega_k = c\,\big|\vec{\mathbf{k}}\big|. \tag{5.7}$$ i7

5.1.3 Interaction hamiltonian

Interaction hamiltonian H_{AF} is essential in our considerations. Due to the analogy to classical physics, we take the interaction hamiltonian in the following form

$$H_{AF} = -\vec{\mathbf{d}} \cdot \vec{\mathbf{E}}(\vec{\mathbf{R}}, t), \tag{5.8}$$ i11

where $\vec{\mathbf{d}} = e\,\vec{\mathbf{r}}$ is the electric dipole moment of the atom, and $\vec{\mathbf{E}}(\vec{\mathbf{R}}, t)$ the electric field of the incident electromagnetic field taken at the position of the atomic nucleus (center of mass). This hamiltonian is called a dipole-interaction one. The given name has two

explanations. Firstly, there appears the dipole moment of an atom which will be discussed later. Secondly, it must be noted that the electric field is taken in the center of the atom $\vec{\mathbf{R}}$, and not at the position $\vec{\mathbf{x}}$ of the electron. This is clearly an approximation justified by the following argument. The influence of the incident light on the atom will be appreciable if its frequency ω_k has the same order of magnitude as some of the atomic frequencies ω_a. The statement that $\omega_a \approx \omega_k$ leads to appreciable effects can be supported, for example, by simple time-dependent perturbation theory. This is a notion of resonance – the nonresonant events are quite improbable. Atomic frequencies are typically within optical range, then field frequencies must also lie in this region. This means that the wavelength λ of light is of the order of 500 nm. The size of an atom is smaller roughly by three orders of magnitude. Therefore $|\vec{\mathbf{r}}| \ll \lambda$. As a conclusion we can say that $\vec{\mathbf{R}} \approx \vec{\mathbf{x}}$ which explains why we used $\vec{\mathbf{R}}$ instead of $\vec{\mathbf{x}}$ in the definition (5.8). This approximation is called a dipole one and explains the name of the interaction hamiltonian.

Electric field of the incident light is written as

$$\vec{\mathbf{E}} = \sum_{\vec{\mathbf{k}}\lambda} \left[\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} + \vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} \right], \tag{5.9}$$

where we have denoted

$$\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} = i \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}}\, \vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda} \exp\left(i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}\right), \tag{5.10a}$$

$$\vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} = -i \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}}\, \vec{\mathbf{e}}^{\,*}_{\vec{\mathbf{k}}\lambda} a^{\dagger}_{\vec{\mathbf{k}}\lambda} \exp\left(i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}\right), \tag{5.10b}$$

according to our discussion in the previous chapters. Let us, however, stress that the quantized electromagnetic field is a dynamic quantity. The time dependence is "hidden" in the annihilation and creation operators. Combining relations (5.8) and (5.9) we write the interaction hamiltonian as

$$H_{AF} = -\sum_{\vec{\mathbf{k}}\lambda} \vec{\mathbf{d}} \cdot \left[\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} + \vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} \right]. \tag{5.11}$$

In priciple, the summation runs over all modes. It may lead to the divergences (as discussed earlier). Hence, in practical case some care might be necessary.

5.1.4 Atomic dipole moment and interaction hamiltonian

It remains to specify the electric dipole moment of the atom. We use eigenstates of the hamiltonian (5.3), which allows us to write

$$\vec{\mathbf{d}} = \sum_a |\, a \,\rangle\langle\, a \,|\; \vec{\mathbf{d}} \sum_b |\, b \,\rangle\langle\, b \,| = \sum_{a,b} |\, a \,\rangle\langle\, b \,|\; \vec{\mathbf{d}}_{ab}, \tag{5.12}$$

where $\vec{\mathbf{d}}_{ab}$ is the matrix element defined as

$$\vec{\mathbf{d}}_{ab} = \langle\, a \,|\, \vec{\mathbf{d}} \,|\, b \,\rangle = \int d^3r\; \langle\, a \,|\, \vec{\mathbf{r}} \,\rangle\langle\, \vec{\mathbf{r}} \,|\, \vec{\mathbf{d}} \,|\, b \,\rangle. \tag{5.13}$$

In the position representation we have $\vec{\mathbf{d}} = q\vec{\mathbf{r}}$, hence we can write (due to principles of quantum mechanics)

$$\vec{\mathbf{d}}_{ab} = \langle\, a \,|\, \vec{\mathbf{d}} \,|\, b \,\rangle = q \int d^3r \; \psi_a^*(\vec{\mathbf{r}}) \; \vec{\mathbf{r}} \; \psi_b(\vec{\mathbf{r}}). \tag{5.14}$$ i16c

In many typical atoms wave functions possess the property of parity, then diagonal elements of the atomic dipole vanish

$$\vec{\mathbf{d}}_{aa} = 0. \tag{5.15}$$ i16d

Usually $\left|\psi_a(\vec{\mathbf{r}})\right|^2$ is an even function, so that the integrand in (5.14) is odd and the integral yields zero. In other words, we consider atoms which do not have any permanent dipole moment.

Introducing Eq.(5.12) into hamiltonian (5.11) we obtain

$$H_{AF} = -\sum_{\vec{\mathbf{k}}\lambda} \sum_{a,b} |\, a \,\rangle\langle\, b \,| \vec{\mathbf{d}}_{ab} \cdot \left[\, \vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} + \vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} \,\right]. \tag{5.16}$$ i17

This hamiltonian (as any quantum-mechanical observable) must be hermitian. To see that this the case, lest us split expression (5.16) and write

$$H_{AF} = -\sum_{\vec{\mathbf{k}}\lambda} \sum_{a,b} \left\{ |\, a \,\rangle\langle\, b \,|\, \vec{\mathbf{d}}_{ab} \cdot \vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} + |\, a \,\rangle\langle\, b \,|\, \vec{\mathbf{d}}_{ab} \cdot \vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} \right\}. \tag{5.17}$$ i18a

The sum over (a, b) runs over all atomic states (the case $\vec{\mathbf{d}}_{aa} = 0$ is allowed), hence in the second term we can interchange indices $a \leftrightarrow b$, moreover, since $\vec{\mathbf{d}}_{ba} = \vec{\mathbf{d}}^*_{ab}$ we get

$$H_{AF} = -\sum_{\vec{\mathbf{k}}\lambda} \sum_{a,b} \left\{ |\, a \,\rangle\langle\, b \,|\, \vec{\mathbf{d}}_{ab} \cdot \vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} + |\, b \,\rangle\langle\, a \,|\, \vec{\mathbf{d}}^*_{ab} \cdot \vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} \right\}, \tag{5.18}$$ i18c

which is clearly hermitian, as it should be. This hamiltonian will be employed in a variety of applications. Obviously, its specific form will have to be adapted to particular physical situations.

5.1.5 Semiclassical approximation

Semiclassical approximation consists in quantum-mechanical description of an atom but in the classical treatment of the field. In such a case annihilation and creation operators in (5.10) are replaced by classical amplitudes $a_{\vec{\mathbf{k}}\lambda} \to \alpha_{\vec{\mathbf{k}},\lambda} \exp\left[-i\omega_k t\right]$. As a result we take

$$\vec{\mathbf{E}}^{(\pm)}_{\vec{\mathbf{k}},\lambda} = \vec{\mathbf{E}}^{(\pm)}_{\vec{\mathbf{k}},\lambda}(0) \exp\left[\pm i \left(\vec{\mathbf{k}} \cdot \vec{\mathbf{R}} - \omega_k t\right)\right], \tag{5.19}$$ i21

where $\vec{\mathbf{E}}^{(\pm)}_{\vec{\mathbf{k}},\lambda}(0)$ are classical field amplitudes (given vectors). Field energy, in the classical case is well-defined and, as such can be omitted in the total hamiltonian. Moreover, we can write

$$H_{AF} = -\sum_{\vec{\mathbf{k}}\lambda} \sum_{a,b} \left\{ |\, a \,\rangle\langle\, b \,|\, \vec{\mathbf{d}}_{ab} \cdot \vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} + |\, b \,\rangle\langle\, a \,|\, \vec{\mathbf{d}}^*_{ab} \cdot \vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} \right\}, \tag{5.20}$$ i22

with fields specified in Eq.(5.19).

5.2 Hamiltonian for two–level atom in radiation field

5.2.1 The two-level atom. Free hamiltonian

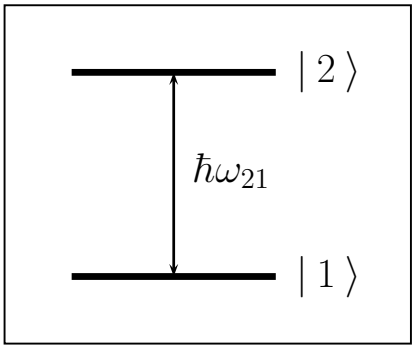

Fig. 5.2: The level scheme of a two-level atom.

4f:tla

In many practical cases the electromagnetic field irradiating an atom is closely tuned to one of the atomic resonances and has a relatively narrow spectral bandwidth equal to $\Delta\omega_L$. In such a case only two atomic levels with energy separation $\hbar\omega_{21}$ close to the central frequency ω_L of the field, are strongly coupled to the incoming radiation. Moreover, if the other levels are separated by much more than $\Delta\omega_L$, we can safely disregard all other levels, except those two coupled to the field. Then we may say that we deal with a two-level approximation to the real atom. We shall still make an additional simplifying assumption. Namely, we will assume that the considered two levels do not exhibit spatial degeneracy. This means, that we do not consider the angular momentum issues, which reduces the atomic basis just to two states, and two quantum numbers (numbering the levels) are sufficient to fully describe the state of the atom. The Hilbert space of these states is, thus, two-dimensional. It may be worth noting, that it is possible to prepare such states of real atoms that are indeed well described by a two-level model. Moreover, investigations of two-level atom give excellent insights in the phenomena occurring in real atoms.

So, we restrict our attention to the simplest two-level atom (TLA) model, and we denote upper (excited) state of a TLA by $|\,2\,\rangle$ and lower (ground) state by $|\,1\,\rangle$. The space spanned by the states $|\,1\,\rangle$ and $|\,2\,\rangle$ is two-dimensional, it is isomorphic to the space of the eigenstates of spin 1/2 states. Therefore, (for future purposes) we make a natural identification

$$|\,2\,\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |\,1\,\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{5.21}$$

i31

The hamiltonian of the free TLA may be then written as it follows from (5.2), that is

i2a

$$H_A = \hbar\omega_1 |\,1\,\rangle\langle\,1\,| + \hbar\omega_2 |\,2\,\rangle\langle\,2\,|. \tag{5.22}$$

i32a

This form is fairly self-evident. We can, however, select other forms of the Hamiltonian for TLA, depending on the choice of the zero on the energy scale. When we take zero energy at the ground level, then we can write

$$H_A = \hbar\omega_{21} |\,2\,\rangle\langle\,2\,|. \tag{5.23}$$

i32b

Another possibility consists in choosing the zero of energy midway between the levels. Then, we can rewrite hamiltonian (5.22) as

i32a

$$H_A = \frac{1}{2}\hbar\omega_{21}\Big[\,|\,2\,\rangle\langle\,2\,| - |\,1\,\rangle\langle\,1\,|\,\Big] = \hbar\omega_{21} S_3, \tag{5.24}$$

i32c

where S_3 is the third component of the quasi–spin operator (for the details see the corresponding appendix). Since the space of $|\,1\,\rangle$ and $|\,2\,\rangle$ is two-dimensional, the corresponding operators can be associated with 2×2 matrices, and are expressible by Pauli matrices. These operators can also be expressed by the so-called pseudo-spin operators introduced and discussed in appendix. We will use pseudo-spin operators without reference to particular formulas given in that appendix, which should be consulted if necessary.

5.2.2 Interaction hamiltonian. Rotating wave approximation

Obviously, the total hamiltonian of TLA-light system contains three terms as in (5.1). The interaction hamiltonian should be, however, transformed to suit our current needs. Moreover, as is was already discussed, we will take

$$\vec{\mathbf{d}}_{11} = \vec{\mathbf{d}}_{22} = 0. \tag{5.25}$$ i34

The specific form of the interaction hamiltonian follows from general expression (5.18), which (due to (5.25)) gives

$$H_{AF} = -\sum_{\vec{\mathbf{k}}\lambda} \Big\{ |\,1\,\rangle\langle\,2\,|\, \vec{\mathbf{d}}_{12} \cdot \vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} \;+\; |\,2\,\rangle\langle\,1\,|\, \vec{\mathbf{d}}^{*}_{12} \cdot \vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} + |\,2\,\rangle\langle\,1\,|\, \vec{\mathbf{d}}_{21} \cdot \vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} \;+\; |\,1\,\rangle\langle\,2\,|\, \vec{\mathbf{d}}^{*}_{21} \cdot \vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda} \Big\}. \tag{5.26}$$ i35

Let us carefully discuss all four terms which appear in the above given expression.

- Operator $|\,1\,\rangle\langle\,2\,|$ corresponds to the transition $|\,2\,\rangle \to |\,1\,\rangle$ (downwards). We expect the photon to be emitted. The field term $\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda}$ contains annihilation operator – photon disappears.

- Operator $|\,2\,\rangle\langle\,1\,|$ corresponds to the transition $|\,1\,\rangle \to |\,2\,\rangle$ (upwards). We expect the photon to be absorbed. The field term $\vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda}$ contains creation operator – a new photon appears.

- Operator $|\,2\,\rangle\langle\,1\,|$ corresponds to the transition $|\,1\,\rangle \to |\,2\,\rangle$ (upwards). We expect the photon to be absorbed. The field term $\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda}$ contains annihilation operator – the photon disappears.

- Operator $|\,1\,\rangle\langle\,2\,|$ corresponds to the transition $|\,2\,\rangle \to |\,1\,\rangle$ (downwards). We expect the photon to be emitted. The field term $\vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda}$ contains creation operator – a new photon appears.

This discussion shows that two first terms in (5.26) are, so to speak, nonresonant. Intuitively speaking, they do not satisfy the principle of energy conservation. For example, the first term describes the process in which an atom losses energy (transition $|\,2\,\rangle \to |\,1\,\rangle$) and also the energy of the field decreases (one photon is annihilated). This heuristic argument justifies the possibility to neglect the first two terms in the hamiltonian (5.26). This is clearly an approximation, which is called *rotating wave approximation (RWA)*. It can be shown, that the neglected terms lead to small corrections called Bloch-Siegert shifts.

Another argument supporting RWA follows from the notions of time-dependent perturbation theory. From this theory we know that nonresonant terms give negligibly small transition probabilities. Thus nonresonant terms may be neglected and droped out of consideration. Thus, we adopt RWA and write our interaction hamiltonian

$$H_{AF} = -\sum_{\vec{\mathbf{k}}\lambda} \Big\{ |\,2\,\rangle\langle\,1\,|\;\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} \;+\; |\,1\,\rangle\langle\,2\,|\;\vec{\mathbf{d}}^{*}_{21}\cdot\vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda}\Big\}, \tag{5.27}$$ i36

with the fields given by Eqs.(5.10). Let us remind, that the dynamical (time) dependence is "hidden" in the annihilation and creation operators.

5.2.3 Semiclassical approximation

The fundamental ideas behind semiclassical approximation were discussed earlier. Here, we only need to adapt what was said before to the present needs. We replace the field operators $\vec{\mathbf{E}}^{(\pm)}_{\vec{\mathbf{k}},\lambda}$ appearing in the hamiltonian (5.27) by classical functions (5.19)

$$H_{AF} = -\sum_{\vec{\mathbf{k}}\lambda} \Big\{ |\,2\,\rangle\langle\,1\,|\;\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda}(0)\;e^{i(\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}-\omega_k t)} \;+\; |\,1\,\rangle\langle\,2\,|\;\vec{\mathbf{d}}_{12}\cdot\vec{\mathbf{E}}^{(-)}_{\vec{\mathbf{k}},\lambda}\;e^{-i(\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}-\omega_k t)}\Big\}, \tag{5.28}$$ i43

It is convenient to introduce the following notation

$$\frac{\hbar}{2}\,\Omega_{\vec{\mathbf{k}},\lambda} = \vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda}(0), \qquad \text{or, equivalently} \qquad \Omega_{\vec{\mathbf{k}},\lambda} = \frac{2}{\hbar}\,\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda}(0), \tag{5.29}$$ i44

where quantities $\Omega_{\vec{\mathbf{k}},\lambda}$ are called *Rabi frequencies*. Then, hamiltonian (5.28) is rewritten as

$$H_{AF} = -\frac{\hbar}{2}\sum_{\vec{\mathbf{k}}\lambda} \Big\{ |\,2\,\rangle\langle\,1\,|\;\Omega_{\vec{\mathbf{k}},\lambda}\;e^{i(\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}-\omega_k t)} \;+\; |\,1\,\rangle\langle\,2\,|\;\Omega^{*}_{\vec{\mathbf{k}},\lambda}\;e^{-i(\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}-\omega_k t)}\Big\}, \tag{5.30}$$ i45

Let us also denote another notational abbreviation, namely

$$\Phi = -\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}, \tag{5.31}$$ i46

which will allow some generalizations. So finally, the semiclassical interaction hamiltonian for a two-level atom, with rotating wave approximation, attains its final form

$$H_{AF} = -\frac{\hbar}{2}\sum_{\vec{\mathbf{k}}\lambda} \Big\{ |\,2\,\rangle\langle\,1\,|\;\Omega_{\vec{\mathbf{k}},\lambda}\;e^{-i(\Phi+\omega_k t)} \;+\; |\,1\,\rangle\langle\,2\,|\;\Omega^{*}_{\vec{\mathbf{k}},\lambda}\;e^{i(\Phi+\omega_k t)}\Big\}, \tag{5.32}$$ i47

which will be used in the next sections.

5.3 Application: Rabi oscillations

5.3.1 Introduction

We will concentrate on the following model. We still consider a two-level atom interacting with the electromagnetic field. However, we will adopt following simplifications. First of

all we will assume that the considered atom is at rest. Hence we can take $\vec{\mathbf{R}} = 0$ (this depends only on the proper choice of the coordinate frame. Moreover, this implies $\Phi = 0$. Finally, we shall assume that the external field can be treated classically (semiclassical approximation) and that it consists of a single monochromatic plane wave. Thus, we deal with a single well-specified mode, so that the indices $(\vec{\mathbf{k}}, \lambda)$ and summation over the modes are not necessary. In the light of these remarks we can write the total hamiltonian as a sum of the atomic one (i32c 5.24) and the interaction one (i47 5.32). So we have

$$H = \frac{1}{2}\,\hbar\omega_{21}\Big[\,|\,2\,\rangle\langle\,2\,| - |\,1\,\rangle\langle\,1\,|\,\Big] - \frac{\hbar}{2}\Big[\,|\,2\,\rangle\langle\,1\,|\,\Omega\,e^{-i\omega t} \;+\; |\,1\,\rangle\langle\,2\,|\,\Omega^*\,e^{i\omega t}\,\Big], \qquad (5.33)$$ i51

where ω denotes the frequency of the mode. Identifications (i31 5.21) allow us to write matrices

$$|\,2\,\rangle\langle\,2\,| - |\,1\,\rangle\langle\,1\,| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad (5.34)$$ i52a

Similarly, we get

$$|\,2\,\rangle\langle\,1\,| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad |\,1\,\rangle\langle\,2\,| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \qquad (5.35)$$ i52b

With the aid of these matrices, hamiltonian (i51 5.33) gets the following matrix form

$$\begin{aligned} H &= \frac{\hbar\omega_{21}}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix} 0 & \Omega\,e^{-i\omega t} \\ \Omega^*\,e^{i\omega t} & 0 \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} \omega_{21} & -\Omega\,e^{-i\omega t} \\ -\Omega^*\,e^{i\omega t} & -\omega_{21} \end{pmatrix}. \end{aligned} \qquad (5.36)$$ i53

Our aim is to solve the time dependent Schrödinger equation for the state of two-level atom interacting with a monochromatic (classical) mode of the electromagnetic field.

5.3.2 Schrödinger equation

As we have already mentioned, the space of the states of a two-level atom is two dimensional. The state of an atom is thus described by the vector

$$|\,\varphi(t)\,\rangle = \begin{pmatrix} \varphi_2(t) \\ \varphi_1(t) \end{pmatrix}, \qquad (5.37)$$ i56

according to identifications (i31 5.21). Obviously, quantity $\varphi_k(t),\ k = 1, 2$, is the probability amplitude of finding the atom in the state $|\,k\,\rangle$. Time-dependent Schrödinger equation is, certainly, of the form

$$i\hbar\frac{\partial}{\partial t}|\,\varphi(t)\,\rangle = H|\,\varphi(t)\,\rangle, \qquad (5.38)$$ i57

where the total hamiltonian is given in (i53 5.36). In order to solve this equation in a unique way we need initial conditions. We shall simply take

$$|\,\varphi(0)\,\rangle = \begin{pmatrix} \varphi_2(0) \\ \varphi_1(0) \end{pmatrix}, \qquad (5.39)$$ i58

which must satisfy the normalization condition

$$\left|\varphi_2(0)\right|^2 \; + \; \left|\varphi_1(0)\right|^2 = 1. \tag{5.40}$$ i58b

Formal Schrödinger equation (i57 5.38) can be written in the matrix form, which follows from (i53 5.36) and is as follows

$$i\hbar\frac{\partial}{\partial t}\left(\begin{array}{c}\varphi_2(t)\\ \varphi_1(t)\end{array}\right) = \frac{\hbar}{2}\left(\begin{array}{cc}\omega_{21} & -\Omega\, e^{-i\omega t}\\ -\Omega^*\, e^{i\omega t} & -\omega_{21}\end{array}\right)\left(\begin{array}{c}\varphi_2(t)\\ \varphi_1(t)\end{array}\right). \tag{5.41}$$ i59a

We see that $\hbar$ cancels out. Multiplying both side by $(-i)$ we obtain an equivalent set of
i62 equations (we discard an obvious time argument)

$$\dot\varphi_2 \;=\; -\,\frac{i\omega_{21}}{2}\,\varphi_2 \;+\; \frac{i\Omega}{2}\,e^{-i\omega t}\,\varphi_1, \tag{5.42a}$$ i62a

$$\dot\varphi_1 \;=\; \frac{i\Omega^*}{2}\,e^{i\omega t}\,\varphi_2 \;+\; \frac{\omega_{21}}{2}\,\varphi_1. \tag{5.42b}$$ i62b

It is a set of the linear, first-order coupled differential equations with time-dependent coefficients. Solution to this set may be sought in several different ways. We will present just one of the methods.

5.3.3 An auxiliary transformation

First of all we intend to get rid of the time-dependent coefficients. This may be achieved by the transformation

$$\varphi_2(t) = c_2(t)\, e^{-i\omega t/2}, \qquad \varphi_1(t) = c_1(t)\, e^{i\omega t/2}. \tag{5.43}$$ i63

Let us note that "new" amplitudes fulfil the same initial conditions

$$\varphi_k(0) = c_k(0), \qquad k = 1, 2. \tag{5.44}$$ i63b

Introducing substitutions (i63 5.43) into Eqs.(i62 5.42) we get a set of equations where the time-
i65 dependent factors $e^{\pm i\omega t}$ cancel out. As a result we get

$$\dot c_2 \;=\; -\,\frac{i}{2}\,\big(\omega_{21}-\omega\big)c_2 \;+\; \frac{i\Omega}{2}\,c_1, \tag{5.45a}$$ i65a

$$\dot c_1 \;=\; \frac{i\Omega^*}{2}\,c_2 \;+\; \frac{i}{2}\big(\omega_{21}-\omega\big)c_1. \tag{5.45b}$$ i65b

Now, we introduce the detuning

$$\Delta = \omega - \omega_{21}, \tag{5.46}$$ i66

i67 due to which the set of equations (i65 5.45) becomes

$$\dot c_2 \;=\; \frac{i\Delta}{2}\,c_2 \;+\; \frac{i\Omega}{2}\,c_1, \tag{5.47a}$$ i67a

$$\dot c_1 \;=\; \frac{i\Omega^*}{2}\,c_2 \;-\; \frac{i\Delta}{2}\,c_1. \tag{5.47b}$$ i67b

This is still a set of linear, coupled differential equations, but with time-independent coefficients.

5.3.4 Solution to the evolution equations

Let us differentiate the first equation of the set (5.47) with respect to time. We obtain a second-order equation

$$\ddot{c}_2 \;=\; \frac{i\Delta}{2}\,\dot{c}_2 \;+\; \frac{i\Omega}{2}\,\dot{c}_1. \tag{5.48}$$

Then, with the aid of the second equation, we eliminate $\dot{c}_1$ obtaining

$$\begin{aligned}\ddot{c}_2 \;&=\; \frac{i\Delta}{2}\,\dot{c}_2 \;+\; \frac{i\Omega}{2}\left(\frac{i\Omega^*}{2}\,c_2 \;-\; \frac{i\Delta}{2}\,c_1\right)\\ &=\; \frac{i\Delta}{2}\,\dot{c}_2 \;-\; \frac{|\Omega|^2}{4}\,c_2 \;-\; \frac{i\Delta}{2}\cdot\frac{i\Omega}{2}\,c_1.\end{aligned} \tag{5.49}$$

Now, from (5.47a) we have

$$\frac{i\Omega}{2}\,c_1 = \dot{c}_2 \;-\; \frac{i\Delta}{2}\,c_2. \tag{5.50}$$

Using this relation in (5.49) we obtain

$$\begin{aligned}\ddot{c}_2 \;&=\; \frac{i\Delta}{2}\,\dot{c}_2 \;-\; \frac{|\Omega|^2}{4}\,c_2 \;-\; \frac{i\Delta}{2}\left(\dot{c}_2 \;-\; \frac{i\Delta}{2}\,c_2\right)\\ &=\; -\frac{1}{4}\left(|\Omega|^2+\Delta^2\right)\,c_2.\end{aligned} \tag{5.51}$$

Introducing the so-called generalized Rabi frequency

$$\Omega_R = \sqrt{|\Omega|^2+\Delta^2}, \tag{5.52}$$

we see, that equation (5.51) is an equation of the type of harmonic oscillator

$$\ddot{c}_2 + \left(\frac{\Omega_R}{2}\right)^2\,c_2 = 0, \tag{5.53}$$

with an obvious solution

$$c_2(t) = A\sin\left(\frac{\Omega_R t}{2}\right) \;+\; B\cos\left(\frac{\Omega_R t}{2}\right). \tag{5.54}$$

Arbitrary constants A and B should be determined from the initial condition (5.44). Before we do so, let us compute amplitude $c_1(t)$. It follows from relation (5.50). Performing the necessary differentiations, we obtain

$$\begin{aligned}c_1 = &-\frac{\Delta}{\Omega}\left[A\sin\left(\frac{\Omega_R t}{2}\right) \;+\; B\cos\left(\frac{\Omega_R t}{2}\right)\right]\\ &-\frac{i\Omega_R}{\Omega}\left[A\cos\left(\frac{\Omega_R t}{2}\right) \;-\; B\sin\left(\frac{\Omega_R t}{2}\right)\right]\\ =&\left(-\frac{\Delta}{\Omega}A+\frac{i\Omega_R}{\Omega}B\right)\sin\left(\frac{\Omega_R t}{2}\right) \;+\; \left(-\frac{\Delta}{\Omega}B-\frac{i\Omega_R}{\Omega}A\right)\cos\left(\frac{\Omega_R t}{2}\right)\end{aligned} \tag{5.55}$$

Summarizing the obtained results we write down the amplitudes of the evolving two-level atom

i73

$$c_2(t) = A\sin\left(\frac{\Omega_R t}{2}\right) \; + \; B\cos\left(\frac{\Omega_R t}{2}\right), \tag{5.56a}$$ i73a

$$c_1(t) = -\frac{1}{\Omega}\big(\Delta A - i\Omega_R B\big)\sin\left(\frac{\Omega_R t}{2}\right) \; - \; \frac{1}{\Omega}\big(\Delta B + i\Omega_R A\big)\cos\left(\frac{\Omega_R t}{2}\right). \tag{5.56b}$$ i73b

This ends the formal solution to the Schrödinger equation, what remains is the determination of constants A and B from initial conditions.

Due to relations (i63b 5.44) and to solutions (i73 5.56) we arrive at the set od equations for constants A and B i74

$$\varphi_2(0) = B, \tag{5.57a}$$ i74a

$$c_1(0) = -\frac{1}{\Omega}\big(\Delta B + i\Omega_R A\big). \tag{5.57b}$$ i74b

i75 Solution to this set of equations is a straightforward matter. They read

$$A = \frac{i\Omega}{\Omega_R}\varphi_1(0) \; + \; \frac{i\Delta}{\Omega_R}\varphi_2(0), \tag{5.58a}$$ i75a

$$B = \varphi_2(0). \tag{5.58b}$$ i75b

Plugging the constants A and B into solutions (i73 5.56) after simple transformations we obtain i77

$$c_2(t) = \varphi_2(0)\cos\left(\frac{\Omega_R t}{2}\right) \; + \; \frac{i}{\Omega_R}\big[\Omega\varphi_1(0) + \Delta\varphi_2(0)\big]\sin\left(\frac{\Omega_R t}{2}\right), \tag{5.59a}$$ i77a

$$c_1(t) = \varphi_1(0)\cos\left(\frac{\Omega_R t}{2}\right) \; + \; \frac{i}{\Omega_R}\big[\Omega\varphi_2(0) - \Delta\varphi_1(0)\big]\sin\left(\frac{\Omega_R t}{2}\right). \tag{5.59b}$$ i77b

Finally, we have to take into account transformation (i63 5.43). Then, we can write down the solutions to the considered problem,as i78

$$\varphi_2(t) = \varphi_2(0)\cos\left(\frac{\Omega_R t}{2}\right)e^{-i\omega t/2} \; + \; \frac{i}{\Omega_R}\big[\Omega\varphi_1(0) + \Delta\varphi_2(0)\big]\sin\left(\frac{\Omega_R t}{2}\right)e^{-i\omega t/2}, \tag{5.60a}$$ i78a

$$\varphi_1(t) = \varphi_1(0)\cos\left(\frac{\Omega_R t}{2}\right)e^{i\omega t/2} \; + \; \frac{i}{\Omega_R}\big[\Omega\varphi_2(0) - \Delta\varphi_1(0)\big]\sin\left(\frac{\Omega_R t}{2}\right)e^{i\omega t/2}. \tag{5.60b}$$ i78b

This is the end of the procedure of finding the solutions to the Schrödinger equation for a two-level atom interacting with (a classical) single, monochromatic mode of light. The initial conditions are fully arbitrary, they only must satisfy the normalization condition (i58b 5.40).

5.3.5 Specific initial conditions

Let us now assume, that the atom was initially in the ground state. This corresponds to the initial conditions

$$\varphi_2(0) = 0, \qquad \text{and} \qquad \varphi_1(0) = 1, \tag{5.61}$$ i81

which clearly satisfy the normalization requirement. In such a case, from general solutions
i82 (i78 5.60) we obtain

$$\varphi_2(t) = \frac{i\Omega}{\Omega_R} \sin\left(\frac{\Omega_R t}{2}\right) e^{-i\omega t/2}, \tag{5.62a}$$ i82a

$$\varphi_1(t) = \cos\left(\frac{\Omega_R t}{2}\right) e^{i\omega t/2} \; - \; \frac{i\Delta}{\Omega_R} \sin\left(\frac{\Omega_R t}{2}\right) e^{i\omega t/2}. \tag{5.62b}$$ i82b

Having the amplitudes, we easily compute the corresponding probabilities of finding the
i83 atom in the excited state and in the ground state

$$P_2(t) = \frac{|\Omega|^2}{\Omega_R^2} \sin^2\left(\frac{\Omega_R t}{2}\right), \tag{5.63a}$$ i83a

$$P_1(t) = \cos^2\left(\frac{\Omega_R t}{2}\right) \; + \; \frac{\Delta^2}{\Omega_R^2} \sin^2\left(\frac{\Omega_R t}{2}\right). \tag{5.63b}$$ i83b

Since $\Omega_R^2 = |\Omega|^2 + \Delta^2$ the obtained probabilities sum up to unity for any moment T , as it should be. Next, we use the simple trigonometric identities

$$\cos^2\left(\frac{\alpha}{2}\right) = \frac{1}{2}\left(1 + \cos\alpha\right), \qquad \sin^2\left(\frac{\alpha}{2}\right) = \frac{1}{2}\left(1 - \cos\alpha\right), \tag{5.64}$$ i84

i85 With the aid of these relations, from (i83 5.63) we get

$$P_2(t) = \frac{|\Omega|^2}{2\,\Omega_R^2} \cdot \left[1 - \cos\left(\Omega_R t\right)\right], \tag{5.65a}$$ i85a

$$P_1(t) = \frac{1}{2}\left[1 + \cos\left(\Omega_R t\right)\right] \; + \; \frac{\Delta^2}{2\,\Omega_R^2} \cdot \left[1 - \cos\left(\Omega_R t\right)\right]. \tag{5.65b}$$ i85b

i86 Since $\Omega^2 = \Omega_R^2 - \Delta^2$, we can eliminate Ω from the above equations, obtaining

$$P_2(t) = \frac{1}{2}\left(1 - \frac{\Delta^2}{\Omega_R^2}\right)\left[\, 1 - \cos\left(\Omega_R t\right) \,\right], \tag{5.66a}$$ i86a

$$P_1(t) = \frac{1}{2}\left(1 + \frac{\Delta^2}{\Omega_R^2}\right) \; + \; \frac{1}{2}\left(1 - \frac{\Delta^2}{\Omega_R^2}\right) \cos\left(\Omega_R t\right). \tag{5.66b}$$ i86b

Using trigonometric relations it is easy to check that these probabilities sum up to unity. Moreover we note that the obtained probabilities do not depend on the sign of detuning only on its absolute value.

5.3.6 Rabi oscillations

Expressions (i86 5.66) clearly exhibit oscillatory behavior. Let us discuss it in some more detail. Let us concentrate on the probability of finding two-level atom in the ground state. $P_1(t)$. As it follows from the obtained results, the time derivative of this probability is

$$\frac{d}{dt}\, P_1(t) = -\, \frac{1}{2}\left(1 - \frac{\Delta^2}{\Omega_R^2}\right) \Omega_R \sin\left(\Omega_R t\right), \tag{5.67}$$ i88b

which is zero for $\Omega_R t = k\pi$ $(k = 0, 1, 2, \ldots)$. let us investigate the values of $P_1(t)$ for the given moments of time. Then, from (5.66b) we get

$$P_1\left(\frac{k\pi}{\Omega_R}\right) = \frac{1}{2}\left(1 + \frac{\Delta^2}{\Omega_R^2}\right) + \frac{1}{2}\left(1 - \frac{\Delta^2}{\Omega_R^2}\right)\cos(k\pi)\,. \tag{5.68}$$ i88c0

Since $\cos(k\pi) = (-1)^k$ we have

$$P_1\left(\frac{k\pi}{\Omega_R}\right) = \frac{1}{2}\left[1 + (-1)^k\right] + \frac{\Delta^2}{2\,\Omega_R^2}\left[1 - (-1)^k\right]. \tag{5.69}$$ i88c

For even $k = 2n$ (in particular for $n = 0$ – initial moment) we get

$$P_1\left(\frac{\pi}{\Omega_R}\cdot 2n\right) = 1. \tag{5.70}$$ i88d

On the other hand, for odd $k = 2n + 1$

$$P_1\left(\frac{\pi}{\Omega_R}\cdot (2n+1)\right) = \frac{\Delta^2}{\Omega_R^2}. \tag{5.71}$$ i88e

Thus, we see that at the initial moment $(t = 0)$ we have $P_1(t) = 1$, the atom is in its ground state. When the time goes probability of finding the atom in the ground state reaches its minimum value Δ^2/Ω_R^2. Next, at the later moment $\Omega_R t = 2\pi$, it reaches unity again. Obviously, with growing time, the oscillations continue.

In a similar way we discuss $P_2(t)$ – probability of finding the atom in the excited state. From (5.66a) we find the derivative

$$\frac{d}{dt}\,P_2(t) = \frac{1}{2}\left(1 - \frac{\Delta^2}{\Omega_R^2}\right)\Omega_R \sin(\Omega_R t)\,, \tag{5.72}$$ i89lb

which is again zero for $\Omega_R t = k\pi$ $(k = 0, 1, 2, \ldots)$. Hence we easily get

$$P_2\left(\frac{k\pi}{\Omega_R}\right) = \frac{1}{2}\left(1 - \frac{\Delta^2}{2\,\Omega_R^2}\right)\left[1 - (-1)^k\right]. \tag{5.73}$$ i89c

Hence, for even $k = 2n$ we get

$$P_2\left(\frac{\pi}{\Omega_R}\cdot 2n\right) = 0. \tag{5.74}$$ i89d

For odd $k = 2n + 1$, on the other hand, we obtain

$$P_2\left(\frac{\pi}{\Omega_R}\cdot (2n+1)\right) = 1 - \frac{\Delta^2}{\Omega_R^2}. \tag{5.75}$$ i89e

Oscillations of the excited state population are, thus, slightly different. At the initial moment $t = 0$ $P_2(0) = 0$, which agrees we the adopted initial conditions. Then, the probability P_2 grows, at the moment $t = \pi/\Omega_R$ attains its maximum equal to $1 - \Delta^2/\Omega_R^2$. when the time passes $P_2(t)$ decreases and reaches zero at the moment $t = 2\pi/\Omega_R$. Afterwards, the oscillations go on.

Let us return to the discussion of $P_2(t)$ – probability of finding the atom in the upper state, which is given in Eq.(5.66a), ie.,

$$P_2(t) = \frac{1}{2}\left(1 - \frac{\Delta^2}{\Omega_R^2}\right)\left[\,1 - \cos\left(\Omega_R t\right)\,\right] = \left(1 - \frac{\Delta^2}{\Omega_R^2}\right)\sin\left(\frac{\Omega_R t}{2}\right). \tag{5.76}$$ i92

Moreover, we recall that $\Delta = \omega - \omega_{21}$, and $\Omega_R^2 = \Delta^2 + |\Omega|^2$. It is important to realize which parameters can be controlled in a real experimental situations. Frequency ω of the incident light can be tuned. This allows an experimentalist to control the detuning Δ (atomic frequency ω_{21} is obviously fixed. Furthermore, application of filters results in the control over the field intensity. This means that the electric $|\vec{\mathbf{E}}|$ can be adjusted. This, in turn, gives a chance to regulate Rabi frequency Ω (see (5.29)). Hence, we see that Δ and Ω are the essential experimental parameters. We will consider several possible choices of these parameters.

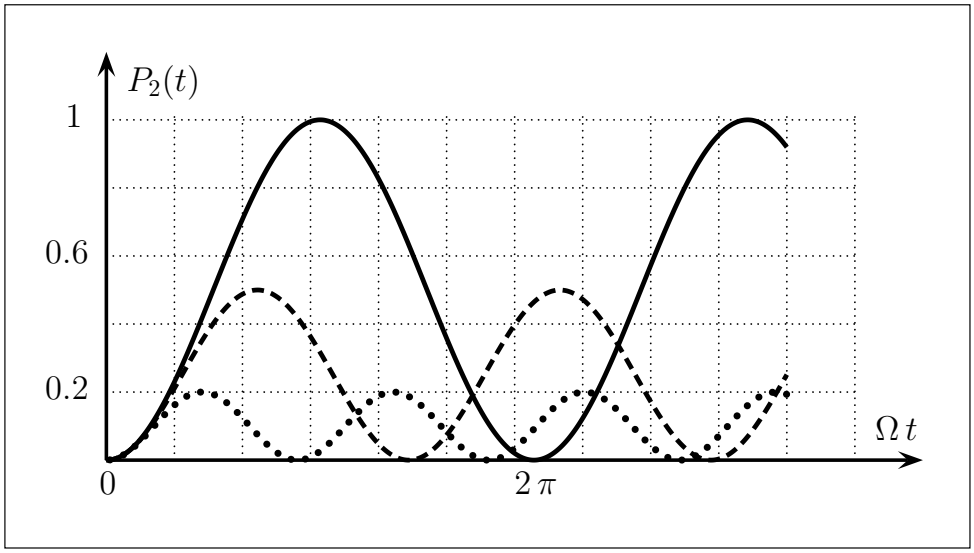

Fig. 5.3: Examples of Rabi oscillations – probability of finding an atom in the upper state. Dotted line: $\Delta = 2\Omega$; dashed line: $\Delta = \Omega$; solid line - resonance: $\Delta = 0$. f:ir

- As the first case we take $|\Delta| = 2\Omega$. This gives $\Omega_R = \sqrt{5}\Omega$. Probability $P_2(t)$ becomes

$$P_2(t) \;=\; \frac{1}{10}\left[1 - \cos\left(\sqrt{5}\,\Omega t\right)\right] \;=\; \frac{1}{5}\,\sin^2\left(\frac{\sqrt{5}}{2}\,\Omega t\right). \tag{5.77}$$ i93

  Rabi frequency Ω_R is relatively large. Probability $P_2(t)$ oscillates quickly. It reaches the first zero (with $t > 0$) in the moment $\sqrt{5}\,\Omega t/2 = 2\pi$, which yields $\Omega t \approx 2.8$. Its maximum value is only 0.2. Rabi oscillations are shown as a dotted line in the figure 5.3. f:ir
- The second case corresponds to $|\Delta| = \Omega$, so that $\Omega_R = \sqrt{2}\,\Omega$. Eq. (5.76)) implies

$$P_2(t) \;=\; \frac{1}{4}\left[1 - \cos\left(\sqrt{2}\,\Omega t\right)\right] \;=\; \frac{1}{2}\,\sin^2\left(\frac{\sqrt{2}}{2}\,\Omega t\right). \tag{5.78}$$ i94

Generalized Rabi frequency decreases so the oscillations are slower than in the previous case. The first zero occurs at $\sqrt{2}\,\Omega t/2 = 2\pi$, so that $\Omega t \approx 4.4$. Maximum value of the probability equals to 0.5. Its behavior is shown in figure 5.3 by a dashed line

- The third case depicted in figure 5.3 is a resonance one. Thus, $\Delta = 0$ and $\Omega_R = \Omega$. In this case from (5.76) we have

$$P_2(t) \;=\; \frac{1}{2}\left[1 - \cos\left(\Omega t\right)\right] \;=\; \sin^2\left(\frac{1}{2}\,\Omega_1 t\right). \tag{5.79}$$ i95

Rabi frequency Ω_R is smallest and Oscillations are slowest. The first zero appears at $\Omega t = 2\pi \approx 6.28$. On the other hand, probability of finding the atom in the upper state reaches maximum possible value equal to 1.

5.3.7 Mollow spectrum – heuristic approach

The operator of the atomic dipole moment (the one for a two-level atom) is of the form

$$\vec{\mathbf{d}} = \vec{\mathbf{d}}_{12}|\,1\,\rangle\langle\,2\,| + \vec{\mathbf{d}}_{21}|\,2\,\rangle\langle\,1\,|. \tag{5.80}$$ iA1

Let us assume that, as previously, the atom is initially in the ground state. The corresponding probability amplitudes ar given in Eqs.(5.62). We intend to find the expectation value of atomic dipole moment. For simplicity, we shall assume that its matrix elements are real $\vec{\mathbf{d}}_{12} = \vec{\mathbf{d}}_{21}$. So, we want to compute the quantity

$$\begin{aligned}\langle\,\vec{\mathbf{d}}\,\rangle &= \langle\,\varphi(t)\,|\,\vec{\mathbf{d}}\,|\,\varphi(t)\,\rangle \\ &= \vec{\mathbf{d}}_{21}\langle\,\varphi(t)\,|\,\big(|\,1\,\rangle\langle\,2\,| + |\,2\,\rangle\langle\,1\,|\big)\,|\,\varphi(t)\,\rangle\end{aligned} \tag{5.81}$$ iA4

Having found the matrices (5.35) we easily construct the matrix corresponding to the operator in the above matrix element. Thus we have

$$\begin{aligned}\langle\,\vec{\mathbf{d}}\,\rangle &= \vec{\mathbf{d}}_{21}\big(\varphi_1^*,\;\varphi_1^*\big)\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\begin{pmatrix}\varphi_1\\ \varphi_2\end{pmatrix} = \vec{\mathbf{d}}_{21}\big(\varphi_1^*,\;\varphi_1^*\big)\begin{pmatrix}\varphi_2\\ \varphi_1\end{pmatrix} \\ &= \vec{\mathbf{d}}_{21}\big[\varphi_1^*\varphi_2 + \varphi_2^*\varphi_1\big] = \vec{\mathbf{d}}_{21}\cdot 2\mathrm{Re}\left\{\varphi_2^*\varphi_1\right\}\end{aligned} \tag{5.82}$$ iA6

The amplitudes φ_j are known, It is easy to get

$$\varphi_2^*\varphi_1 = \frac{i\Omega}{\Omega_R}e^{-i\omega t}\sin\left(\frac{\Omega_R t}{2}\right)\left[\cos\left(\frac{\Omega_R t}{2}\right) + \frac{i\Delta}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right)\right]. \tag{5.83}$$ iA8

To simplify our calculation let us temporarily denote $a = \Omega_R t/2$. Writing trigonometric functions in exponential form, we get

$$\begin{aligned}\varphi_2^*\varphi_1 &= \frac{i\Omega}{\Omega_R}e^{-i\omega t}\,\frac{e^{ia} - e^{-ia}}{2i}\left[\frac{e^{ia} + e^{-ia}}{2} + \frac{i\Delta}{\Omega_R}\frac{e^{ia} - e^{-ia}}{2i}\right] \\ &= \frac{\Omega}{4\,\Omega_R}e^{-i\omega t}\,\left[e^{2ia} - e^{-2ia} + \frac{\Delta}{\Omega_R}\left(e^{2ia} + e^{-2ia} - 2\right)\right] \\ &= -\frac{\Omega}{2\,\Omega_R}e^{-i\omega t}\,\left[\frac{\Delta}{\Omega_R} - \frac{1}{2}\left(1 + \frac{\Delta}{\Omega_R}\right)e^{2ia} + \frac{1}{2}\left(1 - \frac{\Delta}{\Omega_R}\right)e^{-2ia}\right].\end{aligned} \tag{5.84}$$ iA8a

Returning to "old" notation, we finally obtain

$$\varphi_2^*\varphi_1 = -\frac{\Omega}{2\,\Omega_R}\left[\frac{\Delta}{\Omega_R}e^{-i\omega t} - \frac{1}{2}\left(1+\frac{\Delta}{\Omega_R}\right)e^{-i(\omega-\Omega_R)t} + \frac{1}{2}\left(1-\frac{\Delta}{\Omega_R}\right)e^{-i(\omega+\Omega_R)t}\right]. \quad (5.85)$$ iA9

Taking real part and inserting into (5.82) yields

$$\langle\,\vec{\mathbf{d}}\,\rangle = -\vec{\mathbf{d}}_{21}\,\frac{\Omega}{2\,\Omega_R}\left\{\frac{\Delta}{\Omega_R}\cos(\omega t) - \frac{1}{2}\left(1+\frac{\Delta}{\Omega_R}\right)\cos\big[(\omega-\Omega_R)t\big] + \frac{1}{2}\left(1-\frac{\Delta}{\Omega_R}\right)\cos\big[(\omega+\Omega_R)t\big]\right\}. \quad (5.86)$$ iA12

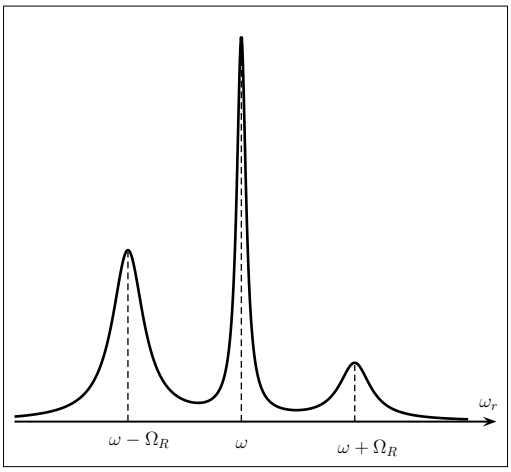

Fig. 5.4: A typical example of the Mollow's spectrum. f:mollow

From this relation we can see that the oscillations of the atomic dipole moment are more complicated than Rabi ones which were discussed above. In this case we deal with the superposition of three oscillations at frequencies: $\omega_r = \omega$ – at the frequency of the incoming light, and at two shifted frequencies $\omega_r = \omega \pm \Omega_R$. We can discuss these oscillations according to the notions known from classical electrodynamics. As we know an oscillating dipole emits electromagnetic waves which have the same frequency as the frequency of dipole's oscillations. Hence, on the basis of Eq.(5.86) we can say that the dipole would emit waves with three frequencies ω_r which follow from our considerations. We expect that that the spectrum of the emitted radiation would consist of three lines, which (after accounting for natural line broadening). Naturally, our present analysis is based on classical notions. Later on we we argue that the full quantum-mechanical analysis (at least quantitatively) leads to the same predictions. Summarizing, we can say, that we expect the spectrum of the light emitted by the two-level atom to consist of three peaks. Such a spectrum is called *Mollow's spectrum.* An example of such a spectrum is given in the figure.

However, one comment is in place. Namely, we know that the spectral lines have some natural linewidth, which usually is expressed by the Einstein's A coefficient. If the generalized Rabi frequency Ω_R (which determines the separation of the spectral lines in the Mollow's spectrum) is less or comparable with A then the three lines strongly overlap. As a result we will see just one line (perhaps somewhat broadened, but single). In order to observe Mollow's three-peaked spectrum the incident field has to be strong enough. We shall return to the discussion of these issues later, in more precise, quantum-mechanical manner.

* *

Chapter 6

Spontaneous emission. Simple treatment

c:sp

6.1 Introduction

In this chapter we shall deal with the physical model much similar to that considered in the previous chapter. Our atom still is a two-level one. hence its free hamiltonian is given by (i32c 5.24). This atom interacts with a single mode of quantized electromagnetic field which is described by a hamiltonian

$$H_F = \hbar\omega_k a^\dagger_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda}. \tag{6.1}$$ s2

We will soon generalize our approach to a multimode situation. The interaction hamiltonian will be taken in the RWA approximation, so it is (for a single mode) of the same form as (i36 5.27)

$$\begin{aligned} H_{AF} &= -|\,2\,\rangle\langle\,1\,|\;\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{E}}^{(+)}_{\vec{\mathbf{k}},\lambda} \;+\; H.C \\ &= -|\,2\,\rangle\langle\,1\,|\;\big(\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\big) i\sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}}\; e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}}\; a_{\vec{\mathbf{k}}\lambda} + H.C. \end{aligned} \tag{6.2}$$ s3a

We stress that all dynamical (ie., time dependent) information is "hidden" in the annihilation and creation operators. For future purposes it is convenient to introduce an abbreviated notation

$$V = \frac{2}{\hbar}\, i\,\big(\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\big)\sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}}\; e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}} \quad\Longrightarrow\quad \frac{\hbar V}{2} = i\,\big(\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\big)\sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}}\; e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}}. \tag{6.3}$$ s4

This allows us to write the interaction hamiltonian as

$$H_{AF} = -\frac{\hbar}{2}\Big[\, V|\,2\,\rangle\langle\,1\,|\; a_{\vec{\mathbf{k}}\lambda} + V^*|\,1\,\rangle\langle\,2\,|\; a^\dagger_{\vec{\mathbf{k}}\lambda}\,\Big]. \tag{6.4}$$ s5b

We will be interested in the following physical situation.

- At the initial moment $t = 0$ the atom is assumed to be in the exited (upper) state, while the field is in the n-photon state. That is, the initial state of the system is

$$|\,i\,\rangle = |\,2\,\rangle \otimes |\,n_{\vec{\mathbf{k}},\lambda}\,\rangle. \tag{6.5}$$ s6

- At some later moment the system is in the final state

$$|\,i\,\rangle = |\,1\,\rangle \otimes |\,n_{\vec{\mathbf{k}},\lambda}+1\,\rangle. \tag{6.6}$$

s7

That is, we assume that within time interval t there occurs a transition $|\,i\,\rangle \to |\,f\,\rangle$ during which, the atom emits a photon (and goes to the ground state).

We note that states $|\,i\,\rangle$ and $|\,f\,\rangle$ are normalized and orthogonal. The latter fact is due to orthogonality of atomic states $|\,1\,\rangle$ and $|\,2\,\rangle$ and of photon states (with different photon numbers.

The problem now, is to find the probability of such a transition. To find such a probability we need to solve Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\,\psi(t)\,\rangle = (H_A + H_F + H_{AF})\,|\,\psi(t)\,\rangle. \tag{6.7}$$

s8

We will seek the solution to this equation in the form of a linear combination

$$|\,\psi(t)\,\rangle = C_i(t)|\,i\,\rangle + C_f(t)|\,f\,\rangle, \tag{6.8}$$

s9

with states $|\,i\,\rangle$ and $|\,f\,\rangle$ defined above. Equation (6.7) needs an initial condition, which is

$$C_i(0) = 1, \qquad C_f(0) = 0, \tag{6.9}$$

s10

as it follows from our discussion. Now, we should construct the explicit form of the Schrödinger equation and the look for the solution. We want to find the probability of finding the atom in the upper state, that is

$$P_{f\leftarrow i}(t) = \big|\langle\, f\,|\,\psi(t)\,\rangle\big|^2 = \big|C_f(t)\big|^2. \tag{6.10}$$

s11

6.2 Schrödinger eqaution

We introduce ansatz (6.8) into Schrödinger equation (6.7) and we get

$$i\hbar\frac{\partial C_i}{\partial t}\,|\,i\,\rangle + i\hbar\frac{\partial C_f}{\partial t}\,|\,f\,\rangle = (H_A + H_F + H_{AF})\,\big[C_i|\,i\,\rangle + C_f|\,f\,\rangle\big]. \tag{6.11}$$

s13a

States $|\,i\,\rangle$ and $|\,f\,\rangle$ are orthogonal so multiplying on the right by $|\,i\,\rangle$ and $|\,f\,\rangle$ we obtain a set of two differential equations

s14

$$i\hbar\dot{C}_i = \langle\, i\,|\,(H_A + H_F + H_{AF})\,|\,i\,\rangle\, C_i + \langle\, i\,|\,(H_A + H_F + H_{AF})\,|\,f\,\rangle\, C_f, \tag{6.12a}$$

s14a

$$i\hbar\dot{C}_f = \langle\, f\,|\,(H_A + H_F + H_{AF})\,|\,i\,\rangle\, C_i + \langle\, f\,|\,(H_A + H_F + H_{AF})\,|\,f\,\rangle\, C_f. \tag{6.12b}$$

s14b

The problem is reduced to a two-dimensional case, the space of the solutions $|\,\psi(t)\,\rangle$ is spanned by vectors $|\,i\,\rangle$ and $|\,f\,\rangle$. Hence we need to construct the corresponding 2×2 matrices of three hamiltonians appearing in the above set of equations.

6.2.1 Matrix elements

From the definition (5.24) we see that

$$H_A|\,i\,\rangle = \frac{\hbar\omega_{21}}{2}\Big[\,|\,2\,\rangle\langle\,2\,|-|\,1\,\rangle\langle\,1\,|\,\Big]|\,2\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}\,\rangle = \frac{\hbar\omega_{21}}{2}\,|\,2\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}\,\rangle$$
$$= \frac{\hbar\omega_{21}}{2}\,|\,i\,\rangle, \tag{6.13}$$ s15a

since H_A does not act on photon states. So the state $|\,i\,\rangle$ is an eigenstate of the atomic hamiltonian. Similarly for state $|\,f\,\rangle$ we have

$$H_A|\,f\,\rangle = \frac{\hbar\omega_{21}}{2}\Big[\,|\,2\,\rangle\langle\,2\,|-|\,1\,\rangle\langle\,1\,|\,\Big]|\,1\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}+1\,\rangle = -\frac{\hbar\omega_{21}}{2}\,|\,1\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}+1\,\rangle$$
$$= -\frac{\hbar\omega_{21}}{2}\,|\,f\,\rangle, \tag{6.14}$$ s15b

and $|\,f\,\rangle$ is also an eigenstate of H_A. Due to orthogonality of states $|\,i\,\rangle$ and $|\,f\,\rangle$ we obtain four necessary matrix elements of the atomic hamiltonian. They are

$$\begin{aligned}&\langle\,i\,|H_A|\,i\,\rangle = \frac{\hbar\omega_{21}}{2}, \qquad &&\langle\,i\,|H_A|\,f\,\rangle = 0,\\ &\langle\,f\,|H_A|\,i\,\rangle = 0, &&\langle\,f\,|H_A|\,i\,\rangle = -\frac{\hbar\omega_{21}}{2}.\end{aligned} \tag{6.15}$$ s16

The field hamiltonian $H_F = \hbar\omega_k a^\dagger_{\vec{\mathbf{k}}\lambda}a_{\vec{\mathbf{k}}\lambda}$ is diagonal in photon numbers and does not affect atomic states. Therefore, we immediately get

$$H_F|\,i\,\rangle = \hbar\omega_k a^\dagger_{\vec{\mathbf{k}}\lambda}a_{\vec{\mathbf{k}}\lambda}|\,2\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}\,\rangle = \hbar\omega_k\,n_{\vec{\mathbf{k}},\lambda}|\,2\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}\,\rangle$$
$$= n_{\vec{\mathbf{k}},\lambda}\hbar\omega_k|\,i\,\rangle, \tag{6.16}$$ s18a
$$H_F|\,f\,\rangle = \hbar\omega_k a^\dagger_{\vec{\mathbf{k}}\lambda}a_{\vec{\mathbf{k}}\lambda}|\,1\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}+1\,\rangle = \hbar\omega_k\,\big(n_{\vec{\mathbf{k}},\lambda}+1\big)|\,1\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}+1\,\rangle$$
$$= \big(n_{\vec{\mathbf{k}},\lambda}+1\big)\hbar\omega_k|\,f\,\rangle. \tag{6.17}$$ s18b

Considered states $|\,i\,\rangle$ and $|\,f\,\rangle$ are, thus, the eigenstates of the field hamiltonian. Similarly as in the case of atomic hamiltonian we obtain

$$\begin{aligned}&\langle\,i\,|H_F|\,i\,\rangle = n_{\vec{\mathbf{k}},\lambda}\hbar\omega_k, \qquad &&\langle\,i\,|H_F|\,f\,\rangle = 0,\\ &\langle\,f\,|H_F|\,i\,\rangle = 0, &&\langle\,f\,|H_F|\,i\,\rangle = \big(n_{\vec{\mathbf{k}},\lambda}+1\big)\hbar\omega_k.q\end{aligned} \tag{6.18}$$ s19

Finally, we analyze matrix elements of the interaction hamiltonian (6.4). Proceeding along the same lines as above, we look at the action of H_{AF} on the basis states $|\,i\,\rangle$ and $|\,f\,\rangle$. For vector $|\,i\,\rangle$ we get

$$H_{AF}|\,i\,\rangle = -\frac{\hbar}{2}\Big[\,V|\,2\,\rangle\langle\,1\,|\,a_{\vec{\mathbf{k}}\lambda}+V^*|\,1\,\rangle\langle\,2\,|\,a^\dagger_{\vec{\mathbf{k}}\lambda}\,\Big]\,|\,2\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}\,\rangle$$
$$= -\frac{\hbar V^*}{2}|\,1\,\rangle a^\dagger_{\vec{\mathbf{k}}\lambda}|\,n_{\vec{\mathbf{k}},\lambda}\,\rangle$$
$$= -\frac{\hbar V^*}{2}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}\,|\,1\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}+1\,\rangle = -\frac{\hbar V^*}{2}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}\,|\,f\,\rangle. \tag{6.19}$$ s23a

Contrary to the previous cases, now matrix elements are off-diagonal. For the second vector we have

$$\begin{aligned} H_{AF}|\,f\,\rangle &= -\frac{\hbar}{2}\Big[\,V|\,2\,\rangle\langle\,1\,|\,a_{\vec{\mathbf{k}}\lambda} + V^*|\,1\,\rangle\langle\,2\,|\,a^\dagger_{\vec{\mathbf{k}}\lambda}\,\Big]\,|\,1\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}+1\,\rangle \\ &= -\frac{\hbar V}{2}|\,2\,\rangle a_{\vec{\mathbf{k}}\lambda}|\,n_{\vec{\mathbf{k}},\lambda}+1\,\rangle \\ &= -\frac{\hbar V}{2}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}\;|\,2\,\rangle|\,n_{\vec{\mathbf{k}},\lambda}\,\rangle = -\frac{\hbar V}{2}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}\;|\,i\,\rangle. \end{aligned} \tag{6.20}$$ s23b

Then, orthogonality of states $|\,i\,\rangle$ and $|\,f\,\rangle$ yields matrix elements of the interaction hamiltonian

$$\begin{aligned} &\langle\,i\,|H_{AF}|\,i\,\rangle = 0, && \langle\,i\,|H_{AF}|\,f\,\rangle = -\frac{\hbar V}{2}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}, \\ &\langle\,f\,|H_{AF}|\,i\,\rangle = -\frac{\hbar V^*}{2}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}, && \langle\,f\,|H_{AF}|\,i\,\rangle = 0. \end{aligned} \tag{6.21}$$ s23c

Having found matrix elements of all contributions to the total hamiltonian we can construct equations of motion (6.12). s14

6.2.2 Equations of motion

Using matrix elements (6.15), (6.18) and (6.21) we introduce necessary matrix elements into equations (6.12). Then we arrive at the set of equations s16 s19 s23c s14 s24

$$i\hbar\dot{C}_i = \left(\frac{\hbar\omega_{21}}{2} + n_{\vec{\mathbf{k}},\lambda}\hbar\omega_k\right)C_i \;-\; \frac{\hbar V}{2}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}\,C_f, \tag{6.22a}$$ s24a

$$i\hbar\dot{C}_f = -\frac{\hbar V^*}{2}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}C_i \;+\; \left[-\frac{\hbar\omega_{21}}{2} + \big(n_{\vec{\mathbf{k}},\lambda}+1\big)\hbar\omega_k\right]C_f. \tag{6.22b}$$ s24b

Analyzing this set of equations we see that it is convenient to introduce the following notation

$$\omega_i = \tfrac{1}{2}\omega_{21} + n_{\vec{\mathbf{k}},\lambda}\omega_k, \qquad \omega_f = -\tfrac{1}{2}\omega_{21} + \big(n_{\vec{\mathbf{k}},\lambda}+1\big)\omega_k, \tag{6.23}$$ s25

moreover we write

$$v = V\sqrt{n_{\vec{\mathbf{k}},\lambda}+1} = \frac{2i}{\hbar}\sqrt{n_{\vec{\mathbf{k}},\lambda}+1}\;\big(\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\big)\sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}}\;e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}} \tag{6.24}$$ s26

With this notation equations (6.22) after multiplication by $(-i)$ can be written as s24 s28

$$\dot{C}_i = -i\omega_i C_i \;+\; \frac{iv}{2}C_f, \tag{6.25a}$$ s28a

$$\dot{C}_f = \frac{iv^*}{2}C_i \;-\; i\omega_f C_f. \tag{6.25b}$$ s28b

This is a set of differential equations with time independent coefficients.

6.2.3 Solution to the equations of motion

The set (6.25) is quite similar to the one considered in the previous chapter (in connection with Rabi equations), see Eqs(5.47). In order to have a full analogy let us perform the following transformation

$$C_i(t) = B_i(t)e^{-i\omega_i t}, \qquad C_f(t) = B_f(t)e^{-i\omega_f t}. \tag{6.26}$$ s29

These transformation leads to the initial conditions $B_k(0) = C_k(0)$ for $k = i, f$. Substituting these into Eqs.(6.25) we obtain equations of motion for amplitudes $B_j(t)$ in the s30 form

$$\dot{B}_i = \frac{iv}{2} B_f e^{-i\omega_{fi}t}, \tag{6.27a}$$ s30a

$$\dot{B}_f = \frac{iv^*}{2} B_i e^{i\omega_{fi}t}, \tag{6.27b}$$ s30b

where $\omega_{fi} = \omega_f - \omega_i$. This set of equations is formally identical to the set (5.42). We can use the solutions of the latter one in the present case. We only need to make the proper identifications. In the case of Eqs.(5.42) the initial conditions were $\varphi_2(0) = 0,\ \varphi_1(0) = 1$. Comparing initial conditions, we make the identifications

$$\varphi_2 \leftrightarrow B_f, \qquad \varphi_1 \leftrightarrow B_i, \tag{6.28}$$ s31a

Moreover, comparing equations (5.42) and (6.27) we should identify

$$\omega_{21} \to 0, \qquad \Omega \to v, \qquad \omega \to \omega_{fi} = \omega_f - \omega_i = \omega_k - \omega_{21}. \tag{6.29}$$ s31b

These substitutions result in some further ones, namely

$$\Delta = \omega - \omega_{21} \to \omega_k - \omega_{21}, \qquad \Omega_R = \sqrt{\Delta^2 + |\Omega|^2} \to \sqrt{v^2 + (\omega_k - \omega_{21})^2}. \tag{6.30}$$ s31c

We are interested in the amplitude $C_f(t)$, ot equivalently in $B_f(t)$. Then using the given identifications in solution (5.62a) for $\varphi_2 \to B_f$ we can write

$$B_f(t) = \frac{iv}{\sqrt{|v|^2 + (\omega_k - \omega_{21})^2}} e^{i(\omega_k - \omega_{21})t} \sin\left[\sqrt{|v|^2 + (\omega_k - \omega_{21})^2}\ \frac{t}{2}\right]. \tag{6.31}$$ s31d

The second coefficient $B_i(t)$ – of the atom remaining in the upper state with the field having $n_{n_{\vec{\mathbf{k}},\lambda}}$ photons is out of our interest.

6.2.4 Transition probability

As indicated in (6.10) we are interested in the transition probability $P_{f\leftarrow i}(t) = \left|C_f(t)\right|^2 = \left|B_f(t)\right|^2$, as it follows from (6.26). Amplitude $B_f(t)$ is found in Eq.(6.31), so we have

$$P_{f\leftarrow i}(t) = \frac{|v|^2}{|v|^2 + (\omega_k - \omega_{21})^2}\ \sin^2\left[\sqrt{|v|^2 + (\omega_k - \omega_{21})^2}\ \frac{t}{2}\right]. \tag{6.32}$$ s32

Coefficient v is defined by relation (6.24), it is proportional to the square root of the light intensity (because $v \propto \sqrt{n_{\vec{\mathbf{k}},\lambda}}$). We are interested in small field intensities, when $n_{\vec{\mathbf{k}},\lambda} \to 0$,

so we can take the lowest order approximation in $|v^2|$. Taking such an approximation in (6.32) we get

$$P_{f\leftarrow i}(t) = |v|^2 \, \frac{\sin^2\left[\frac{1}{2}(\omega_k - \omega_{21}t)\right]}{(\omega_k - \omega_{21})^2}. \tag{6.33}$$

It is worth noting that the same result can be obtained within the first order time-dependent perturbation calculations. Returning to the full notation, as it follows from Eq.(6.24), we get

$$P_{f\leftarrow i}(t) = \frac{\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2}{\hbar^2}\left(\frac{\hbar\omega_k}{2\varepsilon_0 V}\right)\left(n_{\vec{\mathbf{k}},\lambda}+1\right)\frac{4\,\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}. \tag{6.34}$$

Let us stress the very important fact. From the obtained expression we see that the atomic transition $|\,2\,\rangle \rightarrow |\,1\,\rangle$ (that is, downwards with the photon emission) is possible when the number of photons in the considered mode $(\vec{\mathbf{k}},\lambda)$ is zero, ie., $n_{\vec{\mathbf{k}},\lambda}=0$. This corresponds to the spontaneous emission. It is not important what was the reason of finding the atom in the excited (upper) state. The interaction of the atom with the field in the vacuum state ($n_{\vec{\mathbf{k}},\lambda}=0$) results in the spontaneous emission. Thus, the probability of spontaneous emission follows from the last equation with ($n_{\vec{\mathbf{k}},\lambda}=0$), and it is

$$P_{sp}(t) = \frac{4\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2}{\hbar^2}\left(\frac{\hbar\omega_k}{2\varepsilon_0 V}\right)\frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}. \tag{6.35}$$

This probability cannot be obtained within the semiclassical approximation. The reason is simple. In the semiclassical approach the fields are given functions not operators. The essential term $\left(n_{\vec{\mathbf{k}},\lambda}+1\right)$ arises due to annihilation and creation operators so, it is of quantum-mechanical origin.

6.3 Probability of spontaneous emission

6.3.1 Einstein's A-coefficient

Probability given by Eq.(6.35) corresponds to spontaneous emission into one well-defined mode. But we should remember that the vacuum field (and that is what we intend to consider) consists of infinity of modes. Therefore, we shall sum the obtained expression over all modes. Thus, we write

$$P_{sp}(t) = \frac{2}{\hbar\varepsilon_0 V}\sum_{\vec{\mathbf{k}}\lambda}\omega_k\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2\frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}. \tag{6.36}$$

Let us assume that the cavity is large enough so that we can transform the sum over the modes into the corresponding integration(as it was discussed in previous chapters). This transformation is summarized as

$$\sum_{\vec{\mathbf{k}}\lambda}(\,\ldots\,) \;\longrightarrow\; \frac{V}{(2\pi c)^3}\sum_{\lambda}\int_0^\infty d\omega_k\,\omega_k^2\int d\Omega_{\vec{\mathbf{k}}}\,(\,\ldots\,), \tag{6.37}$$

where the angular integral runs over all possible spatial orientations of the wave vector $\vec{\mathbf{k}}$. Combining these relations, we get

$$P_{sp}(t) = \frac{1}{4\pi^3\hbar\varepsilon_0 c^3} \sum_\lambda \int_0^\infty d\omega_k\ \omega_k^3 \int d\Omega_{\vec{\mathbf{k}}}\ \left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2 \frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}. \qquad (6.38)$$ s51a

The term containing matrix elements of the atomic dipole moment does not depend on frequency ω_k, so the integration splits into two independent parts. Hence, it is convenient to introduce an integral

$$J(\omega_{21}) = \int_0^\infty d\omega_k\ \omega_k^3\ \frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}. \qquad (6.39)$$ s51b

Then, expression (6.38) can be written as

$$P_{sp}(t) = \frac{1}{4\pi^3\hbar\varepsilon_0 c^3}\ J(\omega_{21}) \sum_\lambda \int d\Omega_{\vec{\mathbf{k}}}\ \left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2, \qquad (6.40)$$ s51c

and there are two terms which can be computed separately.

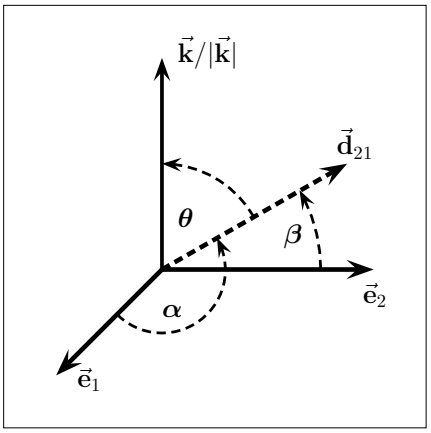

Fig. 6.1: Relative orientations of atomic dipole moment, wave vector and two polarization vectors.

First we deal with the last one – summation over polarizations and angular integration. Atomic dipole moment has a completely arbitrary orientation with respect to wave vector $\vec{\mathbf{k}}$ and two polarization vectors $\vec{\mathbf{e}}_1,\ \vec{\mathbf{e}}_2$. This is illustrated in figure 6.1. We can assume that atomic dipole $\vec{\mathbf{d}}_{21}$ is aligned with the z axis, so the wave vectors makes an angle θ with vector $\vec{\mathbf{d}}_{21}$. Polarization vetors are oriented at angles α and β, respectively (see figure). According to this discussion, the sum over polarization of the scalar products is written as

$$\sum_\lambda \left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2 = \left|\vec{\mathbf{d}}_{21}\right|^2\left(\cos^2\alpha+\cos^2\beta\right), \qquad (6.41)$$ s52a

since polarization vector are of unit length. Three vectors $\vec{\mathbf{k}},\vec{\mathbf{e}}_1,\vec{\mathbf{e}}_2$ are mutually orthogonal, thus the theorem on directional cosines holds, and we have

$$\cos^2\alpha+\cos^2\beta+\cos^2\theta = 1. \qquad (6.42)$$ s52b

Previous relation now becomes

$$\sum_\lambda \left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2 = \left|\vec{\mathbf{d}}_{21}\right|^2\left(1-\cos^2\theta\right), \qquad (6.43)$$ s52c

and now the last term in (6.40) can easily be calculated

$$\sum_\lambda \int d\Omega_{\vec{\mathbf{k}}}\ \left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2 = \left|\vec{\mathbf{d}}_{21}\right|^2 \int d\Omega_{\vec{\mathbf{k}}}\left(1-\cos^2\theta\right)$$
$$= 2\pi\left|\vec{\mathbf{d}}_{21}\right|^2 \int_0^\pi d\theta\ \sin\theta\left(1-\cos^2\theta\right) = \frac{8\pi}{3}\left|\vec{\mathbf{d}}_{21}\right|^2. \qquad (6.44)$$ s52d

So summation over polarizations and integration over all possible orientations is performed, The result is inserted into probability (6.40) giving

$$P_{sp}(t) = \frac{2\left|\vec{\mathbf{d}}_{21}\right|^2}{3\pi^2\hbar\varepsilon_0 c^3}\ J(\omega_{21}). \tag{6.45}$$ s53

It remains to compute the integral J. In order to do so, we take a new integration variable $x = \omega_k - \omega_{21}$ and from (6.39) we obtain

$$J(\omega_{21}) = \int\limits_{-\omega_{21}}^{\infty} dx\ \ (x+\omega_{21})^3\ \ \frac{\sin^2\left[\frac{1}{2}xt\right]}{x^2}. \tag{6.46}$$ s54b

Strictly speaking this integral is divergent, what is typical for quantum-electrodynamical problems. We will give some intuitive arguments which will allow us to find an approximate value of this integral. Due to physical arguments (energy conservation) we expect that emission of a photon with high energy (large frequency) is in fact highly improbable, if not just impossible. Hence, me may expect that some cutoff would be in place. As a result, high frequencies do not contribute to the integral and the main contribution comes from vicinity of $x \sim 0$ where the second (fractional) term the integrand is strongly peaked. Therefore we write approximately

$$J(\omega_{21}) = \omega_{21}^3 \int\limits_{-\infty}^{\infty} dx\ \frac{\sin^2\left[\frac{1}{2}xt\right]}{x^2}. \tag{6.47}$$ s54c

where (due to the given arguments) moved lower bound of integration to minus infinity he remaining integral can be found in the mathematical tables

$$\int\limits_{-\infty}^{\infty} dx\ \frac{\sin^2\left[\frac{1}{2}xt\right]}{x^2} = 2\int\limits_{0}^{\infty} dx\ \frac{\sin^2\left[\frac{1}{2}xt\right]}{x^2} = \frac{\pi t}{2}. \tag{6.48}$$ s54d

Hence the sought integral $J(\omega_{21})$ becomes

$$J(\omega_{21}) = \frac{\pi}{2}\omega_{21}^3 t. \tag{6.49}$$ s54e

This final result is then introduced int (6.45) and the probability of spontaneous emission is given as

$$P_{sp}(t) = \frac{\left|\vec{\mathbf{d}}_{21}\right|^2}{3\pi\hbar\varepsilon_0 c^3}\ \omega_{21}^3 t, \tag{6.50}$$ s55

and the probability per unit time

$$A = \frac{d\,P_{sp}(t)}{dt} = \frac{\omega_{21}^3\left|\vec{\mathbf{d}}_{21}\right|^2}{3\pi\hbar\varepsilon_0 c^3}, \tag{6.51}$$ s56

which is called Einstein's A-coefficient. We note that the probability (per unit time) of spontaneous emission is isotropic. Any direction of emission is as probable as any other one. This is an important feature of spontaneous emission.

6.3.2 Some additional discussion

Let us return to relation (6.36) (with summation over modes)

$$P_{sp}(t) = \frac{2}{\hbar\varepsilon_0 V}\sum_{\vec{\mathbf{k}}\lambda}\ \omega_k \left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2 \frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}. \tag{6.52}$$

Our discussion will consist in performing the summation in a different manner.

Atomic dipole moment has, as previously, arbitrary direction (obviously in the laboratory frame of reference). Let us take one of the polarization vectors, say $\vec{\mathbf{e}}_{\vec{\mathbf{k}}1}$. Then we can write

$$\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2 = \left|\vec{\mathbf{d}}_{21}\right|^2\ \cos^2\theta, \tag{6.53}$$

where θ is an angle between the considered vectors. Since vector $\vec{\mathbf{d}}_{21}$ has arbitrary direction the angle θ is also arbitrary. Therefore we should average over the orientations of the atomic dipole moment

$$\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2_{av} = \frac{1}{4\pi}\int_0^{2\pi}d\varphi\int_0^{\pi}d\theta\ \left|\vec{\mathbf{d}}_{21}\right|^2\ \cos^2\theta = \frac{\left|\vec{\mathbf{d}}_{21}\right|^2}{3}. \tag{6.54}$$

The averaged value of the atomic dipole moment is now inserted into probability (6.52)

$$P_{sp}(t) = \frac{2}{\hbar\varepsilon_0 V}\sum_{\vec{\mathbf{k}}\lambda}\ \frac{\left|\vec{\mathbf{d}}_{21}\right|^2}{3}\ \omega_k\ \frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}. \tag{6.55}$$

For sake of clarity we shall keep numerical factors. Inspecting the terms summed in the above relation, we see that they do no depend on polarizations. Hence, this sum produces a factor equal two. So we have

$$P_{sp}(t) = \frac{2}{\hbar\varepsilon_0 V}\left(\frac{2\left|\vec{\mathbf{d}}_{21}\right|^2}{3}\right)\sum_{\vec{\mathbf{k}}\lambda}\ \omega_k\ \frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}. \tag{6.56}$$

As previously, we transform the sum over wave vectors to the integral, so that

$$\begin{aligned} P_{sp}(t) &= \frac{2}{\hbar\varepsilon_0 V}\left(\frac{2\left|\vec{\mathbf{d}}_{21}\right|^2}{3}\right)\frac{V}{(2\pi c)^3}\int_0^{\infty}d\omega_k\ \omega_k^2\int d\Omega_{\vec{\mathbf{k}}}\ \omega_k\ \frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2} \\ &= \frac{1}{4\hbar\varepsilon_0\pi^3c^3}\left(\frac{2\left|\vec{\mathbf{d}}_{21}\right|^2}{3}\right)\cdot 4\,\pi\int_0^{\infty}d\omega_k\ \omega_k^3\ \frac{\sin^2\left[\frac{1}{2}(\omega_k-\omega_{21})t\right]}{(\omega_k-\omega_{21})^2}, \end{aligned} \tag{6.57}$$

because the integrand does not depend on the orientations of wave vectors. Recognizing integral $J(\omega_{21}$ as in Eq.(6.39), we have

$$P_{sp}(t) = \frac{1}{4\hbar\varepsilon_0\pi^3c^3}\left(\frac{2\left|\vec{\mathbf{d}}_{21}\right|^2}{3}\right)\cdot 4\,\pi\ J(\omega_{21}). \tag{6.58}$$

This expression is exactly the same as (6.45) only obtained in a different way. Previously, we computed $\sum_\lambda\int d\Omega_{\vec{\mathbf{k}}}\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2$ (see Eqs.(6.41)-(6.43)) which lead us to relation (6.44)

and gave a factor $(8\pi/3)\left|\vec{\mathbf{d}}_{21}\right|^2$. In the present case we first averaged over spatial orientations of the atomic dipole moment (see (6.54)) which yielded $\left|\vec{\mathbf{d}}_{21}\right|^2/3$. Polarization summation reduced to multiplication by 2, which appeared in (6.56) (the middle term, in brackets). Since remaining expression is polarization independent, the angular integral in (6.57) became trivial and produced factor 4π. Further discussion is identical as in previous subsection and leads to Einstein's A-coefficient (6.51).

6.3.3 Final remarks

Now we return to expression (6.40), that is to

$$P_{sp}(t) = \frac{1}{4\pi^3\hbar\varepsilon_0 c^3}\; J(\omega_{21}) \sum_{\lambda} \int d\Omega_{\vec{\mathbf{k}}}\; \left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}_{\vec{\mathbf{k}}\lambda}\right|^2, \tag{6.59}$$ s68

Probability of spontaneous emission of a photon with specified polarization $\vec{\mathbf{e}}$ in the given direction $d\Omega_{\vec{\mathbf{k}}}$ can be obtained from (6.59) without any summation. Then we get

$$P_{sp}(t,\vec{\mathbf{e}},d\Omega_{\vec{\mathbf{k}}}) = \frac{\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}\right|^2}{4\pi^3\hbar\varepsilon_0 c^3}\; J(\omega_{21})\; d\Omega_{\vec{\mathbf{k}}}. \tag{6.60}$$ s69a

Taking the integral $J(\omega_{21})$ from Eq.(6.49) we further obtain

$$P_{sp}(t,\vec{\mathbf{e}},d\Omega_{\vec{\mathbf{k}}}) = \frac{\omega_{21}^3\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}\right|^2}{8\pi^2\hbar\varepsilon_0 c^3}\; t\; d\Omega_{\vec{\mathbf{k}}}, \tag{6.61}$$ s69b

hence, per unit time we get

$$p_{sp}(\vec{\mathbf{e}},d\Omega_{\vec{\mathbf{k}}}) = \frac{\omega_{21}^3\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}\right|^2}{8\pi^2\hbar\varepsilon_0 c^3}\; d\Omega_{\vec{\mathbf{k}}}. \tag{6.62}$$ s69c

This is a probability (per unit time) of spontaneous emission of a photon with given polarization in the direction of a solid angle $d\Omega_{\vec{\mathbf{k}}}$. We again see that this expression is fully isotropic (direction independent).

On the other hand, when we integrate expression over all emission angles we would obtain probability (per unit time) of the emission in arbitrary direction but with specified polarization. Due to isotropy such an integral is trivial and produces a factor 4π. We get from

$$p_{sp}(\vec{\mathbf{e}}) = \frac{\omega_{21}^3\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}\right|^2}{2\pi\hbar\varepsilon_0 c^3}. \tag{6.63}$$ s70

Furthermore, the obtained expression can be averaged over the orientations of the atomic dipole. This, according to relation (6.54) gives a factor 1/3, so that

$$p_{sp}(\vec{\mathbf{e}}) = \frac{\omega_{21}^3\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}\right|^2}{6\pi\hbar\varepsilon_0 c^3}. \tag{6.64}$$ s71a

Finally, summation over polarizations will produce factor 2 and we get

$$p_{sp} = \frac{\omega_{21}^3\left|\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{e}}\right|^2}{3\pi\hbar\varepsilon_0 c^3}, \tag{6.65}$$ s71b

and we again arrive at Eistein's A-coefficient.

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Chapter 7

Optical Bloch equations

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7.1 Introduction. General discussion

We return to the more detailed analysis of the interaction of a two-level atom with electromagnetic field. The problem was already discussed in chapter 5, hence we just briefly recall some basic facts.

- The atomic Hamiltonian H_A is taken to be (see (5.24))

$$H_A = \frac{1}{2}\hbar\omega_{21}\ [\,|\,2\,\rangle\langle\,2\,|\,-\,|\,1\,\rangle\langle\,1\,|\,]\,. \tag{7.1}$$ b1

- We shall consider a semiclassical approach. We will assume that an atom interacts with a light beam consisting of a single mode with frequency ω_L and wave vector $\vec{\mathbf{k}}$. Hence, we can take the interaction hamiltonian given in (5.32), where summation and corresponding indices are not necessary.So we have

$$H_{AF} = -\frac{\hbar}{2}\Big\{|\,2\,\rangle\langle\,1\,|\,\Omega\,e^{-i(\Phi+\omega_L t)}\ +\ |\,1\,\rangle\langle\,2\,|\,\Omega^*\,e^{i(\Phi+\omega_L t)}\Big\}, \tag{7.2}$$ b2

where we have typical notation for Rabi frequency Ω and phase factor

$$\Omega = \frac{2}{\hbar}\,\vec{\mathbf{d}}_{21}\cdot\vec{\mathbf{E}}_L^{(+)}, \qquad\qquad \Phi = -\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}, \tag{7.3}$$ b3

with $\vec{\mathbf{d}}_{21}$ being the matrix element of the atomic dipole; $\vec{\mathbf{E}}_L^{(+)}$ – the amplitude of the classical monochromatic incident mode; $\vec{\mathbf{R}}$ – the position of (the center of mass of) the atom. We also note that RWA is silently assumed.

- The total hamiltonian (according to the discussion in chapter 5) of an atom interacting with (classical) radiation mode is of the form

$$H_{AL} = \frac{1}{2}\hbar\omega_{21}\ [\,|\,2\,\rangle\langle\,2\,|\,-\,|\,1\,\rangle\langle\,1\,|\,] - \frac{\hbar}{2}\Big\{|\,2\,\rangle\langle\,1\,|\,\Omega\,e^{-i(\Phi+\omega_L t)}\ +\ |\,1\,\rangle\langle\,2\,|\,\Omega^*\,e^{i(\Phi+\omega_L t)}\Big\}. \tag{7.4}$$ b4

The outlined model does not account for spontaneous emission which consists in the emission of a photon into vacuum modes which are not present here. Therefore we should

account for the coupling with vacuum modes. This implies, that we should consider a physical system consisting of three subsystems

$$\{\, atom\ (A)\,\} \;+\; \{\, laser\ field\ (L)\,\} \;+\; \{\, vacuum\ modes\ (V)\,\}. \tag{7.5}$$ b5

We are, in fact, interested only in the atomic subsystem in the description of which we need to account for spontaneous emission. The laser light is treated classically so there are no problems with it. On the other hand, vacuum modes are necessary for spontaneous emission, but otherwise not interesting. We are describing a compound system, but we are interested only in one part of it. Then, by necessity, we must consider the density matrix approach. The von Neumann equation thus reads

$$i\hbar\frac{\partial}{\partial t}\rho_{A+L+V} = \big[\, H_{A+L+V},\ \rho_{A+L+V}\,\big]. \tag{7.6}$$ b6a

The laser light is treated classically so we can write "AL" instead of separate index "L" in the above equation of motion. Hence we have

$$i\hbar\frac{\partial}{\partial t}\rho_{AL+V} = \big[\, H_{AL+V},\ \rho_{AL+V}\,\big]. \tag{7.7}$$ b6b

This equation should be reduced to the equation for the reduced density operator of an atom only. The mathematically sound reduction technique is quite complicated and difficult. It leads to the so called *Master Equation (ME)*. We shall not discuss the details of the ME methods. We will only state the main results. They follow from the requirements imposed upon atomic reduced density operator. Such an operator must be

- hermitian: $\rho = \rho^\dagger$;
- normalized: $\mathrm{Tr}\,\{\,\rho\,\} = 1$;
- semi-positive definite, ie., its eigenvalues must be nonnegative.

The mathematically strict reduction technique then leads to the following equation of motion for atomic density operator $\rho_{AL} \equiv \rho$:

$$\begin{aligned}\frac{d}{dt}\ \rho(t) &= \frac{1}{i\hbar}\ [\, H_{AL},\ \rho\,] \\ &\quad -\ \frac{A}{2}\Big[\, |\,2\,\rangle\langle\,2\,|\,\rho(t)\ +\ \rho(t)\,|\,2\,\rangle\langle\,2\,|\ -\ 2\,|\,1\,\rangle\langle\,2\,|\,\rho(t)\,|\,2\,\rangle\langle\,1\,|\,\Big],\end{aligned} \tag{7.8}$$ b7

where H_{AL} is the hamiltonian defined in (7.4). A denotes the usual Einstein's coefficient – probability (per unit time) of spontaneous emission. The second line of the above equation stems from reduction of the degrees of freedom to the atom only (which interacts with classical incident field). Sometimes we say that the second line of (7.8) accounts for the radiative damping due to the coupling with vacuum mode, that is, it describes spontaneous emission and ensures that the conditions imposed upon atomic density operator are fulfilled.

7.2 Derivation of optical Bloch equations

7.2.1 Evolution of the atom without damping

We continue our analysis of the two-level atom in the framework presented in the previous section. The evolution without damping is given by the first term in (7.8) in a manner similar to the von Neuman equation

$$i\hbar\frac{\partial}{\partial t}\,\rho(t)\Big|_{free} = [\,H_{AL},\ \rho(t)\,]\,. \tag{7.9}$$ b11

From now on, we we will omit the time argument and we will remember that we analyze the free evolution. Radiative damping will be considered later. Equation (7.8) is an operator equation. We transform it into a set of equations for the matrix elements of the atomic density operator. We multiply from the left by $\langle\, a\,|$ and from the right by $|\, b\,\rangle$ with $a, b = 1, 2$.

$$\begin{aligned}\frac{\partial}{\partial t}\,\langle\, a\,|\,\rho\,|\,b\,\rangle &= \frac{1}{i\hbar}\langle\, a\,|\,(\,H_{AL}\rho - \rho H_{AL}\,)\,|\,b\,\rangle \\ &= \frac{1}{i\hbar}\langle\, a\,|\,H_{AL}\rho\,|\,b\,\rangle - \frac{1}{i\hbar}\langle\, a\,|\,\rho H_{AL}\,|\,b\,\rangle.\end{aligned} \tag{7.10}$$ b12

Between operators in the second line we insert a unit operator $\hat{\mathbf{1}} = |\,1\,\rangle\langle\,1\,| + |\,1\,\rangle\langle\,2\,|$. After minor transformations, we obtain an equation for matrix elements of the atomic density operator

$$\frac{\partial}{\partial t}\,\rho_{ab} = \frac{1}{i\hbar}\Big((H_{AL})_{a1}\,\rho_{1b} + (H_{AL})_{a2}\,\rho_{2b} - (H_{AL})_{1b}\,\rho_{a1} - (H_{AL})_{2b}\,\rho_{a2}\Big). \tag{7.11}$$ b14

The hamiltonian H_{AL} is given in (7.8). It is straightforward to find its matrix elements. They are

$$\begin{aligned}(H_{AL})_{11} &= -\frac{\hbar\omega_{21}}{2}, & (H_{AL})_{12} &= -\frac{\hbar\Omega^*}{2}\,e^{i(\omega_L t+\Phi)}, \\ (H_{AL})_{21} &= -\frac{\hbar\Omega}{2}\,e^{-i(\omega_L t+\Phi)}, & (H_{AL})_{22} &= \frac{\hbar\omega_{21}}{2}.\end{aligned} \tag{7.12}$$

Having matrix elements of the Hamiltonian it is an easy matter to construct the equations of motion for the matrix elements of the atomic density operator which follow from Eq.(7.11)). We obtain the set of equations b21

$$\dot\rho_{11} = \frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\rho_{21} \;-\; \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\rho_{12}, \tag{7.13a}$$ b21a

$$\dot\rho_{22} = -\frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\rho_{21} \;+\; \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\rho_{12}, \tag{7.13b}$$ b21b

$$\dot\rho_{21} = \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\,(\rho_{11}-\rho_{22}) - i\,\omega_{21}\,\rho_{21}, \tag{7.13c}$$ b21c

$$\dot\rho_{12} = -\frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\,(\rho_{11}-\rho_{22}) + i\,\omega_{21}\,\rho_{21}. \tag{7.13d}$$ b21d

These equations describe the free evolution of the two-level atom in the field of classical monochromatic field. It remains to account for spontaneous emission.

7.2.2 Radiative and collisional damping

Radiative damping (spontaneous emission) is accounted for by the last term in Eq.(7.8). For matrix elements we easily obtain

$$\frac{\partial}{\partial t}\,\rho_{ab}\Big|_{sp} = -\frac{A}{2}\Big(\delta_{a2}\,\rho_{2b} + \rho_{a2}\,\delta_{2b} - 2\,\delta_{a1}\,\rho_{22}\,\delta_{1b}\Big). \tag{7.14}$$

The contributions due to this term are as follows

$$\frac{\partial}{\partial t}\,\rho_{11}\Big|_{sp} = A\,\rho_{22}, \qquad \frac{\partial}{\partial t}\,\rho_{12}\Big|_{sp} = -\frac{A}{2}\,\rho_{12},$$
$$\frac{\partial}{\partial t}\,\rho_{21}\Big|_{sp} = -\frac{A}{2}\,\rho_{21}, \qquad \frac{\partial}{\partial t}\,\rho_{22}\Big|_{sp} = -A\,\rho_{22}. \tag{7.15}$$

These equations must be now combined with free evolution ones (7.13). This results in the following set of equations

$$\dot\rho_{11} = A\,\rho_{22} \;+\; \frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\rho_{21} \;-\; \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\rho_{12} \tag{7.16a}$$

$$\dot\rho_{22} = -A\,\rho_{22} \;-\; \frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\rho_{21} \;+\; \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\rho_{12} \tag{7.16b}$$

$$\dot\rho_{21} = \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\,(\rho_{11}-\rho_{22}) - \left(\frac{A}{2} + i\,\omega_{21}\right)\rho_{21} \tag{7.16c}$$

$$\dot\rho_{12} = -\frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\,(\rho_{11}-\rho_{22}) - \left(\frac{A}{2} - i\,\omega_{21}\right)\rho_{12} \tag{7.16d}$$

This set of equations constitutes optical Bloch equations (OBE) for a two-level atom interacting with the single-mode (monochromatic) electromagnetic field which is assumed to be classical. Since OBE play an extremely important role in quantum optics we summarize the notation.

- ω_{21} denotes the atomic frequency;
- ω_L is the frequency of the incoming (classical) electromagnetic field;
- Ω is the Rabi frequency, defined in (7.3).
- The phase factor $\Phi = -\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}$, where $\vec{\mathbf{R}}$ is the position of the atom.
- A is Einstein's coefficient for spontaneous emission.

Let us note that OBE preserve the trace of the atomic density matrix. From Eqs.(7.16a) and (7.16b) we see that

$$\dot\rho_{11} + \dot\rho_{22} = 0 \quad\Longrightarrow\quad = \varrho_{11} + \varrho_{22} = const., \tag{7.17}$$

so if normalization is imposed at the initial moment, it will be conserved for any later moment of time. The requirement (which follows from the hermiticity of the density operator) that $\rho_{12} = \rho_{21}^*$ is also clearly satisfied by the OBE.

It is also evident that the optical Bloch equations are not independent. The first two equations are actually the same, while two last equation are complex conjugates of each

other. Therefore, the trace conservation requirement (7.17)) plays an essential role in any attempts to find the solution to Eqs.(7.16).

Before proceeding further we note the presence of the term $e^{\pm(i\Phi+i\omega t)}$ in equations (7.13). Certainly the presence of a time dependent factor makes the solution to the set of equations more difficult. Therefore, it is desirable to eliminate the time dependent factor. We will do this in the further sections, transforming the OBE to such a form, that right-hand sides of the equations will not include any time dependencies.

In many practical cases there are some other mechanisms which lead to the damping of the atomic dipole moment. For example, our atom may collide with some other atoms. General analysis of atomic collisions id pretty difficult. During the collision the oscillations of atomic dipole are disturbed and caused to decay. The matrix elements of atomic dipole are proportional to the coherences. Hence the collisional damping of the dipole moment can be accounted for in a phenomenological manner. We will assume that atomic coherences decay not only due to spontaneous emission but also due to collisions. This effect can be included in our picture by introducing an additional damping rate of the coherences. In the equations (7.16) we will replace the decay rate $A/2$ by

$$\Gamma_c = \frac{A}{2} + \gamma_{ph}, \tag{7.18}$$ b28a

where γ_{ph} describes the dephasing of the atomic dipole moment. The physical reasons for the dephasing will be discussed elsewhere. At present, we will simply include it into the optical Bloch equations. We arrive at the following set of equations b29

$$\dot\rho_{11} = A\,\rho_{22} \;+\; \frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\rho_{21} \;-\; \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\rho_{12}, \tag{7.19a}$$ b29a

$$\dot\rho_{22} = -A\,\rho_{22} \;-\; \frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\rho_{21} \;+\; \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\rho_{12}, \tag{7.19b}$$ b29b

$$\dot\rho_{21} = \frac{i\Omega}{2}e^{-i(\omega_L t+\Phi)}\,(\rho_{11}-\rho_{22}) - (\Gamma_c + i\,\omega_{21})\,\rho_{21}, \tag{7.19c}$$ b29c

$$\dot\rho_{12} = -\frac{i\Omega^*}{2}e^{i(\omega_L t+\Phi)}\,(\rho_{11}-\rho_{22}) - (\Gamma_c - i\,\omega_{21})\,\rho_{12}, \tag{7.19d}$$ b29d

which constitute the final form of the optical Bloch equations.

7.2.3 Simple elimination of time dependence

The set of equations (7.19) is linear, first order and with time-dependent coefficients. This is very inconvenient for practical solutions. It is desirable to transform out the unnecessary time dependence. To achieve this end we introduce new auxiliary variables

$$\begin{aligned} \rho_{11} &= \sigma_{11}, & \rho_{12} &= \sigma_{12}\,e^{i(\omega_L t+\Phi)}, \\ \rho_{21} &= \sigma_{21}\,e^{-i(\omega_L t+\Phi)}, & \rho_{22} &= \sigma_{22}. \end{aligned} \tag{7.20}$$

Transformation (7.20) allows us to write

$$\dot\rho_{21} = -i\big(\omega_L + \dot\Phi\big)\sigma_{21}\,e^{-i(\omega_L t+\Phi)} \;+\; \dot\sigma_{21}\,e^{-i(\omega_L t+\Phi)}, \tag{7.21}$$ b31

and similarly (by complex conjugation) for ρ_{12}. Let us stress that $\dot{\Phi} = -\vec{\mathbf{k}} \cdot \dot{\vec{\mathbf{R}}} = -\vec{\mathbf{k}} \cdot \vec{\mathbf{v}}$, where $\vec{\mathbf{V}}$ is the velocity of the atom. Transformation (7.20) in the two first equations of the set (7.16) leads to cancellation of the time-dependent exponential factors. Then, we use (7.21) in the equations for coherences, and we get from (7.16c)

$$-i\big(\omega_L + \dot{\Phi}\big)\sigma_{21}\, e^{-i(\omega_L t+\Phi)} \;+\; \dot{\sigma}_{21}\, e^{-i(\omega_L t+\Phi)} = \\ = \frac{i\Omega}{2} e^{-i(\omega_L t+\Phi)}\,(\rho_{11}-\rho_{22}) - (\Gamma_c + i\,\omega_{21})\,\rho_{21}. \tag{7.22}$$

b33a

Time-dependent factors cancel out. Introducing the generalized detuning defined as

$$\Delta = \omega_L - \omega_{21} - \dot{\Phi} = \omega_L - \omega_{21} - \vec{\mathbf{k}} \cdot \vec{\mathbf{v}}, \tag{7.23}$$

b34

we rewrite Eq.(7.22) in the form

$$\dot{\sigma}_{21} = \frac{i\Omega}{2}\,(\rho_{11}-\rho_{22}) - (\Gamma_c - i\,\Delta)\,\rho_{21}. \tag{7.24}$$

b35

Combining the results of our discussion, we transform the set (7.19) into one with time-independent coefficients. This is

b36

$$\dot{\sigma}_{11} = A\,\sigma_{22} \;+\; \frac{i\Omega^*}{2}\sigma_{21} \;-\; \frac{i\Omega}{2}\sigma_{12}, \tag{7.25a}$$

b36a

$$\dot{\sigma}_{22} = -A\,\sigma_{22} \;-\; \frac{i\Omega^*}{2}\sigma_{21} \;+\; \frac{i\Omega}{2}\sigma_{12}, \tag{7.25b}$$

b36b

$$\dot{\sigma}_{21} = \frac{i\Omega}{2}\,(\sigma_{11}-\sigma_{22}) - (\Gamma_c - i\,\Delta)\,\sigma_{21}, \tag{7.25c}$$

b36c

$$\dot{\sigma}_{12} = -\frac{i\Omega^*}{2}\,(\sigma_{11}-\sigma_{22}) - (\Gamma_c + i\,\Delta)\,\sigma_{12}. \tag{7.25d}$$

b36d

This is an alternative form of OBE. However it must be remembered that if we intend to give physical predictions, then we must use matrix elements of ρ. So the solutions to the set (7.25) must always be transformed back into elements of ρ according to relations (7.20).

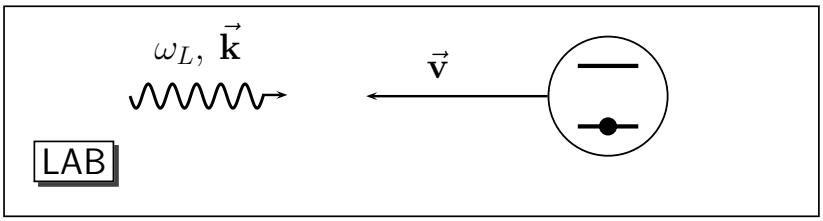

Fig. 7.1: Illustration to the discussion of the Doppler shift.

f:do

The generalized detuning is defined as $\Delta = \omega_L - \omega_{21} - \vec{\mathbf{k}} \cdot \vec{\mathbf{v}}$. The term $\vec{\mathbf{k}} \cdot \vec{\mathbf{v}}$ is just a Doppler shift. To see this note that the laser light is resonant when $\Delta = 0$. This means (according to Eq.(7.23)) that

$$\omega_L - \vec{\mathbf{k}} \cdot \vec{\mathbf{v}} = \omega_{21}. \tag{7.26}$$

b37

When the atom moves toward the light source, the atom (which plays the role of the "observer") sees the light of the "shorter" wavelength. Since $\lambda\nu = c$, the smaller λ means larger frequency $\omega_L = 2\pi\nu$. Therefore, when the atom moves towards the light source, it must "see" the light of resonant frequency $\omega_L' = \omega_L - \vec{\mathbf{k}} \cdot \vec{\mathbf{v}}$ greater than ω_L because the scalar product $\vec{\mathbf{k}} \cdot \vec{\mathbf{v}}$ is negative as is clearly seen from figure 7.1.

It is convenient to write set of equations (7.25) in the matrix form

$$\frac{d}{dt}\begin{pmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{21}\\ \sigma_{12}\end{pmatrix} = \begin{pmatrix} 0 & A & \frac{i}{2}\Omega^* & -\frac{i}{2}\Omega^* \\ 0 & -A & -\frac{i}{2}\Omega^* & \frac{i}{2}\Omega^* \\ \frac{i}{2}\Omega^* & -\frac{i}{2}\Omega^* & -\Gamma_c + i\Delta & 0 \\ -\frac{i}{2}\Omega^* & \frac{i}{2}\Omega^* & -\Gamma_c - i\Delta & 0 \end{pmatrix}\begin{pmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{21}\\ \sigma_{12}\end{pmatrix}. \tag{7.27}$$

The matrix has vanishing determinant (first two lines are linearly dependent). This indicates that one of the eigenvalues of the above given matrix is equal to zero. Moreover, it can be shown that the remaining three eigenvalues have negative real parts. As a consequence we can say that the solution to set (7.27) consists of two parts. One part (due to negative real parts of three eigenvalues) leads to quickly decaying transients. They decays in time exponentially, roughly speaking during the time comparable to several atomic lifetimes $\tau_A = 1/A$. The other part (corresponding to the zero eigenvalue) survives when time t is long enough. This part of the solutionis called a stationary one. This reasoning has also physical counterpart. When the laser is switch on some transient and fast phenomena occur. Afterwards we expect that some kind of dynamical equilibrium is established. The system stabilizes and no more changes occur. This clearly corresponds to the stationary behavior.

7.3 Stationary optical Bloch equations

Following the argument given in the previous section we will find stationary solutions to OBE (7.25) or (7.27).

7.3.1 Stationary solutions

Stationary optical Bloch equations follow, when we take the left-hand sides of equations (7.25)) to be equal zero. So we have

$$0 = A\bar{\sigma}_{22} + \frac{i}{2}\Omega^*\,\bar{\sigma}_{21} - \frac{i}{2}\Omega\,\bar{\sigma}_{12}, \tag{7.28a}$$

$$0 = -A\bar{\sigma}_{22} - \frac{i}{2}\Omega^*\,\bar{\sigma}_{21} + \frac{i}{2}\Omega\,\bar{\sigma}_{12}, \tag{7.28b}$$

$$0 = \frac{i}{2}\Omega\,(\,\bar{\sigma}_{11} - \bar{\sigma}_{22}\,) - (\Gamma_c - i\,\Delta)\,\bar{\sigma}_{21}, \tag{7.28c}$$

$$0 = -\frac{i}{2}\Omega^*\,(\bar{\sigma}_{11} - \bar{\sigma}_{22}\,) - (\Gamma_c + i\,\Delta)\,\bar{\sigma}_{12}. \tag{7.28d}$$

The bar indicates that we deal with stationary solutions, in the sense

$$\bar{\sigma}_{ab} = \lim_{t\to\infty}\sigma_{ab}(t). \tag{7.29}$$

The obtained set is homogeneous, moreover, it is straightforward to see that the first two equations differ only by a sign, so they are linearly dependent. It may seem that there are no nontrivial solution. This not the case since we must account for the trace conservation. We discard the first equation of the above set, and instead, we adopt the trace conservation requirement as the first equation. As a result we arrive at the set of equations

b48

$$1 = \bar{\sigma}_{11} + \bar{\sigma}_{22}, \tag{7.30a}$$ b48a

$$0 = -A\bar{\sigma}_{22} - \frac{i}{2}\,\Omega^*\,\bar{\sigma}_{21} + \frac{i}{2}\,\Omega\,\bar{\sigma}_{12}, \tag{7.30b}$$ b48b

$$0 = \frac{i\,\Omega}{2}\,(\bar{\sigma}_{11} - \bar{\sigma}_{22}) - (\Gamma_c - i\Delta)\,\bar{\sigma}_{21}, \tag{7.30c}$$ b48c

$$0 = -\frac{i\,\Omega^*}{2}\,(\bar{\sigma}_{11} - \bar{\sigma}_{22}) - (\Gamma_c + i\Delta)\,\bar{\sigma}_{12}. \tag{7.30d}$$ b48d

From two last equations we express coherences as functions of populations

$$\bar{\sigma}_{21} = \frac{i\Omega}{2(\Gamma_c - i\Delta)}\,(\bar{\sigma}_{11} - \bar{\sigma}_{22})\,, \tag{7.31}$$ b48e

while the second coherence $\bar{\sigma}_{12}$ follows by complex conjugation. Inserting these expressions into the first two equations of the set (7.30) we get two, closed equations for populations only

b48x

$$\bar{\sigma}_{11} = 1 - \bar{\sigma}_{22}, \tag{7.32a}$$ b48xa

$$A\bar{\sigma}_{22} = \frac{|\Omega|^2}{2}\,(\bar{\sigma}_{11} - \bar{\sigma}_{22})\,\frac{\Gamma_c}{\Gamma_c^2 + \Delta^2}, \tag{7.32b}$$ b48xb

Solution to these equations poses no difficulties. The obtained populations are then substituted into Eq.(7.31) which yield the coherences. Straightforward algebra leads to the following stationary solutions to optical Bloch equations

b49

$$\bar{\sigma}_{11} = \frac{A(\Gamma_c^2 + \Delta^2) + \frac{1}{2}|\Omega|^2\Gamma_c}{A(\Gamma_c^2 + \Delta^2) + |\Omega|^2\Gamma_c}, \tag{7.33a}$$ b49a

$$\bar{\sigma}_{22} = \frac{\frac{1}{2}|\Omega|^2\Gamma_c}{A(\Gamma_c^2 + \Delta^2) + |\Omega|^2\Gamma_c}, \tag{7.33b}$$ b49b

$$\bar{\sigma}_{21} = \bar{\sigma}_{12}^{\,*} \;=\; \frac{\frac{1}{2}\Omega A(i\Gamma_c - \Delta)}{A(\Gamma_c^2 + \Delta^2) + |\Omega|^2\Gamma_c}. \tag{7.33c}$$ b49c

The trace conservation requirement is obviously satisfied. Moreover, we note the inequality

$$\bar{\sigma}_{11} > \bar{\sigma}_{22} \tag{7.34}$$ b51

7.3.2 Stationary energy balance

Our present discussion of atom-light interaction is semiclassical. The atom is coupled to the electric field

$$\begin{aligned}\vec{\mathbf{E}}(\vec{\mathbf{R}},t) &= \vec{\mathbf{E}}^{(+)}(\vec{\mathbf{R}},t) + \vec{\mathbf{E}}^{(-)}(\vec{\mathbf{R}},t)\\ &= \vec{\mathbf{E}}_0^{(+)}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}} - i\omega_L t} + \vec{\mathbf{E}}_0^{(-)}\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}} + i\omega_L t}.\end{aligned} \tag{7.35}$$

This field acts upon the atom and within the time interval performs the elementary work

$$dW = q\vec{\mathbf{E}}(\vec{\mathbf{R}},t)\cdot d\vec{\mathbf{r}}, \tag{7.36}$$ b57

where $d\vec{\mathbf{r}}$ is the displacement of the electron. Thus, the power absorbed by the atom is given as

$$\frac{d}{dt}\ W = \vec{\mathbf{E}}(\vec{\mathbf{R}},t)\cdot\frac{d}{dt}\ (q\vec{\mathbf{r}})\,, = \vec{\mathbf{E}}(\vec{\mathbf{R}},t)\cdot\frac{d}{dt}\ \left(\vec{\mathbf{d}}(t)\right), \tag{7.37}$$ b58

with $\vec{\mathbf{d}}(t)$ being the operator of the atomic dipole moment. We average the obtained relation both quantum-mechanically and over time (we denote the latter averaging by the bar)

$$\overline{\langle\ \frac{d}{dt}\ W\ \rangle}\ =\ \overline{\vec{\mathbf{E}}(\vec{\mathbf{R}},t)\cdot\frac{d}{dt}\ \langle\ \vec{\mathbf{d}}(t)\ \rangle}. \tag{7.38}$$ b59

Quantum-mechanical averaging refers only to the atomic dipole, because the field is treated classically.

$$\begin{aligned}\langle\ \vec{\mathbf{d}}(t)\ \rangle &= \mathrm{Tr}\left\{\vec{\mathbf{d}}\,\rho(t)\right\} &(7.39)\\ &= \mathrm{Tr}\left\{\left[\vec{\mathbf{d}}_{12}|\,1\,\rangle\langle\,2\,| + \vec{\mathbf{d}}_{21}|\,2\,\rangle\langle\,1\,|\right]\rho(t)\right\} &(7.40)\\ &= \vec{\mathbf{d}}_{12}\rho_{21}(t) + \vec{\mathbf{d}}_{21}\rho_{12}(t). &(7.41)\end{aligned}$$ b60

In this section we are interested only in the stationary regime, hence we can use Eq.(7.20) b30 to express matrix elements of ρ by the corresponding elements of σ. Thus, we get

$$\rho_{21} = \bar{\sigma}_{21}\,e^{-i(\omega_L t+\Phi)}, \qquad \rho_{12} = \bar{\sigma}_{12}\,e^{i(\omega_L t+\Phi)}. \tag{7.42}$$ b61

Hence the expectation value for the atomic dipole moment becomes

$$\langle\ \vec{\mathbf{d}}(t)\ \rangle = \vec{\mathbf{d}}_{12}\,\bar{\sigma}_{21}\,e^{-i(\omega_L t+\Phi)} + \vec{\mathbf{d}}_{21}\,\bar{\sigma}_{12}\,e^{i(\omega_L t+\Phi)}. \tag{7.43}$$ b62

The needed time derivative is

$$\frac{d}{dt}\ \langle\ \vec{\mathbf{d}}(t)\ \rangle = i\left(\omega_L+\dot{\Phi}\right)\vec{\mathbf{d}}_{21}\,\bar{\sigma}_{12}\,e^{i(\omega_L t+\Phi)} - i\left(\omega_L+\dot{\Phi}\right)\vec{\mathbf{d}}_{12}\,\bar{\sigma}_{21}\,e^{-i(\omega_L t+\Phi)}. \tag{7.44}$$ b63a

According to relation (7.26) b37 we have $\omega_L+\dot{\Phi} = \omega_L - \vec{\mathbf{k}}\cdot\vec{\mathbf{v}} = \omega_{21}$. Hence

$$\frac{d}{dt}\ \langle\ \vec{\mathbf{d}}(t)\ \rangle = i\omega_{21}\,\vec{\mathbf{d}}_{21}\,\bar{\sigma}_{12}\,e^{i(\omega_L t+\Phi)} - i\omega_{21}\,\vec{\mathbf{d}}_{12}\,\bar{\sigma}_{21}\,e^{-i(\omega_L t+\Phi)}. \tag{7.45}$$ b63b

Now, we substitute the obtained time derivative into (7.38) b59 to get the average absorbed power

$$\begin{aligned}\overline{\langle\ \frac{d}{dt}\ W\ \rangle}\ =\ &\overline{\left[\vec{\mathbf{E}}_0^{(+)}\,e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}-i\omega_L t} + \vec{\mathbf{E}}_0^{(-)}\,e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}+i\omega_L t}\right]}\\ &\overline{\cdot\left[\ i\omega_{21}\vec{\mathbf{d}}_{21}\,\bar{\sigma}_{12}\,e^{i(\omega_L t+\Phi)} - i\omega_{21}\vec{\mathbf{d}}_{12}\,\bar{\sigma}_{21}\,e^{-i(\omega_L t+\Phi)}\right]},\end{aligned} \tag{7.46}$$

We are averaging over time, therefore we can neglect the quickly oscillating terms. We arrive at the expression

$$\overline{\langle \frac{d}{dt}\ W \rangle} \ = \ i\omega_{21} \left(\vec{\mathbf{E}}_0^{(+)} \cdot \vec{\mathbf{d}}_{21} \right) \bar{\sigma}_{12} - i\omega_{21} \left(\vec{\mathbf{E}}_0^{(+)} \cdot \vec{\mathbf{d}}_{12} \right) \bar{\sigma}_{21}. \tag{7.47}$$ b65

According to Eq.(7.3) we recognize the Rabi frequency $\Omega/2$ and its complex conjugate. We obtain

$$\overline{\langle \frac{d}{dt}\ W \rangle} \ = \ i\omega_{21} \frac{\hbar\Omega}{2} \bar{\sigma}_{12} - i\omega_{21} \frac{\hbar\Omega^*}{2} \bar{\sigma}_{21} \ = \ -\hbar\omega_{21} \mathrm{Im}\{\Omega\bar{\sigma}_{12}\}. \tag{7.48}$$ b66a

We now take $\bar{\sigma}_{12}$ from Eq.(7.33c)) and we obtain

$$\overline{\langle \frac{d}{dt}\ W \rangle} \ = \ \hbar\omega_{21} \ \frac{\frac{1}{2}|\Omega|^2 A\Gamma_c}{A(\Gamma_c^2 + \Delta^2) + \Gamma_c|\Omega|^2} \ = \ \hbar\omega_{21}\, A \ \frac{\frac{1}{2}|\Omega|^2 \Gamma_c}{A(\Gamma_c^2 + \Delta^2) + \Gamma_c|\Omega|^2}. \tag{7.49}$$ b68

Finally, we see that the fraction reproduces the stationary-state upper state population $\bar{\sigma}_{22}$ as given in (7.33b). Therefore we have

$$\overline{\langle \frac{d}{dt}\ W \rangle} \ = \ \hbar\omega_{21} A\, \bar{\sigma}_{22}. \tag{7.50}$$ b69

We have calculated the average power absorbed by the atom from the incident field. Let us denote

$$\bar{N}_{abs} \ = \ A\, \bar{\sigma}_{22}. \tag{7.51}$$ b70

and call this quantity an average absorption rate. Then we can write

$$\overline{\langle \frac{d}{dt}\ W \rangle} \ = \ \hbar\omega_{21}\, \bar{N}_{abs}. \tag{7.52}$$ b71

The average absorption rate can be interpreted as the average number od absorbed photons (per unit time), each photon carrying the resonant energy $\hbar\omega_{21}$. In this sense expression (7.52) is understandable.

On the other hand, the term $A\,\bar{\sigma}_{22}$ is the rate of spontaneous emission, because it appears in the right-hand side of the equation of motion (7.25b) as the rate of the decay of the upper state population. So the quantity $\bar{N}_{abs}$ may be interpreted as the average number (per unit time) of spontaneous emissions. At first it may seem difficult to explain this apparent discrepancy.

The sequence of photon absorption and stimulated emission do not result in the weakening of the light beam. It is impossible to say whether a photon appeared in the beam due to stimulated emission or it just was not absorbed. When a photon is absorbed from the beam by an atom which afterwards emits spontaneously (in arbitrary direction) then the former one is truly lost from the beam. This explains the equivalence between the average rate of absorption (from the incident beam) and the average rate of spontaneous emission. This seems to be an intuitively plausible conclusion.

7.4 Population inversion

7.4.1 Population inversion. Introduction

bb1 Let us return to OBE, as given in Eqs.(b36 7.25)

$$\dot{\sigma}_{11} = A\,\sigma_{22} \;+\; \frac{i\Omega^*}{2}\sigma_{21} \;-\; \frac{i\Omega}{2}\sigma_{12}, \tag{7.53a}$$ bb1a

$$\dot{\sigma}_{22} = -A\,\sigma_{22} \;-\; \frac{i\Omega^*}{2}\sigma_{21} \;+\; \frac{i\Omega}{2}\sigma_{12}, \tag{7.53b}$$ bb1b

$$\dot{\sigma}_{21} = \frac{i\Omega}{2}\,(\sigma_{11}-\sigma_{22}) - (\Gamma_c - i\,\Delta)\,\sigma_{21}, \tag{7.53c}$$ bb1c

$$\dot{\sigma}_{12} = -\frac{i\Omega^*}{2}\,(\sigma_{11}-\sigma_{22}) - (\Gamma_c + i\,\Delta)\,\sigma_{12}. \tag{7.53d}$$ bb1d

We construct a new physical quantity, the so-balled population inversion

$$w(t) = \sigma_{22} - \sigma_{11}, \tag{7.54}$$ bb2

note that it is independent of the transformation (b30 7.20). Inversion is greatest when all population is in the upper state, that is when $\sigma_{22} = 1$. The minimum value of inversion corresponds to $\sigma_{11} = 1$ – all atoms in in the ground state. Hence we see that population inversion is a real number within an interval

$$w(t) \in \big[\,-1,\,1\,\big]. \tag{7.55}$$ bb2e

First two out of Eqs.(bb1 7.53) yield an equation of motion for population inversion.

$$\dot{w}(t) = -2A\sigma_{22} \;-\; i\Omega^*\sigma_{21} \;+\; i\Omega\sigma_{12}. \tag{7.56}$$ bb3a

Due to normalization condition $\sigma_{22} = 1 - \sigma_{11}$ we can write

$$2\sigma_{22} = \sigma_{22} + \sigma_{22} = \sigma_{22} + 1 - \sigma_{11} = 1 + w(t). \tag{7.57}$$ bb3b

Hence, equation of motion becomes

$$\dot{w}(t) = A\big[-1 - w(t)\big] \;-\; i\Omega^*\sigma_{21} \;+\; i\Omega\sigma_{12}. \tag{7.58}$$ bb3c

Let us modify this equation. We shall replace the number (-1) in the brackets by a unspecified number λ, so our equation of motion reads

$$\dot{w}(t) = A\big[\lambda - w(t)\big] \;-\; i\Omega^*\sigma_{21} \;+\; i\Omega\sigma_{12}. \tag{7.59}$$ bb4

Our present aim is to investigate the physical sense of the parameter λ. In order to do so, we consider a simplified physical situation, assuming that there is no incident light, which entails that $\Omega = 0$. So we investigated the equation

$$\dot{w}(t) = A\lambda - Aw(t). \tag{7.60}$$ bb5

This is an inhomogeneous differential equation. The heomogeneous one is $\dot{w}(t) = -Aw(t)$, with an obvious solution $w_h(t) = C\exp(-At)$. We postulate, that the solution to Eq.(7.60) is

$$w(t) = C(t)\exp(-At). \tag{7.61}$$ bb7a

This leads to the equation for the unknown function $C(t)$

$$\dot{C}(t) = A\lambda\exp(At). \tag{7.62}$$ bb7c

Integration is trivial, and gives

$$C(t) = \lambda\exp(At) + C_0, \tag{7.63}$$ bb7d

where the constant C_0 has to be found. Inserting (7.63) into (7.61) yields

$$w(t) = [\lambda\exp(At) + C_0]\exp(-At) = \lambda + C_0\exp(-At). \tag{7.64}$$ bb8a

Assuming that in the initial moment $w(0) = w_0$ we get $C_0 = w_0 - \lambda$. This allows us to write

$$w(t) = w_0\exp(-At) + \lambda\big[1 - \exp(-At)\big]. \tag{7.65}$$ bb9

This relation enables us to determine the physical sense of the parameter λ. We see that

$$w(t) \xrightarrow[t\to\infty]{} \lambda. \tag{7.66}$$ bb10

So λ equals the value to which population inversion tends, after the decay of all possible initial excitations. In principle, we expect the atom to arrive at the ground state, which in turn, correspond to $\lambda = -1$. In fact we have replaced -1 by λ, so this conclusion should not be surprising.

Let us, however, generalize our approach. Let us call the parameter λ the equilibrium population inversion

$$\lambda \equiv w_{eq} \in \big[\,-1,\ 1\,\big]. \tag{7.67}$$ bb11

Such a generalization results in the modification of equation (7.59) which now is of the form

$$\dot{w}(t) = A\big[w_{eq} - w(t)\big] \ - \ i\Omega^*\sigma_{21} \ + \ i\Omega\sigma_{12}. \tag{7.68}$$ bb12

This equation was derived from optical Bloch equations, so the introduced modification must lead to the corresponding modification of OBE. The question is whether such modification is really necessary. To answer the question we must investigate w_{eq} in much more detail.

7.4.2 Analysis of equilibrium population inversion

In this subsection we use the concepts of statistical physics. Let us assume that our atomic system st in thermodynamical equilibrium (and the atoms are not irradiated). The canonical density operator follows from Gibbs theory and it is

$$\varrho_{eq} = \frac{1}{Z}\ \exp\left(-\frac{H_A}{k_B T}\right). \tag{7.69}$$ bb15

H_A is the (free) atomic hamiltonian (b1 7.1), k_B is the Boltzmann constant, and T the temperature. Finally Z denotes the statistical sum

$$Z = \mathrm{Tr}\left\{\exp\left(-\frac{H_A}{k_B T}\right)\right\}. \tag{7.70}$$ bb17

Since the atomic hamiltonian is known, it is not difficult to find Z.

$$Z = \left\langle 1 \left| \exp\left(-\frac{H_A}{k_B T}\right) \right| 1 \right\rangle \ + \ \left\langle 2 \left| \exp\left(-\frac{H_A}{k_B T}\right) \right| 2 \right\rangle. \tag{7.71}$$ bb18a

States $|\,1\,\rangle$ and $|\,2\,\rangle$ are the eigenstates of H_A so we easily get

$$Z = \exp\left(\frac{\hbar\omega_{21}}{2k_B T}\right) \ + \ \exp\left(-\frac{\hbar\omega_{21}}{2k_B T}\right). \tag{7.72}$$ bb18b

Let us introduce a temporary symbol

$$\kappa = \frac{\hbar\omega_{21}}{2k_B T}. \tag{7.73}$$ bb19

Combining the result, we write the equilibrium density operator (bb15 7.69) as

$$\varrho_{eq} = \frac{1}{e^{\kappa} + e^{-\kappa}}\ \exp\left(-\frac{H_A}{k_B T}\right). \tag{7.74}$$ bb20

Then we can compute the equilibrium populations. For the ground state we get

$$\langle\,1\,|\,\varrho_{eq}\,|\,1\,\rangle = \left\langle 1 \left| \frac{1}{e^{\kappa} + e^{-\kappa}}\ \exp\left(-\frac{H_A}{k_B T}\right) \right| 1 \right\rangle = \frac{e^{\kappa}}{e^{\kappa} + e^{-\kappa}}, \tag{7.75}$$ bb21

while for the excited state we have

$$\langle\,2\,|\,\varrho_{eq}\,|\,2\,\rangle = \left\langle 2 \left| \frac{1}{e^{\kappa} + e^{-\kappa}}\ \exp\left(-\frac{H_A}{k_B T}\right) \right| 2 \right\rangle = \frac{e^{-\kappa}}{e^{\kappa} + e^{-\kappa}}. \tag{7.76}$$ bb22

Thus, in the thermodynamical equilibrium the population inversion is equal to

$$w_{eq} = \langle\,2\,|\,\varrho_{eq}\,|\,2\,\rangle - \langle\,1\,|\,\varrho_{eq}\,|\,1\,\rangle = -\frac{e^{\kappa} - e^{-\kappa}}{e^{\kappa} + e^{-\kappa}} = -\tanh(\kappa) = -\tanh\left(\frac{\hbar\omega_{21}}{2k_B T}\right). \tag{7.77}$$ bb23

Obviously, the argument of the hyperbolic tangent is positive. Let us consider the case of high and low temperatures.

- For large temperatures, such that $k_B T \gg \hbar\omega_{21}$, the argument of the hyperbolic tangent is very small and the tangent itself is very close to zero. Therefore, we can say that

$$w_{eq} \xrightarrow[T \to \infty]{} 0_-, \tag{7.78}$$

bb24

that is w_{eq} tends to zero from the negative side. This means, that in high temperatures $w_{eq} = (\varrho_{eq})_{22} - (\varrho_{eq})_{11}$ is very small but negative. Almost half of the atoms are in the excited (upper) state, while slightly more than half are still in the ground state.

- In the case of low temperatures, that is when $\hbar\omega_{21} \gg k_B T$, the argument of the hyperbolic tangent is quite large and the value of tangent is close to unity. Therefore, in this case we have

$$w_{eq} \xrightarrow[T \to 0]{} -1_+. \tag{7.79}$$

bb25

Equilibrium population inversion tends from above to -1. It means that almost all atoms are in the ground state and only a very small fraction of them may be found in the excited state.

The presented reasoning is certainly sound, but what does it mean that temperature is high or low ? To answer this question we need some numerical estimates.

7.4.3 Numerical estimates and conclusions

We are interested in the estimates, not in precise calculations for any specific physical situations. For this purpose, we will consider an atomic transition corresponding to the light of wavelength

$$\lambda = 500 \text{ nm}. \tag{7.80}$$

bb31a

Since $c = 3{\cdot}10^8$ m/s, the assumed wavelength corresponds to the frequency $f = c/\lambda = 0.6{\cdot}10^{15}$ s^{-1}. The angular frequency (usually used in our calculations) $\omega = 2\pi f \approx 3.8{\cdot}10^{15}$ s^{-1}. Atomic frequency ω_{21} must be of the same order of magnitude. For our estimates we shall, thus, adopt

$$\omega_{21} = 4 \cdot 10^{15} \text{ s}^{-1}. \tag{7.81}$$

bb32b

We stress that we are making estimates, not exact calculations, thereby it is reasonable to assume that

$$\hbar = \frac{h}{2\pi} = \frac{6.6256 \cdot 10^{-34} \text{ J/s}}{2\pi} \approx 10^{-34} \text{ J/s}. \tag{7.82}$$

bb32c

Then, the energy $\hbar\omega_{21}$ is estimated as

$$\hbar\omega_{21} \approx 4 \cdot 10^{15} \cdot 10^{-34} \text{ J} = 4 \cdot 10^{-19} \text{ J} = \frac{4}{1.6} \text{ eV} = 2.5 \text{ eV}, \tag{7.83}$$

bb32d

which is quite a reasonable result. On the other hand, Boltzmann constant is $k_B = 1.38 \cdot 10^{-23}$ J/K. Let us now consider room temperature $T = 300$ K. This corresponds to thermal energy

$$k_B T \approx 1.38 \cdot 10^{-23} \cdot 300 \text{ J} \approx 4.2 \cdot 10^{-21} \text{ J} = \frac{4.2}{1.6} \cdot 10^{-2} \text{ eV} \approx 2.6 \cdot 10^{-2} \text{ eV}. \quad (7.84)$$ bb33b

Hence we have an estimate

$$\kappa = \frac{\hbar\omega_{21}}{2k_B T} \approx \frac{2.5 \text{ eV}}{2 \cdot 2.6 \cdot 10^{-2} \text{ eV}} \approx 0.5 \cdot 10^2 = 50. \quad (7.85)$$ bb34

Obviously, for lower temperatures the parameter κ will be still larger. Now according to Eq. (7.77) for κ estimated above, we get for $T = 300$ K

$$w_{eq} = -\tanh(\kappa) = -1. \quad (7.86)$$ bb35

This is a result given by three (quite different) calculators. We conclude that the substitution $\lambda = w_{eq} > -1$ (as it was done when passing from Eq.(7.58) to (7.59)) is completely not necessary when temperatures are reasonable.

It is straightforward to repeat this estimate for temperature $T = 1000$ K. This gives $k_B T \approx 0.09$ eV. This, in turn, leads to $\kappa = \hbar\omega_{21}/2k_B T = 13.9$. Then, one calculator gives $\tanh(13.9) = 1$ and the second calculator showed 11 digits 9 after the decimal point. The conclusion stated above still holds with extremely good approximation even for relatively high temperatures.

We have established that for temperature below 1000 K we ar fully justified to put $w_{eq} = -1$ and forget about any modifications to OBE as given by Eqs.(7.25) ot (7.16). At reasonable temperatures (in equilibrium) all atoms are in the ground state. Reasonable temperatures in practice mean temperatures of the order of several hundreds of kelvins or less.

An interesting question is as follows. What is the temperature at which (in equilibrium) 1 per cent of atoms is in the excited state while 99 % remain in the ground state ? This corresponds to the population inversion

$$w_{eq} = (\varrho_{eq})_{22} - (\varrho_{eq})_{11} = \frac{1}{100} - \frac{99}{100} = -\frac{98}{100}. \quad (7.87)$$ bb41

According to Eq.(7.77) this requirement corresponds to the equation

$$\tanh\left(\frac{\hbar\omega_{21}}{2k_B T}\right) = \tanh(\kappa) = \frac{98}{100}. \quad (7.88)$$ bb42a

Calculator estimates are as follows

$$\tanh(2.29) = 0.9797, \qquad \tanh(2.30) = 0.9801, \qquad \tanh(2.31) = 0.9805. \quad (7.89)$$ bb42x

So we see that 1 per cent of excited atoms corresponds to $\kappa = \hbar\omega_{21}/2k_B T \approx 2.3$. This leads to the simple estimate

$$k_B T \approx \frac{\hbar\omega_{21}}{5} = 0.5 \text{ eV} = 0.8 \cdot 10^{-19} \text{ J}. \quad (7.90)$$ bb42d

Having estimated the thermal energy, we translate it into temperature estimate

$$T \approx \frac{0.8 \cdot 10^{-19}\ \mathrm{J}}{1.38 \cdot 10^{-23}\ \mathrm{J/K}} \approx 0.6 \cdot 10^{4}\ \mathrm{K} = 6000\ K. \tag{7.91}$$ bb43

We conclude that the appreciable number of atoms (1 %) in the upper state (in thermal equilibrium) occurs at the temperatures corresponding to the star's atmospheres. In practical laboratory experiments virtually all atoms are in the ground state, $w_{eq} = -1$, and no modifications to the optical Bloch equations (7.19) or (7.25) are necessary.

* *

Part II

AUXILIARY CHAPTERS

Chapter 8

Classical harmonic oscillator in external field

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8.1 Discussion of the roots and solutions

In the main part of the lectures we considered the roots of the characteristic polynomial (os6a) of the damped harmonic oscillator. These roots ω_1 and ω_2 are given in (os6d). They govern the behavior of the solution of the homogeneous equation. They are also important for the solution of the inhomogeneous one, therefore we will discuss their properties. Let us recall that the considered roots are as follows

$$\omega_{1,2} = -\frac{i\Gamma}{2} \pm \Omega, \qquad \text{with} \qquad \Omega = \sqrt{\omega_0^2 - \frac{1}{4}\Gamma^2}. \tag{8.1}$$

aos15

We stress that from the physical point of view, we require that the damping parameter $\Gamma \geq 0$, while the oscillator frequency $\omega_0 > 0$. Negative parameters are unphysical, so we do not consider such a case. First of all, we note that for arbitrary values of the parameters Γ and ω_0, the characteristic roots have the property

$$|\omega_{1,2}| = \omega_0. \tag{8.2}$$

aos16

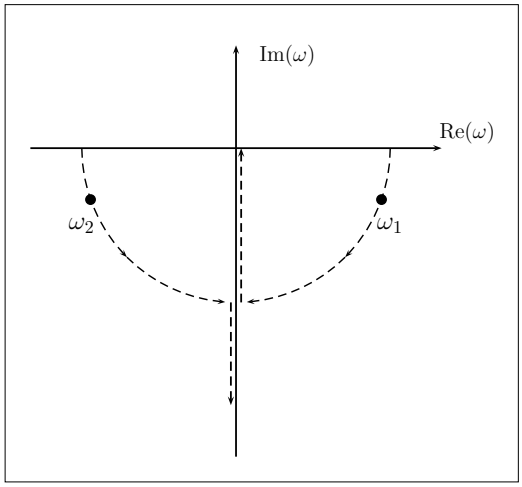

Fig. 8.1: Behaviour of the characteristic roots for fixed frequency ω_0 for parameter Γ varying from zero to infinity.

1f:osc

We start our discussion taking the lowest value of damping parameter, that is $\Gamma = 0$. Then $\Omega = \omega_0$ and characteristic roots are simply $\omega_{1,2} = \pm\omega_0$, so they lie on the real axis in the plane of complex ω, see figure 8.1. The solution to homogeneous equation follows easily from (os12), and it is $x(t) = x_0 \cos(\omega_0 t) + (v_0/\omega_0)\sin(\omega_0 t)$, which are standard undamped oscillations satisfying arbitrary initial conditions.

When Γ grows from zero, but satisfies $\frac{1}{2}\Gamma < \omega_0$, the roots have the form (aos15) and Ω is real. Both roots have nonzero (negative) imaginary part and as Γ grows they move in the complex plane downwards along the arcs of the radius ω_0, as it follows from the relation (aos16). The oscillator performs typical damped oscillations and the

general solution of the homogeneous equation is as given in Eq. (1.11).

The situation changes at the point where $\frac{1}{2}\Gamma = \omega_0$. Then $\Omega = 0$ and both roots coincide, possessing the values $\omega_{1,2} = \omega_0 = -\frac{i}{2}\Gamma$. So we do not have two linearly independent solutions as it was in the case of Eq. (1.8). For the case of $\Omega = 0$ we can, however, take the limit in Eq. (1.11). Taking the limit carefully we obtain the following result

$$x(t) \xrightarrow[\Omega \to 0]{} \exp\left(-\frac{1}{2}\Gamma t\right)\left[x_0 + \left(v_0 + \frac{1}{2}\Gamma x_0\right) t\right]. \tag{8.3}$$ aos19d

This solution corresponds to exponential decay without oscillations.

When parameter Γ still grows, i.e., $\frac{1}{2}\Gamma > \omega_0$, then Ω becomes purely imaginary. We can then write

$$\Omega = i\sqrt{\frac{1}{4}\Gamma^2 - \omega_0^2} = i\widetilde{\Omega}, \tag{8.4}$$ aos20a

where $\widetilde{\Omega}$ is again real. The general solution (1.11) changes its character because substitution (8.4) must be made. Hence, from Eqs. (1.10) and (8.4) we obtain

$$x(t) \xrightarrow[\frac{1}{2}\Gamma > \omega_0]{} \exp\left(-\frac{1}{2}\Gamma t\right)\left[x_0 \cos\left(i\widetilde{\Omega}t\right) + \frac{v_0 + \frac{1}{2}\Gamma x_0}{i\widetilde{\Omega}} \sin\left(i\widetilde{\Omega}t\right)\right]. \tag{8.5}$$ aos20d

Then, trigonometric function are transformed into hyperbolic ones, and we obtain

$$x(t) \xrightarrow[\frac{1}{2}\Gamma > \omega_0]{} \exp\left(-\frac{1}{2}\Gamma t\right)\left[x_0 \operatorname{ch}\left(\widetilde{\Omega}t\right) + \frac{v_0 + \frac{1}{2}\Gamma x_0}{\widetilde{\Omega}} \operatorname{sh}\left(\widetilde{\Omega}t\right)\right]. \tag{8.6}$$ aos20e

This solution quickly decays in time because $\widetilde{\Omega} < \frac{1}{2}\Gamma$ and may be called an overdamped one, since it corresponds to strong damping.

aos20b In this case two characteristic roots are purely imaginary and have the property

$$\omega_1 = -\frac{i\Gamma}{2} + i\,\widetilde{\Omega} \xrightarrow[\Gamma \to \infty]{} 0, \tag{8.7a}$$ aos20ba

$$\omega_2 = -\frac{i\Gamma}{2} - i\,\widetilde{\Omega} \xrightarrow[\Gamma \to \infty]{} -i\infty, \tag{8.7b}$$ aos20bb

Therefore, as presented in Fig. 8.1, we see that when Γ grows ω_1 moves upward the imaginary axis towards zero, while $\omega_2 \to -i\infty$ downwards along the imaginary axis.

1f:osc Fig.8.1 illustrates the behaviour of the roots $\omega_{1,2}$ as functions of the varying parameter Γ. It is important to note that only for $\Gamma = 0$ the roots are real, for $\Gamma > 0$ the roots are always in the lower half of the complex ω–plane.

8.2 Green's function

8.3 Solution to inhomogeneous equation – Green's function

Our next aim is to find the Green's function leading to an elegant method of finding a particular solution to the inhomogeneous equation of motion for driven harmonic oscillator. We will apply the method to a particular case, but it seems clear that it can be

generalized to other differential equations. So, now we consider the equation (1.1) which we write as follows

$$\ddot{x} + \Gamma\dot{x} + \omega_0^2 x = f(t), \qquad \text{with} \qquad f(t) = (q/m)E(t). \tag{8.8}$$ ano01

We seek a particular solution to the inhomogeneous equation (8.8) in the form

$$x(t) = \int_{-\infty}^{\infty} dt'\; g(t-t')\, f(t'), \tag{8.9}$$ ano02

where $g(\tau)$ is an unknown function. We will first discuss the conditions imposed on function $g(\tau)$ which follow for the physics of the problem. Then, we will explicitly construct this function and check that it satisfies all the requirements.

8.3.1 Requirement of causality

We seek the particular solution to the inhomogeneous equation in the postulated form of (8.9). We require that this solution is causal. This means that the force $f(t')$ can affect the displacement $x(t)$ only at the instants earlier than the current moment. In other words, this means that the displacement $x(t)$ can depend on the force $f(t')$ only when $t' \leq t$. We may also say that the *current* state of the oscillator can be influenced by the *earlier* magnitude of the force, and not by the *later* ones. Therefore, requirement of causality can be written as ano03

$$g(t-t') \neq 0 \quad \text{for } t' < t, \tag{8.10a}$$ ano03a

$$g(t-t') = 0 \quad \text{for } t' \geq t. \tag{8.10b}$$ ano03b

Relation (8.10a) should be understood in the sense that the function $g(t-t')$ is not identically zero for times t' earlier than t. Let us note, that since $g(t-t') = 0$ for $t' > t$ the upper limit of the integral in (8.9) is effectively equal to t and not $+\infty$. Hence, instead of (8.9), we can write

$$x(t) = \int_{-\infty}^{t} dt'\; g(t-t')\, f(t'), \tag{8.11}$$ ano04

which, in an evident manner, displays the causality requirement. Only moments t' earlier than t give nonzero contributions to the current value of the displacement, so that $x(t)$ is determined solely by the earlier magnitudes of the driving force.

The condition (8.10) can be put into somewhat more formal way. We write

$$g(t-t') = \Theta(t-t')\, g(t-t'), \tag{8.12}$$ ano05

which is an equality in the sense of generalized functions. $\Theta(t-t')$ denotes the Heaviside function, which is defined as

$$\Theta(t-t') = \begin{cases} 1 & \text{for } t' < t, \\ 0 & \text{for } t' \geq t. \end{cases} \tag{8.13}$$ ano06

At this stage it is perhaps worthwhile to give some comments. Searching for the Green's function in the form of the product $\Theta(t-t')\,g(t-t')$ requires a careful approach within the theory of generalized functions, which is not easy. It seems that it is more convenient to seek the Green's function $g(t-t')$ via the particular solution (8.9) of the inhomogeneous equation with additional conditions summarized by relations (8.10). On the other hand, relation (8.12) may be useful in practical applications, because it automatically restricts the integration domain to times earlier than the current moment. Hence, the causality requirement is then explicitly seen. This is put clearly via the equation

$$x(t) = \int_{-\infty}^{\infty} dt'\ \Theta(t-t')g(t-t')\ f(t'), = \int_{-\infty}^{t} dt'\ g(t-t')\ f(t'), \tag{8.14}$$ ano06x

Although this relation seems "tempting", we will seek the Green's function via relations (8.9) and (8.10).

8.3.2 Green's function

As we have discussed, one of the ways to construct the particular solution to inhomogeneous equation is to look for the function $g(t-t')$. In order to do so, we substitute (8.9) into equation (8.8).Thus, we find an equation which must be satisfied by $g(t-t')$ – the Green's function

$$\int_{-\infty}^{\infty} dt' \left[\frac{d^2g(t-t')}{dt^2} + \Gamma\frac{dg(t-t')}{dt} + \omega_0^2 g(t-t') \right]\ f(t') = f(t). \tag{8.15}$$ ano09

Since the right-hand side can be written as

$$f(t) = \int_{-\infty}^{\infty} dt'\ \delta(t-t')\ f(t'), \tag{8.16}$$ ano09x

it is straightforward to see that Eq. (8.15) is equivalent to the equation

$$\frac{d^2g(\tau)}{d\tau^2} + \Gamma\frac{dg(\tau)}{d\tau} + \omega_0^2 g(\tau) = \delta(\tau), \tag{8.17}$$ ano10

where we have put $t-t'=\tau$. Eq (8.16) is a differential equation for generalized functions of the form typical for the equations determining the Green's function.

Solution to (8.17) is best sought in the Fourier domain. The fundamentals of Fourier transform theory are briefly presented in *Appendix A*. Following this theory, we introduce a pair of Fourier transforms

$$G(\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\ g(t), \qquad g(t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\ G(\omega), \tag{8.18}$$ ano12

and we recall the relation well-known from generalized functions (distribution) theory

$$\delta(t) = \frac{1}{2\pi}\ \int_{-\infty}^{\infty} d\omega\ e^{-i\omega t}. \tag{8.19}$$ ano13

Transforming equation (8.17) into the Fourier domain we obtain

$$\int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}} \left[(-i\omega)^2 - i\omega\Gamma + \omega_0^2\right]\ e^{-i\omega t}\, G(\omega)\ =\ \frac{1}{2\pi}\ \int_{-\infty}^{\infty} d\omega\ e^{-i\omega t}, \tag{8.20}$$ ano14

where we used (8.19) in the right-hand side. Hence, the last relation entails the equality of the Fourier transforms and we get the algebraic equation for the Fourier transform $G(\omega)$ of the Green's function $g(\tau)$. The result is

$$\left(-\omega^2 - i\omega\Gamma + \omega_0^2 \right) G(\omega) = \frac{1}{\sqrt{2\pi}}, \tag{8.21}$$

or, equivalently

$$G(\omega) = \frac{1}{\sqrt{2\pi}} \, \frac{(-1)}{\omega^2 + i\omega\Gamma - \omega_0^2} = \frac{1}{\sqrt{2\pi}} \, \frac{(-1)}{(\omega - \omega_1)(\omega - \omega_2)}, \tag{8.22}$$

where $\omega_{1,2} = -\frac{i}{2}\Gamma \pm \Omega$ are the previously discussed roots (8.1). This is so, because the denominator in the first equality is exactly the same as the discussed characteristic equation (1.5) of the homogeneous equation. Hence, we have easily found the Fourier transform of the Green's function for the driven and damped harmonic oscillator. Moreover, due to previous discussion of the roots of characteristic equation we automatically have discussed the poles of the complex valued Fourier transform of the Green's function.

In order to find the Green's function $g(\tau)$ we must invert the Fourier transform. This is equivalent to compute the integral

$$g(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}} \, e^{-i\omega\tau} \, G(\omega) = \frac{-1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \frac{\exp(-i\omega\tau)}{(\omega - \omega_1)\,(\omega - \omega_2)}. \tag{8.23}$$

Computation of this integral is simple when one uses the residue theory. For time $\tau < 0$ we close the contour in the upper half–plane of complex ω as indicated in Fig.8.2 by the dashed line. The radius of the semicircle goes to infinity and from the Jordan lemma the integral over the upper semicircle vanishes (because $\tau < 0$ and $-i\omega\tau$ possesses negative real part).The integral reduces to the one over the real axis and since there are no poles within the contour (which has the positive direction) the integral vanishes, yielding $g(\tau) = 0$ for $\tau < 0$.

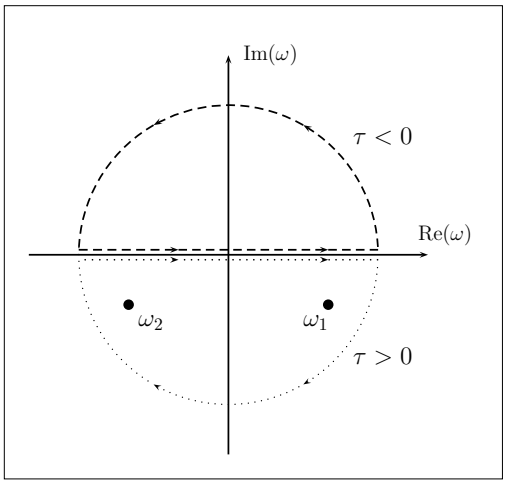

Fig. 8.2: Integration contours for evaluation of Green's function from Eq.(8.23).

Similarly, for positive argument, (i.e. for $\tau > 0$) we close the contour in the lower half–plane as indicated by dotted line. This contour has negative direction. The integral over the semicircle vanishes again due to Jordan lemma for $\tau > 0$ when the radius goes to infinity. Since the poles are within the contour we obtain non-vanishing result which is easily computed via the residues in the first order poles ω_1 and ω_2 given in (8.1). The obtained Green's function follows by evaluation of the residues

$$g(\tau) = -2\pi i \left(\frac{-1}{2\pi}\right) \left[\frac{\exp\left[-i\tau\left(-\frac{i}{2}\Gamma + \Omega\right)\right]}{-\frac{i}{2}\Gamma + \Omega + \frac{i}{2}\Gamma + \Omega} + \frac{\exp\left[-i\tau\left(-\frac{i}{2}\Gamma - \Omega\right)\right]}{-\frac{i}{2}\Gamma - \Omega + \frac{i}{2}\Gamma - \Omega} \right]. \tag{8.24}$$

Simple manipulation of this result allows us to write the resulting Green's function for $\tau > 0$ as

$$g(\tau) \;=\; \frac{-i}{2\Omega}\, e^{-\frac{1}{2}\Gamma\tau}\left(e^{i\Omega\tau} - e^{-i\Omega\tau}\right) \;=\; \frac{1}{\Omega}\, e^{-\frac{1}{2}\Gamma\tau}\sin\left(\Omega\tau\right) \tag{8.25}$$

ano20b

Summarizing, the Green's function for the damped harmonic oscillator is given as follows

ano21

$$g(\tau) \;=\; 0, \qquad \text{for} \;\; \tau < 0 \tag{8.26a}$$

ano21a

$$\;=\; \frac{1}{\Omega}\exp\left(-\frac{\Gamma\tau}{2}\right)\sin(\Omega\tau), \qquad \text{for} \;\; \tau > 0, \tag{8.26b}$$

ano21b

which completes the computation of the Green's function for the damped, driven harmonic oscillator.

* *

Chapter 9

ac:ae

Electrodynamics in Fourier space

In some applications it is convenient to express Maxwell's equations (ce1 2.1) in Fourier space. The basic review of the properties of Fourier transforms is given in the appendix ap:ff A. For vector fields such as $\vec{\mathbf{E}}$ or $\vec{\mathbf{B}}$ the Fourier transform can be defined for each Cartesian component separately, so that again a vector field results. For example, we define Fourier ae1 transform of the electric field and its inverse as

$$\vec{\mathcal{E}}(\vec{\mathbf{k}},t) = \frac{1}{(2\pi)^{3/2}}\int d^3r\; e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\;\vec{\mathbf{E}}(\vec{\mathbf{r}},t), \tag{9.1a}$$ ae1a

$$\vec{\mathbf{E}}(\vec{\mathbf{r}},t) = \frac{1}{(2\pi)^{3/2}}\int d^3k\; e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\;\vec{\mathcal{E}}(\vec{\mathbf{k}},t). \tag{9.1b}$$ ae1b

Note that time dependence is explicitly accounted for. Completely analogously we intro- ae2 duce the corresponding relations for other fields

$$\vec{\mathbf{B}}(\vec{\mathbf{r}},t) \longleftrightarrow \vec{\mathcal{B}}(\vec{\mathbf{k}},t), \tag{9.2a}$$ ae2a

$$\vec{\mathbf{D}}(\vec{\mathbf{r}},t) \longleftrightarrow \vec{\mathcal{D}}(\vec{\mathbf{k}},t), \tag{9.2b}$$ ae2b

$$\vec{\mathbf{H}}(\vec{\mathbf{r}},t) \longleftrightarrow \vec{\mathcal{H}}(\vec{\mathbf{k}},t). \tag{9.2c}$$ ae2c

ae3 Moreover, similarly as in (ae1 9.1) we have Fourier pairs

$$\rho(\vec{\mathbf{r}},t) \longleftrightarrow \widetilde{\rho}(\vec{\mathbf{k}},t), \tag{9.3a}$$ ae3a

$$\vec{\mathbf{j}}(\vec{\mathbf{r}},t) \longleftrightarrow \vec{\mathcal{J}}(\vec{\mathbf{k}},t), \tag{9.3b}$$ ae3b

Electrodynamics in the Fourier space consists in expressing the laws of classical theory in the language of the defined Fourier transforms. Therefore, the sections in the present chapter would have the same titles as the sections in the chapter in the *Main Part*.

9.1 Maxwell's equation

Using the connections between differentiation in normal space and vector multiplications by vector $\vec{\mathbf{k}}$ in the Fourier space (see Appendix ap:ff A) we rewrite Maxwell's equations (ce1 2.1) in the Fourier domain as follows (we suppress the arguments, which should not cause any

ae5 problems)

$$i\vec{\mathbf{k}}\cdot\vec{\mathcal{D}} = \widetilde{\rho}, \tag{9.4a}$$ ae5a

$$i\vec{\mathbf{k}}\cdot\vec{\mathcal{B}} = 0, \tag{9.4b}$$ ae5b

$$i\vec{\mathbf{k}}\times\vec{\mathcal{E}} = -\frac{\partial}{\partial t}\vec{\mathcal{B}}, \tag{9.4c}$$ ae5c

$$i\vec{\mathbf{k}}\times\vec{\mathcal{H}} = \vec{\mathcal{J}} + \frac{\partial}{\partial t}\vec{\mathcal{D}}, \tag{9.4d}$$ ae5d

It should be, however, noted that in case of dispersive media (that is, media for which the dielectric and magnetic susceptibilities depend on frequency, which is proportional to the absolute value of wave vector $\vec{\mathbf{k}}$) and/or are position dependent, the material relations lead to serious complications. The same applies to nonlinear media (when susceptibilities depend on fields, usually in a nonlinear manner). The problem of the electromagnetic fields in the media is still not fully understood. Therefore, we will mainly focus our attention on the case of the fields in vacuum. In such a case the corresponding Maxwell's equations (ce17 2.15) in coordinate space and in the Fourier space are simpler, and are of the

ae6 form

$$i\vec{\mathbf{k}}\cdot\vec{\mathcal{E}} = \frac{1}{\epsilon_o}\widetilde{\rho}, \tag{9.5a}$$ ae6a

$$i\vec{\mathbf{k}}\cdot\vec{\mathcal{B}} = 0, \tag{9.5b}$$ ae6b

$$i\vec{\mathbf{k}}\times\vec{\mathcal{E}} = -\frac{\partial}{\partial t}\vec{\mathcal{B}}, \tag{9.5c}$$ ae6c

$$i\vec{\mathbf{k}}\times\vec{\mathcal{B}} = \frac{1}{\epsilon_0\, c^2}\vec{\mathcal{J}} + \frac{1}{c^2}\frac{\partial}{\partial t}\vec{\mathcal{E}}, \tag{9.5d}$$ ae6d

It is perhaps worth stressing that the time derivatives of the Fourier transforms of the fields depend on the values of the transforms taken at the same point $\vec{\mathbf{k}}$ of the Fourier space. Hence, Maxwell's equation in the Fourier domain are local.

Let us also note that Eqs.(ae5b 9.4b) and (ae6b 9.5b) clearly show that the Fourier field $\mathcal{B}(\vec{\mathbf{k}},t)$ are perpendicular to the wave vector $\vec{\mathbf{k}}$. This notion leading to the concepts of transverse (orthogonal to $\vec{\mathbf{k}}$) and longitudinal (parallel to $\vec{\mathbf{k}}$) fields will be discussed later. It also explains why we say that magnetic field is purely transverse.

Finally, we express the charge conservation equation (ce6 2.7) in the Fourier domain. According to the rules of Fourier transformation it now reads

$$i\vec{\mathbf{k}}\cdot\vec{\mathcal{J}} + \frac{\partial}{\partial t}\widetilde{\rho} = 0. \tag{9.6}$$ ae7

9.2 Potentials

9.2.1 Introduction and basic definitions

Discussing potentials in Fourier space we follow similar lines of reasoning as it was done in the main part of these lectures. For vector potential we write the pair of Fourier

ae10 transforms

$$\vec{\mathcal{A}}(\vec{\mathbf{k}},t) = \frac{1}{(2\pi)^{3/2}}\int d^3r\; e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\;\vec{\mathbf{A}}(\vec{\mathbf{r}},t), \tag{9.7a}$$ ae10a

$$\vec{\mathbf{A}}(\vec{\mathbf{r}},t) = \frac{1}{(2\pi)^{3/2}}\int d^3k\; e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\;\vec{\mathcal{A}}(\vec{\mathbf{r}},t). \tag{9.7b}$$ ae10b

where we have included the time dependencies. Obviously we similarly have for scalar potential

$$\phi(\vec{\mathbf{r}},t) \longleftrightarrow \widetilde{\phi}(\vec{\mathbf{k}},t), \tag{9.8}$$ ae11

As in the case of Maxwell's equations we use the connections between spatial derivatives and wave vectors as discussed in Appendix A. Then, the Fourier transforms of the electric and magnetic fields $\vec{\mathcal{E}}(\vec{\mathbf{k}},t)$ and $\vec{\mathcal{B}}(\vec{\mathbf{k}},t)$ are given by the transforms of potentials in the ae12 following manner

$$\vec{\mathcal{E}}(\vec{\mathbf{k}},t) = -\frac{\partial}{\partial t}\,\vec{\mathcal{A}}(\vec{\mathbf{k}},t) - i\vec{\mathbf{k}}\,\widetilde{\phi}(\vec{\mathbf{k}},t) \tag{9.9a}$$ ae12a

$$\vec{\mathcal{B}}(\vec{\mathbf{k}},t) = i\vec{\mathbf{k}}\times\vec{\mathcal{A}}(\vec{\mathbf{k}},t). \tag{9.9b}$$ ae12b

Note that the electric field in the Fourier domain contains a longitudinal component (parallel to wave vector $\vec{\mathbf{k}}$) and proportional to scalar potential $\widetilde{\phi}(\vec{\mathbf{k}},t)$.

9.2.2 Wave equations for potentials

General wave equations in normal space are given by Eqs.(2.21) and (2.24). In Fourier ae13 domain they become

$$k^2\,\widetilde{\phi}(\vec{\mathbf{k}},t) = \frac{1}{\epsilon_0}\,\widetilde{\rho}(\vec{\mathbf{k}},t) + i\vec{\mathbf{k}}\cdot\frac{\partial}{\partial t}\,\vec{\mathcal{A}}(\vec{\mathbf{k}},t), \tag{9.10a}$$ ae13a

$$\left[k^2 + \frac{1}{c^2}\,\frac{\partial^2}{\partial t^2}\right]\vec{\mathcal{A}}(\vec{\mathbf{k}},t) = \frac{1}{c^2\epsilon_0}\,\vec{\mathcal{J}}(\vec{\mathbf{k}},t) - i\vec{\mathbf{k}}\left[i\vec{\mathbf{k}}\cdot\vec{\mathcal{A}}(\vec{\mathbf{k}},t) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\widetilde{\phi}(\vec{\mathbf{k}},t)\right], \tag{9.10b}$$ ae13b

9.2.3 Potentials – gauge invariance

Gauge transformation are specified by equations (2.28). The corresponding relations in ae14 the Fourier domain are as follows is of the form

$$\vec{\mathcal{A}}(\vec{\mathbf{k}},t) \xrightarrow[gauge]{} \vec{\mathcal{A}}'(\vec{\mathbf{k}},t) = \vec{\mathcal{A}}(\vec{\mathbf{k}},t) + i\vec{\mathbf{k}}\,\widetilde{F}(\vec{\mathbf{k}},t), \tag{9.11a}$$ ae14a

$$\widetilde{\phi}(\vec{\mathbf{k}},t) \xrightarrow[gauge]{} \widetilde{\phi}'(\vec{\mathbf{k}},t) = \widetilde{\phi}(\vec{\mathbf{k}},t) - \frac{\partial}{\partial t}\,\widetilde{F}(\vec{\mathbf{k}},t), \tag{9.11b}$$ ae14b

where $\widetilde{F}(\vec{\mathbf{k}},t)$ is the Fourier transform of the gauge function $F(\vec{\mathbf{r}},t)$.

9.2.4 Lorentz gauge

Lorentz gauge (2.30) in the Fourier domain reads

$$i\vec{\mathbf{k}}\cdot\vec{\mathcal{A}}(\vec{\mathbf{k}},t) + \frac{1}{c^2}\frac{\partial}{\partial t}\,\widetilde{\phi}(\vec{\mathbf{k}},t) = 0, \tag{9.12}$$ ae15

ae16 and the corresponding wave equations (9.11) become

$$\left[\vec{\mathbf{k}}^2 + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\widetilde{\phi}(\vec{\mathbf{k}},t) = \frac{1}{\epsilon_0}\,\widetilde{\rho}(\vec{\mathbf{k}},t) \tag{9.13a}$$ ae16a

$$\left[\vec{\mathbf{k}}^2 + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\vec{\mathcal{A}}(\vec{\mathbf{k}},t) = \frac{1}{\epsilon_0\,c^2}\,\vec{\mathcal{J}}(\vec{\mathbf{k}},t). \tag{9.13b}$$ ae16b

9.2.5 Coulomb gauge

Next we discuss Coulomb gauge (2.35), which in the Fourier domain attains the form

$$\vec{\mathbf{k}}\cdot\vec{\mathcal{A}}(\vec{\mathbf{k}},t) = 0. \tag{9.14}$$ ae17

We see that in this gauge the Fourier transform of the vector potential is perpendicular (or transverse) to the wave vector $\vec{\mathbf{k}}$. This explains why the Coulomb gauge is sometimes ae17a called the transverse one. Wave equations (9.10)) in the Coulomb gauge become

$$\vec{\mathbf{k}}^2\,\widetilde{\phi}(\vec{\mathbf{k}},t) = \frac{1}{\epsilon_0}\,\widetilde{\rho}(\vec{\mathbf{k}},t), \tag{9.15a}$$ ae17aa

$$\left[\vec{\mathbf{k}}^2 + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\vec{\mathcal{A}}(\vec{\mathbf{k}},t) = \frac{1}{\epsilon_0\,c^2}\,\vec{\mathcal{J}}(\vec{\mathbf{k}},t) - \frac{i\vec{\mathbf{k}}}{c^2}\,\frac{\partial}{\partial t}\,\widetilde{\phi}(\vec{\mathbf{k}},t), \tag{9.15b}$$ ae17ab

and deserve some further attention. During our discussion of wave equations in Coulomb gauge we noted that causality is lost. The solution for scalar potential was shown to give instantaneous electric field due to charge distribution $\rho(\vec{\mathbf{r}},t)$, (see (2.37)). Let us repeat similar analysis in Fourier domain. Wave equation (9.15a) may be written

$$\widetilde{\phi}(\vec{\mathbf{k}},t) = \frac{1}{\epsilon_0}\,\widetilde{\rho}(\vec{\mathbf{k}},t)\,(2\pi)^{3/2}\,\frac{1}{(2\pi)^{3/2}\,k^2}. \tag{9.16}$$ ae18

In Appendix A we show that $[(2\pi)^{3/2}k^2]^{-1}$ is a Fourier transform of $1/4\pi r$. So $\widetilde{\phi}$ given in Eq.(9.16) is a product of two Fourier transforms. It follows that the inverse transform, being the potential $\phi(\vec{\mathbf{r}},t)$ is a convolution of two functions

$$\frac{1}{\epsilon_0}\,\rho(\vec{\mathbf{r}},t) \qquad \text{and} \qquad (2\pi)^{3/2}\,\frac{1}{4\pi|\,\vec{\mathbf{r}}\,|} \tag{9.17}$$ ae19

where the second one follows from (A.96). Therefore we have the potential $\phi(\vec{\mathbf{r}},t)$ – the inverse of $\widetilde{\phi}$ given as the convolution, that is

$$\phi(\vec{\mathbf{r}},t) = \frac{1}{4\pi\epsilon_o}\int d\vec{\mathbf{r}}'\,\frac{\rho(\vec{\mathbf{r}}',t)}{|\,\vec{\mathbf{r}}-\vec{\mathbf{r}}'\,|}, \tag{9.18}$$ ae20

so we reproduce the well-known Coulomb potential, the Fourier transform of which satisfies equation (9.16). This solution exactly reproduces (2.37) obtained as in usual electrostatics.

9.3 Longitudinal and transverse fields

9.3.1 Introduction

Let us translate the concepts of transverse and longitudinal components of vector fields. Fourier transforms are linear so the decomposition $\vec{\mathbf{E}}(\vec{\mathbf{r}}) = \vec{\mathbf{E}}_{\parallel}(\vec{\mathbf{r}}) + \vec{\mathbf{E}}_{\perp}(\vec{\mathbf{r}})$ transforms into

$$\vec{\mathcal{E}}(\vec{\mathbf{k}}) = \vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) + \vec{\mathcal{E}}_{\perp}(\vec{\mathbf{k}}), \tag{9.19}$$ ae25

while the requirements $\operatorname{div} \vec{\mathbf{E}}_{\perp}(\vec{\mathbf{r}}) = 0$ and $\operatorname{rot} \vec{\mathbf{E}}_{\perp}(\vec{\mathbf{r}}) = 0$ become

$$i\,\vec{\mathbf{k}} \cdot \vec{\mathcal{E}}_{\perp}(\vec{\mathbf{k}}) = 0, \qquad i\,\vec{\mathbf{k}} \times \vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) = 0. \tag{9.20}$$ ae26

These relations clearly imply that $\vec{\mathcal{E}}_{\perp}(\vec{\mathbf{k}})$ is a component orthogonal (transverse) to wave vector $\vec{\mathbf{k}}$, while $\vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}})$ is aligned along $\vec{\mathbf{k}}$ – longitudinal. We also see that in the Fourier space the separation (9.19) is local and obviously unique. This clear picture shows why the Fourier domain is sometimes advantageous. Introducing a unit vector

$$\vec{\mathbf{n}}_k = \frac{\vec{\mathbf{k}}}{|\,\vec{\mathbf{k}}\,|} \tag{9.21}$$ ae27

ae28 we may also write

$$\vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) \;=\; \vec{\mathbf{n}}_k \left[\, \vec{\mathbf{n}}_k \cdot \vec{\mathcal{E}}(\vec{\mathbf{k}}) \,\right], \tag{9.22a}$$ ae28a

$$\vec{\mathcal{E}}_{\perp}(\vec{\mathbf{k}}) \;=\; \vec{\mathcal{E}}(\vec{\mathbf{k}}) - \vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) \;=\; \vec{\mathcal{E}}(\vec{\mathbf{k}}) - \vec{\mathbf{n}}_k \left[\, \vec{\mathbf{n}}_k \cdot \vec{\mathcal{E}}(\vec{\mathbf{k}}) \,\right], \tag{9.22b}$$ ae28b

It is straightforward to check that vectors (9.22) satisfy requirements (9.20).

Introducing the discussed separation in normal space we mentioned that it is not an easy problem. There, the requirements $\operatorname{div} \vec{\mathbf{E}}_{\perp}(\vec{\mathbf{r}}) = 0$ and $\operatorname{rot} \vec{\mathbf{E}}_{\perp}(\vec{\mathbf{r}}) = 0$ must be satisfied for all positions $\vec{\mathbf{r}}$. Similarly, relations (9.20) must hold for any wave vector $\vec{\mathbf{k}}$. This may be a tricky problem. To clarify it, let us consider an example, a point charge Q located at a position $\vec{\mathbf{r}}_0$. In this case the charge density is $\rho(\vec{\mathbf{r}}) = Q\,\delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}_0)$. Then, Gauss' law states that

$$\epsilon_o \operatorname{div} \vec{\mathbf{E}} = Q\,\delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}_0). \tag{9.23}$$ ae31

Right hand side is zero almost everywhere (except at the point at which the charge is located). taking Fourier transforms

$$\frac{\epsilon_o}{(2\pi)^{3/2}} \int d^3r\; e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}} \operatorname{div} \vec{\mathbf{E}} = \frac{Q}{(2\pi)^{3/2}} \int d^3r\; e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\, \delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}_0). \tag{9.24}$$ ae32

Thus, we get

$$i\epsilon_0\, \vec{\mathbf{k}} \cdot \vec{\mathcal{E}}(\vec{\mathbf{k}}) \;=\; \frac{Q}{(2\pi)^{3/2}}\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}_0}. \tag{9.25}$$ ae33

Here we see that $\vec{\mathbf{k}} \cdot \vec{\mathbf{cal}}\mathbf{E} \neq 0$ except for a trivial case $\vec{\mathbf{k}} = 0$. The field $\vec{\mathcal{E}}(\vec{\mathbf{k}})$ and wave vectors $\vec{\mathbf{k}}$ are not orthogonal almost everywhere. Although $\operatorname{div} \vec{\mathbf{E}} = 0$ almost everywhere, the field is not transverse. This explains, that in presence of charges the problem of separating the electric field into longitudinal and transverse components can be really difficult. Secondly, the separation into longitudinal and transverse parts is not relativistically invariant. A vector which is transverse in one reference (coordinate) frame, usually is not transverse in another frame – obtained via Lorentz transformation.

9.3.2 Longitudinal Maxwell's equations

We shall again restrict our attention to the vacuum fields. Maxwell's equations (2.1) in coordinate space, or (9.4) in Fourier space, can now be expressed as separate equations for the longitudinal and transverse parts of the fields and the current density. Firstly, we discuss the longitudinal components. Maxwell's equation (9.4b) clearly indicates that the transform of magnetic field is purely transverse. This automatically implies that

$$\vec{\mathcal{B}}_{\parallel}(\vec{\mathbf{k}}) = 0, \tag{9.26}$$ ae35

and the longitudinal component of $\vec{\mathbf{B}}$ must always be zero. The other longitudinal Maxwell's equation (2.42) translates into

$$i\vec{\mathbf{k}} \cdot \vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) = \frac{\widetilde{\rho}(\vec{\mathbf{k}})}{\epsilon_o}, \tag{9.27}$$ ae36

in the Fourier domain. It is interesting to look for the solution to the above equation. Using relation (9.22a) we can write

$$\vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) \;=\; \frac{\vec{\mathbf{k}}}{|\,\vec{\mathbf{k}}\,|^2}\,\left[\vec{\mathbf{k}}\cdot\left(\,\vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) + \vec{\mathcal{E}}_{\perp}(\vec{\mathbf{k}})\,\right)\right] \;=\; \frac{\vec{\mathbf{k}}}{|\,\vec{\mathbf{k}}\,|^2}\,\left(\vec{\mathbf{k}}\cdot\vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}})\right), \tag{9.28}$$ ae37

because $\vec{\mathbf{k}}\cdot\vec{\mathcal{E}}_{\perp} = 0$. The scalar product in right hand side is replaced by Maxwell's equation (9.27) yielding

$$\vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) \;=\; -\,\frac{i\,\vec{\mathbf{k}}}{\epsilon_0\,|\,\vec{\mathbf{k}}\,|^2}\,\widetilde{\rho}(\vec{\mathbf{k}}). \tag{9.29}$$ ae38

Once again we have a product of Fourier transforms (see the Appendix A)

$$\vec{\mathcal{E}}_{\parallel}(\vec{\mathbf{k}}) \;=\; -\,\frac{i\,\vec{\mathbf{k}}}{\epsilon_0\,|\,\vec{\mathbf{k}}\,|^2}\,\widetilde{\rho}(\vec{\mathbf{k}}). \tag{9.30}$$ ae39

So the inverse transform to $\vec{\mathcal{E}}(\vec{\mathbf{k}})$ is a convolution

$$\vec{\mathbf{E}}_{\parallel}(\vec{\mathbf{r}}) \;=\; \frac{1}{4\pi\epsilon_o}\int d\vec{\mathbf{r}}'\;\rho(\vec{\mathbf{r}}\,',t)\;\frac{\vec{\mathbf{r}}-\vec{\mathbf{r}}\,'}{|\vec{\mathbf{r}}-\vec{\mathbf{r}}\,'|^3}. \tag{9.31}$$ ae40

So we indeed see that Maxwell's equation (9.27) leads to the correct solution (2.45b).

Longitudinal Maxwell's equation in the Fourier domain summarize to Eqs.(9.26) and (9.29) (the latter one is equivalent to (9.31)).

9.3.3 Transverse Maxwell's equations

Faraday's law reduces to the transverse equation (2.46) and in Fourier domain it reads

$$i\vec{\mathbf{k}} \times \vec{\mathcal{E}}_{\perp}(\vec{\mathbf{k}}) = -\frac{\partial}{\partial t}\vec{\mathcal{B}}_{\perp}(\vec{\mathbf{k}}). \tag{9.32}$$ ae44

The same follows from Maxwell's equation (9.4c), because longitudinal part of electric field does not contribute to its left hand side, while magnetic field is purely transverse.

Let us now turn to the discussion of the modified Ampere's law

$$\mathrm{rot}\,\vec{\mathbf{B}}(\vec{\mathbf{r}}) = \frac{1}{\epsilon_0\, c^2}\,\vec{\mathbf{j}}(\vec{\mathbf{r}}) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\vec{\mathbf{E}}(\vec{\mathbf{r}}), \tag{9.33}$$ ae45

Which, in the Fourier domain reads directly as

$$i\vec{\mathbf{k}}\times\vec{\mathcal{B}}(\vec{\mathbf{k}}) = \frac{1}{\epsilon_0\, c^2}\,\vec{\mathcal{J}}(\vec{\mathbf{k}}) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\vec{\mathcal{E}}(\vec{\mathbf{k}}). \tag{9.34}$$ ae46

Longitudinal magnetic field $\vec{\mathcal{B}}(\vec{\mathbf{k}}) = 0$ so we can rewrite the above equation as

$$i\vec{\mathbf{k}}\times\vec{\mathcal{B}}_\perp(\vec{\mathbf{k}}) = \frac{1}{\epsilon_0\, c^2}\,\left(\,\vec{\mathcal{J}}_\perp(\vec{\mathbf{k}}) + \vec{\mathcal{J}}_\parallel(\vec{\mathbf{k}})\,\right) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\left(\,\vec{\mathcal{E}}_\perp(\vec{\mathbf{k}}) + \vec{\mathcal{E}}_\parallel(\vec{\mathbf{k}})\,\right). \tag{9.35}$$ ae47

Vector product $\vec{\mathbf{k}}\times\vec{\mathcal{B}}_\perp(\vec{\mathbf{k}})$ is obviously transverse (perpendicular to $\vec{\mathbf{k}}$). So, the last equation splits into two parts. The first one, the transverse one is

$$i\vec{\mathbf{k}}\times\vec{\mathcal{B}}_\perp(\vec{\mathbf{k}}) \;=\; \frac{1}{\epsilon_0\, c^2}\,\vec{\mathcal{J}}_\perp(\vec{\mathbf{k}}) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\vec{\mathcal{E}}_\perp(\vec{\mathbf{k}}), \tag{9.36}$$ ae48a

and the longitudinal part

$$0 \;= \frac{1}{\epsilon_0\, c^2}\,\vec{\mathcal{J}}_\parallel(\vec{\mathbf{k}}) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\vec{\mathcal{E}}_\parallel(\vec{\mathbf{k}}). \tag{9.37}$$ ae48b

As we may suspect (9.37) does not bring any new information, since it reduces to charge conservation requirement and therefore, usually can be discarded. To see this, let us multiply both sides of Eq.(9.37) by $i\vec{\mathbf{k}}$. We get

$$\frac{i}{\epsilon_0}\,\vec{\mathbf{k}}\cdot\vec{\mathcal{J}}_\parallel(\vec{\mathbf{k}}) = -i\,\frac{\partial}{\partial t}\,\vec{\mathbf{k}}\cdot\vec{\mathcal{E}}_\parallel(\vec{\mathbf{k}}). \tag{9.38}$$ ae49a

Longitudinal equation (9.27) allows us to write

$$i\,\vec{\mathbf{k}}\cdot\vec{\mathcal{J}}_\parallel(\vec{\mathbf{k}}) = -\frac{\partial}{\partial t}\,\widetilde{\rho}(\vec{\mathbf{k}}). \tag{9.39}$$ ae49b

Projection of the part $\vec{\mathcal{J}}_\parallel$ onto $\vec{\mathbf{k}}$ is obviously equivalent to the projection of a whole vector. Hence, instead of (9.39) we can write

$$i\,\vec{\mathbf{k}}\cdot\vec{\mathcal{J}}(\vec{\mathbf{k}}) = -\frac{\partial}{\partial t}\,\widetilde{\rho}(\vec{\mathbf{k}}), \tag{9.40}$$ ae49c

which is clearly seen to be the charge continuity equation in the Fourier space. Hence we conclude that (9.37) really does not bring any new information. In the case when we consider free fields only, it can indeed be discarded.

ae50 Summarizing, the transverse Maxwell's equations in the Fourier domain are

$$i\vec{\mathbf{k}}\times\vec{\mathcal{E}}_\perp(\vec{\mathbf{k}},t) = -\frac{\partial}{\partial t}\vec{\mathcal{B}}_\perp(\vec{\mathbf{k}},t), \tag{9.41a}$$ ae50a

$$i\vec{\mathbf{k}}\times\vec{\mathcal{B}}_\perp(\vec{\mathbf{k}},t) = \frac{1}{\epsilon_0\, c^2}\,\vec{\mathcal{J}}_\perp(\vec{\mathbf{k}},t) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\vec{\mathcal{E}}_\perp(\vec{\mathbf{k}},t). \tag{9.41b}$$ ae50b

These equations are fully equivalent (in the Fourier domain) to transverse Maxwell's equations (2.52) in normal space.

9.3.4 Discussion of the potentials

As it was done in the main part of the lectures, we continue the discussion of the transverse and longitudinal fields in the Fourier domain. As we know, (see (A.95a)) the gradient of an arbitrary scalar function $\boldsymbol{\nabla}\phi(\vec{\mathbf{r}})$ transforms into $i\vec{\mathbf{k}}\widetilde{(\vec{\mathbf{k}})}$, hence transforms into a vector parallel to $\vec{\mathbf{k}}$ – the transform is purely longitudinal.

We already know that the magnetic field is purely transverse. It follows that the transverse part of $\vec{\mathcal{A}}(\vec{\mathbf{k}},t)$ is sufficient to specify the magnetic field in the Fourier domain

$$\vec{\mathcal{B}}(\vec{\mathbf{k}},t) \;=\; \vec{\mathcal{B}}_\perp(\vec{\mathbf{k}},t) \;=\; i\,\vec{\mathbf{k}}\times\vec{\mathcal{A}}_\perp(\vec{\mathbf{k}},t), \tag{9.42}$$ ae54

because the component $\vec{\mathcal{A}}_\parallel$ does not contribute anyway. For electric field in the Fourier domain (as it follows from Eqs.(9.9a)) we have

$$\vec{\mathcal{E}}_\perp(\vec{\mathbf{k}},t) = -\frac{\partial}{\partial t}\,\vec{\mathcal{A}}_\perp(\vec{\mathbf{k}},t), \tag{9.43a}$$ ae55a

$$\vec{\mathcal{E}}_\parallel(\vec{\mathbf{k}},t) = -\frac{\partial}{\partial t}\,\vec{\mathcal{A}}_\parallel(\vec{\mathbf{k}},t) - i\vec{\mathbf{k}}\,\widetilde{\phi}(\vec{\mathbf{k}},t). \tag{9.43b}$$ ae55b

Again the role of $\vec{\mathcal{A}}_\parallel$ is unclear. Can we take $\vec{\mathcal{A}}_\parallel = 0$ as indicated in the main part of the lectures. We shall consider this question in terms of wave equations (9.10). We focus our attention on Eq.(9.10b) which we split into longitudinal and transverse parts ae56

$$\left[k^2 + \frac{1}{c^2}\,\frac{\partial^2}{\partial t^2}\right]\vec{\mathcal{A}}_\parallel(\vec{\mathbf{k}},t) = \frac{1}{c^2\epsilon_o}\vec{\mathcal{J}}_\parallel(\vec{\mathbf{k}},t) - i\vec{\mathbf{k}}\,\left[i\vec{\mathbf{k}}\cdot\vec{\mathcal{A}}_\parallel(\vec{\mathbf{k}},t) + \frac{1}{c^2}\,\frac{\partial}{\partial t}\,\widetilde{\phi}(\vec{\mathbf{k}},t)\right]. \tag{9.44a}$$ ae56a

$$\left[k^2 + \frac{1}{c^2}\,\frac{\partial^2}{\partial t^2}\right]\vec{\mathcal{A}}_\perp(\vec{\mathbf{k}},t) = \frac{1}{c^2\epsilon_0}\vec{\mathcal{J}}_\perp(\vec{\mathbf{k}},t) \tag{9.44b}$$ ae56b

Note that $\vec{\mathbf{k}}\cdot\vec{\mathcal{A}}_\perp = 0$ so it does not contribute to the first of the above equations. Note also that these equations are the Fourier domain equivalents of Eqs.(2.56). We have mentioned that Eq.(2.56a) (and also its equivalent (9.44a)) does not bring any new information. This is difficult in normal space, but relatively easy in Fourier domain. To show that, we take scalar product of both its sides with the vector $i\vec{\mathbf{k}}$. We note that the second term in the left-hand side cancels with the second one in right-hand side, and we get

$$i\,\vec{\mathbf{k}}\cdot\frac{\partial^2}{\partial t^2}\vec{\mathcal{A}}_\parallel = \frac{1}{\epsilon_0}\,i\,\vec{\mathbf{k}}\cdot\vec{\mathcal{J}}_\parallel + k^2\,\frac{\partial}{\partial t}\,\widetilde{\phi}. \tag{9.45}$$ ae57

Then, differentiating Eq.(9.10a) over time, we eliminate the second order time derivative of the longitudinal component of the vector potential, so the terms containing the time derivative of scalar potential cancel out and we obtain

$$i\,\vec{\mathbf{k}}\cdot\frac{\partial^2}{\partial t^2}\vec{\mathcal{A}}_\parallel = \frac{1}{\epsilon_o}\,i\,\vec{\mathbf{k}}\cdot\vec{\mathcal{J}}_\parallel + \frac{1}{\epsilon_o}\,\frac{\partial}{\partial t}\,\widetilde{\rho} + i\,\vec{\mathbf{k}}\cdot\frac{\partial^2}{\partial t^2}\vec{\mathcal{A}}_\parallel, \tag{9.46}$$ ae58

since, by definition, $\vec{\mathbf{k}}\cdot\vec{\mathcal{A}}_\perp = 0$ in the last term wich cancels with the one in the left hand side. So, Eq.(9.44a) reduces to

$$0 \;=\; \frac{\partial}{\partial t}\,\widetilde{\rho} \;+\; i\,\vec{\mathbf{k}}\cdot\vec{\mathcal{J}}_\parallel, \tag{9.47}$$ ae59

The vector $\vec{\mathcal{J}}_\parallel$ can be replaced by the total one $\vec{\mathcal{J}} = \vec{\mathcal{J}}_\parallel + \vec{\mathcal{J}}_\perp$ and (ae59 9.47) is then a transform of the charge conservation requirement. Hence wave equation (ae56a 9.44a) does not bring anything new and can be discarded. We conclude that the longitudinal component $\vec{\mathcal{A}}_\parallel$ is not really important.

The discussed problem is fully solved in the Coulomb gauge where $\operatorname{div} \vec{\mathbf{A}}(\vec{\mathbf{r}}, t) = 0$. In the Fourier domain this corresponds to Eq.(ae17 9.14) which indicates that the transform of the vector potential is transverse. The simplest way to assure the transversality of vector potential is to demand that

$$\vec{\mathcal{A}}_\parallel(\vec{\mathbf{k}}, t) = 0. \tag{9.48}$$ ae60

Wave equation (ae58 9.46) automatically reduces to charge conservation demand and the only remaining wave equations (in Fourier domain) are ae61

$$\vec{\mathbf{k}}^2\, \widetilde{\phi}(\vec{\mathbf{k}}, t) \;=\; \frac{1}{\epsilon_0}\, \widetilde{\rho}(\vec{\mathbf{k}}, t), \tag{9.49a}$$ ae61a

$$\left[\vec{\mathbf{k}}^2 + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] \vec{\mathcal{A}}_\perp(\vec{\mathbf{k}}, t) \;=\; \frac{1}{\epsilon_o\, c^2}\, \vec{\mathcal{J}}_\perp(\vec{\mathbf{k}}, t), \tag{9.49b}$$ ae61b

which are Fourier domain ones corresponding to Eqs.(ce77 2.57).

We conclude stating that the longitudinal component of the vector potential (at least in the Coulomb gauge) can be safely assumed to be zero (as in (ae60 9.48)).

Finally, let us make one additional remark. Any gauge transformation for vector potential in the Fourier domain is given by relation (ae14a 9.11a), that is

$$\vec{\mathcal{A}}(\vec{\mathbf{k}}, t) \;\xrightarrow[gauge]{}\; \vec{\mathcal{A}}'(\vec{\mathbf{k}}, t) \;=\; \vec{\mathcal{A}}(\vec{\mathbf{k}}, t) + i\vec{\mathbf{k}}\, \widetilde{F}(\vec{\mathbf{k}}, t), \tag{9.50}$$ ae63

with arbitrary function F. The last term - transforming $\vec{\mathcal{A}}(\vec{\mathbf{k}}, t)$ into $\vec{\mathcal{A}}'(\vec{\mathbf{k}}, t)$ is purely longitudinal (parallel to the wave vector $\vec{\mathbf{k}}$). It follows that gauge transformation changes only the longitudinal component of vector potential. It means that in any gauge the transverse component

$$\vec{\mathcal{A}}_\perp(\vec{\mathbf{k}}, t) \;\xrightarrow[gauge]{}\; \vec{\mathcal{A}}_\perp{}'(\vec{\mathbf{k}}, t) \;=\; \vec{\mathcal{A}}_\perp(\vec{\mathbf{k}}, t), \tag{9.51}$$ ae64

so it is unchanged, hence the transverse part of vector potential $\vec{\mathcal{A}}_\perp$ is gauge invariant. Therefore, wave equation for $\vec{\mathbf{A}}_\perp(\vec{\mathbf{r}}, t)$ (that is, Eq.(ce77b 2.57b)) has the same for as the corresponding transverse equation which follows from (ce42b 2.34b) in the Lorentz gauge. It will have such form in any gauge due to gauge invariance of $\vec{\mathcal{A}}_\perp$ either in normal space or in the Fourier domain.

* *

Chapter 10

Annihilation and creation operators

ac:ac

10.1 General properties

We introduce two nonhermitian operators which, by definition, satisfy the canonical commutation relation:

$$\left[\,\hat{a},\,\hat{a}^\dagger\,\right] \;=\; 1. \tag{10.1}$$ x1ccom

By $|\,z\,\rangle$ we denote a normalized eigenstate of the operator $\hat{N} = \hat{a}^\dagger\,\hat{a}$. We assume that such states are orthogonal, since operator $\hat{N}$ is hermitian. So we have

$$\hat{N}|\,z\,\rangle \;=\; \hat{a}^\dagger\,\hat{a}|\,z\,\rangle \;=\; z\,|\,z\,\rangle, \qquad\qquad \langle\,z\,|\,z'\,\rangle \;=\; \delta_{zz'}. \tag{10.2}$$ x1est

x1le1 **Lemma 10.1** *Eigenvalue of the operator $\hat{N}$ is real and nonnegative: $z \in \mathbb{R}_+$.*

Proof. Since $|\,z\,\rangle$ denotes the normalized eigenvector of $\hat{N}$, we have

$$\begin{aligned} z \;&=\; z\,\langle\,z\,|\,z\,\rangle \;=\; \langle\,z\,|\,z\,|\,z\,\rangle \;=\; \langle\,z|\,\hat{a}^\dagger\,\hat{a}\,|\,z\,\rangle \;=\; \big(\,\langle\,z\,|\,\hat{a}^\dagger\,\big)\,(\,\hat{a}\,|\,z\,\rangle\,) \\ &=\; (\,\hat{a}\,|\,z\,\rangle\,)^\dagger\,(\,\hat{a}\,|\,z\,\rangle\,) \;=\; ||\,\hat{a}\,|\,z\,\rangle\,||^2. \end{aligned} \tag{10.3}$$ x1lem1

So we see that z is equal to a norm of a certain vector, and as such is real and nonnegative. ■

x1le2 x1com **Lemma 10.2** *The following commutation relations hold*

$$\left[\,\hat{a}^\dagger\,\hat{a},\,\hat{a}\,\right] = -\hat{a}, \tag{10.4a}$$ x1coma

$$\left[\,\hat{a}^\dagger\,\hat{a},\,\hat{a}^\dagger\,\right] = \hat{a}^\dagger. \tag{10.4b}$$ x1comb

Proof. By simple calculation, we get from the canonical relation (10.1): x1ccom

$$\begin{aligned} \left[\,\hat{a}^\dagger\,\hat{a},\,\hat{a}\,\right] &= \hat{a}^\dagger\,\left[\,\hat{a},\,\hat{a}\,\right] \;+\; \left[\,\hat{a}^\dagger,\,\hat{a}\,\right]\,\hat{a} \;=\; \hat{a}^\dagger\cdot 0 \;+\; (-1)\hat{a}. \\ \left[\,\hat{a}^\dagger\,\hat{a},\,\hat{a}^\dagger\,\right] &= \hat{a}^\dagger\,\left[\,\hat{a},\,\hat{a}^\dagger\,\right] \;+\; \left[\,\hat{a}^\dagger,\,\hat{a}^\dagger\,\right]\,\hat{a} \;=\; \hat{a}^\dagger \;+\; 0\cdot\hat{a}, \end{aligned} \tag{10.5}$$ x1lem2

which completes the proof. ■

x1le3 **Lemma 10.3** *The ket $\hat{a}\,|\,z\,\rangle$ is an eigenstate of the operator $\hat{N} = \hat{a}^\dagger\,\hat{a}$, and it belongs to an eigenvalue $(z-1)$, that is*

$$\hat{N}\,\hat{a}\,|\,z\,\rangle \;=\; (z-1)\,\hat{a}\,|\,z\,\rangle. \tag{10.6}$$ x1lem3

Proof. If $\hat{a}\,|\,z\,\rangle \neq 0$, then we have

$$\hat{N}\,\hat{a}\,|\,z\,\rangle \;=\; \hat{a}^\dagger\,\hat{a}\,\hat{a}\,|\,z\,\rangle. \tag{10.7}$$ x1lem3a

Due to commutation relation (x1coma 10.4a) we can write $\hat{a}^\dagger\,\hat{a}\,\hat{a} = \hat{a}\,\hat{a}^\dagger\,\hat{a} - \hat{a}$, and hence

$$\hat{N}\,\hat{a}\,|\,z\,\rangle \;=\; \hat{a}\,(\hat{a}^\dagger\,\hat{a} - 1)\,|\,z\,\rangle \;=\; \hat{a}\,z\,|\,z\,\rangle - \hat{a}\,|\,z\,\rangle \;=\; (z-1)\,\hat{a}\,|\,z\,\rangle. \tag{10.8}$$ x1lem3b

This shows that vector $\hat{a}\,|\,z\,\rangle$ is an eigenstate of $\hat{N}$ with an eigenvalue $(z-1)$. ■

x1le4 **Lemma 10.4** *The ket $\hat{a}^\dagger\,|\,z\,\rangle$ is an eigenstate of the operator $\hat{N} = \hat{a}^\dagger\,\hat{a}$, and it belongs to an eigenvalue $(z+1)$, that is*

$$\hat{N}\,\hat{a}^\dagger\,|\,z\,\rangle \;=\; (z+1)\,\hat{a}\,|\,z\,\rangle. \tag{10.9}$$ x1lem4

Proof. The proof is analogous to that of the previous lemma, only we use commutation relation (x1comb 10.4b) instead of (x1coma 10.4a). ■

x1le5 **Lemma 10.5** *Norms of the vectors $\hat{a}\,|\,z\,\rangle$ and $\hat{a}^\dagger\,|\,z\,\rangle$ are given as*

$$||\,\hat{a}\,|\,z\,\rangle\,|| \;=\; \sqrt{z}\,, \qquad\qquad ||\,\hat{a}^\dagger\,|\,z\,\rangle\,|| \;=\; \sqrt{z+1}\,. \tag{10.10}$$ x1lem5

Proof. The first norm follows automatically from the proof of the first lemma, see relation (x1lem1 10.3). The second relation is proved similarly. We have

$$||\hat{a}^\dagger\,|\,z\,\rangle||^2 \;=\; \big(\,\hat{a}^\dagger\,|\,z\,\rangle\big)^\dagger\,\big(\,\hat{a}^\dagger\,|\,z\,\rangle\big) \;=\; \langle\,z\,|\,\hat{a}\,\hat{a}^\dagger\,|\,z\,\rangle. \tag{10.11}$$ x1lem5a

Using the canonical commutation relation we have $\hat{a}\,\hat{a}^\dagger = \hat{a}^\dagger\,\hat{a} + 1$, thus, we get

$$||\hat{a}^\dagger\,|\,z\,\rangle||^2 \;=\; \langle\,z\,|\,\hat{a}^\dagger\hat{a}+1\,|\,z\,\rangle \;=\; \langle\,z\,|\,\hat{a}^\dagger\hat{a}\,|\,z\,\rangle+\langle\,z\,|\,z\,\rangle \;=\; ||\hat{a}|\,z\,\rangle||^2+1 \;=\; z+1, \tag{10.12}$$ x1lem5b

since vector $|\,z\,\rangle$ is normalized and $||\,\hat{a}\,|\,z\,\rangle\,||^2 = z$. Second relation (x1lem5 10.10) follows immediately. ■

x1le6 **Lemma 10.6** *If a vector $\hat{a}^n\,|\,z\,\rangle \neq 0$, then it is an eigenvector of $\hat{N}$ belonging to the eigenvalue $(z-n)$:*

$$\hat{N}\,\hat{a}^n\,|\,z\,\rangle \;=\; (z-n)\,\hat{a}^n\,|\,z\,\rangle \tag{10.13}$$ x1lem6

Proof. The proof follows by mathematical induction. The case $n = 1$ was already shown in (x1lem3 10.6). In the proof essential role is played by the relation $\hat{N}\hat{a} = \hat{N}\hat{a} - \hat{a}$, which follows from (x1coma 10.4a). We easily have

$$\hat{N}\left[\hat{a}^{n+1}\,|\,z\,\rangle\right] \;=\; \hat{N}\hat{a}\,[\hat{a}^n\,|\,z\,\rangle] \;=\; (\hat{a}\hat{N}-\hat{a})\,[\hat{a}^n\,|\,z\,\rangle] \;=\; \hat{a}\hat{N}\,[\hat{a}^n\,|\,z\,\rangle]-\hat{a}^{n+1}\,|\,z\,\rangle \tag{10.14}$$ x1lem6a

By induction assumption, we further get

$$\hat{N}\left[\hat{a}^{n+1}\,|\,z\,\rangle\right] \;=\; \hat{a}(z-n)\hat{a}^n\,|\,z\,\rangle - \hat{a}^{n+1}\,|\,z\,\rangle \;=\; (z-n-1)\hat{a}^{n+1}\,|\,z\,\rangle. \tag{10.15}$$ x1lem6b

and the lemma follows. ■

x1le7 **Lemma 10.7** *There exists such an integer n, that*

$$\hat{a}^n \,|\, z \,\rangle \neq 0, \qquad \text{but} \qquad \hat{a}^{n+1} \,|\, z \,\rangle = 0, \tag{10.16}$$ x1lem7

Proof. From the previous lemma it follows that $\hat{a}^n|\, z \,\rangle$ is an eigenvector of the operator $\hat{N}$ and it belongs to the eigenvalue $(z-n)$. Lemma (x1le1 10.1) states that eigenvalues of $\hat{N}$ are nonnegative. For n sufficiently large we would have $(z-n) < 0$. This contradicts lemma (x1le1 10.1). Hence, there must exist an integer n such that relations (x1lem7 10.16) are satisfied. This completes the proof. ■

x1th1 **Theorem 10.1** *The eigenvalues z of the operator $\hat{N}$ defined in Eq.(x1est 10.2) are nonnegative integers. Moreover, there exists such a normalized eigenvector $|\, 0 \,\rangle$ of $\hat{N}$ that*

$$\hat{a} \,|\, 0 \,\rangle = 0 \tag{10.17}$$ x1t11

which will be called the vacuum state.

Proof. Since a vector $\hat{a}^n|\, z \,\rangle$ is an eigenvector of $\hat{N}$ belonging to the eigenvalue $z-n$, we can normalize it and write it as

$$|\, z-n \,\rangle \;=\; \frac{\hat{a}^n \,|\, z \,\rangle}{||\hat{a}^n \,|\, z \,\rangle||}. \tag{10.18}$$ x1t12

Let the integer n be such, that Eq.(x1lem7 10.16) is satisfied. This means that

$$\hat{a} \,|\, z-n \,\rangle \;=\; 0, \tag{10.19}$$ x1t13

and the norm of the obtained vector is

$$||\, \hat{a} \,|\, z-n \,\rangle \,|| \;=\; 0. \tag{10.20}$$ x1t14

Now, from the first of relations (x1lem5 10.10) it follows that

$$||\, \hat{a} \,|\, z-n \,\rangle \,|| \;=\; \sqrt{z-n} \;=\; 0. \tag{10.21}$$ x1t15

This implies that $z = n$. Hence the eigenvalues z of the operator $\hat{N} = \hat{a}^\dagger \hat{a}$ are nonnegative integers. We also conclude that there exists a normalized vector $|\, 0 \,\rangle$ for which eq.(x1lem7 10.16) is satisfied for $n = 0$. ■

x1th2 **Theorem 10.2** *According to the previous theorem, we denote by $|\, n \,\rangle$ the normalized eigenstate of the operator $\hat{N}$ belonging to the eigenvalue n – nonnegative integer. Then, the vectors*

$$|\, n-1 \,\rangle \;=\; \frac{\hat{a} \,|\, n \,\rangle}{\sqrt{n}}, \qquad \text{and} \qquad |\, n+1 \,\rangle \;=\; \frac{\hat{a}^\dagger \,|\, n \,\rangle}{\sqrt{n+1}}, \tag{10.22}$$ x1t21

are the eigenstates of $\hat{N}$. These relations enable us to construct all the eigenstates of operator $\hat{N}$, provided one of the states $|\, n \,\rangle$ is given.

Proof. In lemma (10.3) we have shown that the vector $\hat{a}\,|\,n\,\rangle$ is an eigenstate of $\hat{N}$ belonging to the eigenvalue $(n-1)$. This means (according to the introduced notation), that $\hat{a}\,|\,n\,\rangle$ is proportional to the vector $|\,n-1\,\rangle$. It remains to find the coefficient of proportionality. From lemma (10.5) we have the norm $||\,\hat{a}\,|\,n\,\rangle\,|| = \sqrt{n}$. Thus the vector

$$\frac{\hat{a}\,|\,n\,\rangle}{||\,\hat{a}\,|\,n\,\rangle\,||} \;=\; \frac{\hat{a}\,|\,n\,\rangle}{\sqrt{n}}, \tag{10.23}$$ x1t22

is a normalized eigenvector of $\hat{N}$ with eigenvalue $(n-1)$. Hence it is equal to $|\,n-1\,\rangle$. So the first part of the theorem is proved. The second part can be shown in the same manner.■

x1def Let us note that relations (10.22) can be rewritten as

$$\hat{a}\,|\,n\,\rangle = \sqrt{n}\;|\,n-1\,\rangle \tag{10.24a}$$ x1defa

$$\hat{a}^\dagger\,|\,n\,\rangle = \sqrt{n+1}\;|\,n+1\,\rangle \tag{10.24b}$$ x1defb

x1le8 **Lemma 10.8** *The eigenstate $|\,n\,\rangle$ of the operator $\hat{N} = \hat{a}^\dagger\,\hat{a}$ can be constructed as*

$$|\,n\,\rangle \;=\; \frac{1}{\sqrt{n!}}\;\left(\,\hat{a}^\dagger\,\right)^n\;|\,0\,\rangle, \tag{10.25}$$ x1lem8

if the vacuum state $|\,0\,\rangle$ defined in eq.(10.17) is given.

Proof. The proof follows by induction from relation (10.24b). For $n = 1$ we have

$$|\,1\,\rangle \;=\; \frac{1}{\sqrt{1!}}\,\hat{a}^\dagger\,|\,0\,\rangle \;=\; \frac{1}{\sqrt{1!}}\,\sqrt{1}\;|\,1\,\rangle \;=\; |\,1\,\rangle, \tag{10.26}$$ x1lem8a

as it should be. Now, we have

$$\begin{aligned} |\,n+1\,\rangle &= \frac{1}{\sqrt{(n+1)!}}\,(\hat{a}^\dagger)^{n+1}\,|\,0\,\rangle \;=\; \frac{1}{\sqrt{n+1}}\,\frac{1}{\sqrt{n!}}\,\hat{a}^\dagger\,(\hat{a}^\dagger)^n|\,0\,\rangle \\ &= \frac{\hat{a}^\dagger}{\sqrt{n+1}}\,|\,n\,\rangle \;=\; \sqrt{n+1}\;\frac{|\,n+1\,\rangle}{\sqrt{n+1}} \;=\; |\,n+1\,\rangle. \end{aligned} \tag{10.27}$$ x1lem8b

Going from the first to the second line we have employed the principle of mathematical induction, and thus the proof is completed. ■

This lemma clearly indicates the manner of construction of the eigenstates of the operator $\hat{N} = \hat{a}^\dagger\,\hat{a}$. We must find the ground state – the vacuum one $|\,0\,\rangle$ which should be unique. If this is not the case, we must find a complete set of commuting observables and classify the vacuum states with the aid of additional quantum numbers. Normalizing the vacuum state we apply the creation operators to construct the eigenstates $|\,n\,\rangle$.

x1le9 **Lemma 10.9** *The eigenstates $|\,n\,\rangle$ specified in (10.25) are orthonormal, that is*

$$\langle\,n\,|\,m\,\rangle \;=\; \delta_{nm}. \tag{10.28}$$ x1lem9

Orthogonality follows from the fact that $|\,n\,\rangle$ are eigenstates of the hermitian operator $\hat{N} = \hat{a}^\dagger\,\hat{a}$, so it is sufficient to prove that the are normalized.

Proof. Without loss of generality we can assume $n \geq m$. Then from (10.25) we have

$$\langle\, n \,|\, m \,\rangle \;=\; \frac{1}{\sqrt{n!\, m!}}\, \langle\, 0 \,|\, \hat{a}^n\, (\hat{a}^\dagger)^m \,|\, 0 \,\rangle. \tag{10.29}$$ x1lem9a

But

$$\begin{aligned} \hat{a}\, (\hat{a}^\dagger)^m - (\hat{a}^\dagger)^m\, \hat{a} = \big[\, \hat{a},\, (\hat{a}^\dagger)^m \,\big] \;&=\; \hat{a}^\dagger\, \big[\, \hat{a},\, (\hat{a}^\dagger)^{m-1} \,\big] \;+\; \big[\, \hat{a},\, \hat{a}^\dagger \,\big]\, (\hat{a}^\dagger)^{m-1} \\ &= \hat{a}^\dagger\, \big[\, \hat{a},\, (\hat{a}^\dagger)^{m-1} \,\big] \;+\; (\hat{a}^\dagger)^{m-1}. \end{aligned} \tag{10.30}$$ x1lem9b

Continuing such a reasoning we finally obtain

$$\hat{a}\, (\hat{a}^\dagger)^m - (\hat{a}^\dagger)^m\, \hat{a} \;=\; m\, (\hat{a}^\dagger)^{m-1}, \tag{10.31}$$ x1lem9c

which can easily be verified by mathematical induction. Therefore, we obtain

$$\begin{aligned} \langle\, n \,|\, m \,\rangle &= \frac{1}{\sqrt{n!\, m!}}\, \langle\, 0 \,|\, \hat{a}^{n-1}\, \big[m (\hat{a}^\dagger)^{m-1} + (\hat{a}^\dagger)^m\, \hat{a} \big] \,|\, 0 \,\rangle \\ &= \frac{1}{\sqrt{n!\, m!}}\, m\, \langle\, 0 \,|\, \hat{a}^{n-1}\, (\hat{a}^\dagger)^{m-1} \,|\, 0 \,\rangle, \end{aligned} \tag{10.32}$$ x1lem9d

because $\hat{a}\,|\,0\,\rangle = 0$. Repeating such a procedure m times we will arrive at the relation

$$\langle\, n \,|\, m \,\rangle \;=\; \sqrt{\frac{m!}{n!}}\; \langle\, 0 \,|\, \hat{a}^{n-m} \,|\, 0 \,\rangle. \tag{10.33}$$ x1lem9e

For $n > m$ we have $\hat{a}^{n-m}\,|\,0\,\rangle = 0$, which follows from the definition of the vacuum state. When $n = m$ we get $\langle\, n \,|\, m \,\rangle = \langle\, 0 \,|\, 0 \,\rangle = 1$. So the states $|\, n \,\rangle$ are orthogonal (which is not unexpected) and normalized, as it should be. ■

10.2 Annihilation and creation operators – summary

Annihilation and creation operators (non-hermitian) are specified by the commutation relation

$$\big[\, \hat{a},\, \hat{a}^\dagger \,\big] \;=\; 1. \tag{10.34}$$ x1scom

The number states $|\, n \,\rangle$ are the eigenstates of the number operator $\hat{N} = \hat{a}^\dagger\, \hat{a}$, that is

$$\hat{N}\,|\, n \,\rangle \;=\; \hat{a}^\dagger\, \hat{a} |\, n \,\rangle \;=\; n\,|\, n \,\rangle, \qquad \text{with} \qquad n = 0,\, 1,\, 2,\, \ldots\ldots \tag{10.35}$$ x1sest

The state $|\, 0 \,\rangle$ is called a vacuum state and it satisfies the condition

$$\hat{a}\,|\, 0 \,\rangle \;=\; 0. \tag{10.36}$$ x1svac

Number states $|\, n \,\rangle$ are orthonormal (eigenstates of the Hermitian operator $\hat{N}$)

$$\langle\, m \,|\, n \,\rangle \;=\; \delta_{mn}. \tag{10.37}$$ x1snorm

Annihilation and creation are sometimes called ladder operators. This follows from the x1sac properties of lowering and raising the number of the state

$$\hat{a}\,|\,n\,\rangle = \sqrt{n}\;|\,n-1\,\rangle, \tag{10.38a}$$ x1saca

$$\hat{a}^\dagger\,|\,n\,\rangle = \sqrt{n+1}\;|\,n+1\,\rangle. \tag{10.38b}$$ x1sacb

Let us note that these relations are fully consistent with the previous ones. Relation (x1saca 10.38a) agrees with the definition (x1svac 10.36) of the vacuum state. Moreover, we have

$$\begin{aligned}\hat{a}^\dagger\,\hat{a}\,|\,n\,\rangle = \hat{a}^\dagger\,\sqrt{n}\;|\,n-1\,\rangle \;&=\; \sqrt{n}\;\hat{a}^\dagger\,|\,n-1\,\rangle \\ = \sqrt{n}\;\sqrt{(n-1)+1}\;|\,n\,\rangle \;&=\; n\,|\,n\,\rangle,\end{aligned} \tag{10.39}$$ x1scon

as it should be, when compared to definition (x1sest 10.35). Matrix elements of the annihilation and creation operators follow immediately from Eqs.(x1sac 10.38)and from orthonormality x1se requirement. We have

$$\langle\,m\,|\,\hat{a}\,|\,n\,\rangle = \sqrt{n}\;\langle\,m\,|\,n-1\,\rangle \;=\; \sqrt{n}\;\delta_{m,n-1}, \tag{10.40a}$$ x1sea

$$\langle\,m\,|\,\hat{a}^\dagger\,|\,n\,\rangle = \sqrt{n+1}\;\langle\,m\,|\,n+1\,\rangle \;=\; \sqrt{n+1}\;\delta_{m,n+1}. \tag{10.40b}$$ x1seb

Finally, practical construction goes along the following way

- Construct annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$, check their commutation relation (to reproduce the canonical one (x1scom 10.34)).
- Find (construct) the vacuum state $|\,0\,\rangle$.
- Construct the number states by using the relation

$$|\,n\,\rangle \;=\; \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|\,0\,\rangle. \tag{10.41}$$ x1snn

10.3 Application to harmonic oscillator

10.3.1 Annihilation and creation operators for harmonic oscillator

Hamiltonian of the quantum–mechanical harmonic oscillator is of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} \;+\; \frac{1}{2}\,m\omega^2\hat{x}^2, \tag{10.42}$$ x1hosc

and the momentum and position operators satisfy the canonical commutation relation

$$[\,\hat{x},\,\hat{p}\,] \;=\; i\hbar. \tag{10.43}$$ x1hocom

It is an easy matter to check that two operators

$$\sqrt{\frac{m\omega}{\hbar}}\,\hat{x} \qquad \text{and} \qquad \frac{\hat{p}}{\sqrt{m\omega\hbar}}, \tag{10.44}$$ x1xpops

are dimensionless.

x1th2 x1b **Theorem 10.3** *Two dimensionless, nonhermitian operators $\hat{a}$ and $\hat{a}^\dagger$ defined as*

$$\hat{b} = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}}\, \hat{x} \;+\; \frac{i\hat{p}}{\sqrt{m\omega\hbar}} \right) \;=\; \frac{1}{\sqrt{2m\omega\hbar}}\, (\, m\omega\, \hat{x} \;+\; i\hat{p}\,)\,, \tag{10.45a}$$ x1ba

$$\hat{b}^\dagger = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}}\, \hat{x} \;-\; \frac{i\hat{p}}{\sqrt{m\omega\hbar}} \right) \;=\; \frac{1}{\sqrt{2m\omega\hbar}}\, (\, m\omega\, \hat{x} \;-\; i\hat{p}\,)\,, \tag{10.45b}$$ x1bb

satisfy the commutation relation

$$\Big[\, \hat{b},\, \hat{b}^\dagger \,\Big] \;=\; 1. \tag{10.46}$$ x1aac

Hence we may identify: $\hat{b}$ – annihilation, and $\hat{b}^\dagger$ – creation operators.

Proof. The facts that these operators are nonhermitian and dimensionless are evident. We show the commutation relation.

$$\begin{aligned}
\Big[\, \hat{b},\, \hat{b}^\dagger \,\Big] &= \frac{1}{2m\omega\hbar}\, [\, m\omega\, \hat{x} \;+\; i\hat{p},\; m\omega\, \hat{x} \;-\; i\hat{p}\,] \\
&= \frac{1}{2m\omega\hbar}\, \big\{\, m^2\omega^2\, [\hat{x},\, \hat{x}] \;-\; im\omega\, [\hat{x},\, \hat{p}] \;+\; im\omega\, [\hat{p},\, \hat{x}] \;+\; [\hat{p},\, \hat{p}]\, \big\} \\
&= \frac{im\omega}{2m\omega\hbar}\, \big\{ \;-\; [\hat{x},\, \hat{p}] \;+\; [\hat{p},\, \hat{x}]\, \big\} \;=\; \frac{i}{2\hbar}\, \big\{ \;-\; i\hbar \;+\; (-i\hbar)\, \big\} \;=\; 1.
\end{aligned} \tag{10.47}$$

Since operators $\hat{b}$ and $\hat{b}^\dagger$ satisfy commutation relation typical for annihilation and creation operators, they posses all the necessary properties and the identification made in the theorem is fully justified and correct. ■

x1b Relations (10.45) can easily be inverted, and we can express the position and momentum operators via annihilation and creation ones

x1xpac

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\, \Big(\hat{b} \;+\; \hat{b}^\dagger \Big)\,, \tag{10.48a}$$ x1xpaca

$$\hat{p} = -i\, \sqrt{\frac{m\omega\hbar}{2}}\, \Big(\hat{b} \;-\; \hat{b}^\dagger \Big)\,, \tag{10.48b}$$ x1xpacb

Having expressions (10.48) we can now express the Hamiltonian of the oscillator in terms of the annihilation and creation operators. We obtain

$$\begin{aligned}
\hat{H} &= \frac{1}{2m} \left[-i\, \sqrt{\frac{m\omega\hbar}{2}}\, \Big(\hat{b} \;-\; \hat{b}^\dagger \Big) \right]^2 \;+\; \frac{1}{2}\, m\omega^2 \left[\sqrt{\frac{\hbar}{2m\omega}}\, \Big(\hat{b} \;+\; \hat{b}^\dagger \Big) \right]^2 \\
&= -\, \frac{\hbar\omega}{4} \Big(\hat{b} \;-\; \hat{b}^\dagger \Big)^2 \;+\; \frac{\hbar\omega}{4} \Big(\hat{b} \;+\; \hat{b}^\dagger \Big)^2 \\
&= -\, \frac{\hbar\omega}{4} \Big(\hat{b}\hat{b} - \hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} + \hat{b}^\dagger\hat{b}^\dagger \Big) \;+\; \frac{\hbar\omega}{4} \Big(\hat{b}\hat{b} + \hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b} + \hat{b}^\dagger\hat{b}^\dagger \Big) \\
&= \frac{\hbar\omega}{2} \Big(\hat{b}\, \hat{b}^\dagger + \hat{b}^\dagger\, \hat{b} \Big)
\end{aligned} \tag{10.49}$$ x1hac1

Using the commutation relation (10.46) we have $\hat{b}\, \hat{b}^\dagger = 1 + \hat{b}^\dagger\hat{b}$, thus from the above we finally get

$$\hat{H} \;=\; \frac{\hbar\omega}{2} \Big(2\, \hat{b}^\dagger\, \hat{b} + 1 \Big) \;=\; \hbar\omega \left(\hat{b}^\dagger\, \hat{b} + \frac{1}{2} \right) \;=\; \hbar\omega \left(\hat{N} + \frac{1}{2} \right) \tag{10.50}$$ x1hac

where, as previously, we introduced the number operator $\hat{N} = \hat{b}^\dagger\, \hat{b}$.

x1th4 **Theorem 10.4** *Energy eigenstates of the quantum-mechanical harmonic oscillator are the number states* $|\,n\,\rangle$ *– the eigenstates of the number operator* $\hat{N} = \hat{b}^\dagger\,\hat{b}$*. The energy eigenvalues are*

$$E_n = \hbar\omega\left(\,n + \frac{1}{2}\,\right). \tag{10.51}$$ x1enei

Proof. The proof follows immediately from relation (x1hac 10.50) and from the properties of the number operator, as discussed in the previous section. ■

10.3.2 Construction of the vacuum state

Construction of the vacuum state is the first step in building the energy eigenstates of the harmonic oscillator. We will do this in the position representation, that is we are looking for the wave function $\varphi_0(x) = \langle\, x\,|\,0\,\rangle$. The vacuum state is defined by eq.(x1t11 10.17), so using the annihilation operator $\hat{b}$ as given in (x1ba 10.45a), we get

$$0 \;=\; \hat{b}\,|\,0\,\rangle \;=\; \frac{1}{\sqrt{2m\omega\hbar}}\;(\,m\omega\,\hat{x} \;+\; i\hat{p}\,)\;|\,0\,\rangle. \tag{10.52}$$ x1vac1

In position representation, this equation reads

$$\begin{aligned} 0 &= \langle\, x\,|\,\frac{1}{\sqrt{2m\omega\hbar}}\;(\,m\omega\,\hat{x} \;+\; i\hat{p}\,)\;|\,0\,\rangle \\ &= \frac{1}{\sqrt{2m\omega\hbar}}\left[\,m\omega\,x \;+\; i\left(-i\hbar\,\frac{d}{dx}\right)\right]\,\varphi_0(x). \end{aligned} \tag{10.53}$$ x1vac2

The latter relation is a simple differential equation of the first order

$$0 \;=\; \left(\lambda x \;+\; \frac{d}{dx}\right)\,\varphi_0(x), \qquad \text{with} \qquad \lambda \;=\; \frac{m\omega}{\hbar}. \tag{10.54}$$ x1vac3

Solution to this equation is very simple. It is

$$\varphi_0(x) \;=\; A_o\,\exp\left(-\frac{\lambda x^2}{2}\right), \tag{10.55}$$ x1vac4

where A_o is a normalization constant. Computation of this constant yields

$$1 \;=\; |\,A_o\,|^2\int_{-\infty}^{\infty} dx\;\exp\left(-\frac{\lambda x^2}{2}\right) \;=\; |\,A_o\,|^2\,\sqrt{\frac{\pi}{\lambda}}. \tag{10.56}$$ x1vac5

Choosing the arbitrary phase of the constant A_o to be zero we obtain the wave function of the ground state of the oscillator, or in other words, the vacuum state in the position representation

$$\varphi_0(x) \;=\; \left(\frac{\lambda}{\pi}\right)^{1/4}\;\exp\left(-\frac{\lambda x^2}{2}\right), \tag{10.57}$$ x1vac6

which is properly normalized.

10.3.3 Construction of the number states $|\, n \,\rangle$

Having constructed the vacuum state in the position representation, we proceed to construct further states. To do so, we use relation (10.41) in position representation

$$\varphi_n(x) \;=\; \langle\, x \,|\, n \,\rangle \;=\; \frac{1}{\sqrt{n!}} \langle\, x \,|\, (\hat{b}^\dagger)^n \,|\, 0 \,\rangle. \tag{10.58}$$

x1n1

In order to deal with this expression let us consider a bra (dual form) $\langle\, x \,|\, \hat{b}^\dagger$. Using Eq.(10.45b) we get

$$\begin{aligned} \langle\, x \,|\, \hat{b}^\dagger = \langle\, x \,|\, \frac{1}{\sqrt{2m\omega\hbar}} \,(\, m\omega\hbar\, \hat{x} \;-\; i\hat{p}\,) \;&=\; \sqrt{\frac{m\omega}{2\hbar}}\, \langle\, x \,|\, \left(\, \hat{x} \;-\; \frac{i}{m\omega}\, \hat{p}\, \right) \\ = \sqrt{\frac{\lambda}{2}}\, \left[\left(\, \hat{x} \;+\; \frac{i}{m\omega}\, \hat{p}\, \right) |\, x \,\rangle \right]^\dagger \;&=\; \sqrt{\frac{\lambda}{2}}\, \left[\left(\, x \;+\; \frac{\hbar}{m\omega}\, \frac{d}{dx}\, \right) |\, x \,\rangle \right]^\dagger. \end{aligned}$$

Since the differential operator d/dx is antihermitian, we get

$$\langle\, x \,|\, \hat{b}^\dagger \;=\; \sqrt{\frac{\lambda}{2}}\, \left(\, x \;-\; \frac{1}{\lambda}\, \frac{d}{dx}\, \right) \langle\, x \,|. \tag{10.59}$$

x1n3

Using this relation n times in (10.58), we get

$$\varphi_n(x) \;=\; \left(\, \frac{\lambda}{2}\, \right)^{n/2} \frac{1}{\sqrt{n!}}\, \left(\, x \;-\; \frac{1}{\lambda}\, \frac{d}{dx}\, \right)^n \langle\, x \,|\, 0 \,\rangle. \tag{10.60}$$

x1n4

Inserting the wave function (10.57), we obtain the differential relation specifying the n-th eigenstate of the harmonic oscillator

$$\varphi_n(x) \;=\; \left(\, \frac{\lambda}{\pi}\, \right)^{1/4} \sqrt{\frac{1}{2^n\, n!}}\, \lambda^{n/2}\, \left(\, x \;-\; \frac{1}{\lambda}\, \frac{d}{dx}\, \right)^n \;\exp\, \left(\, -\frac{\lambda x^2}{2}\, \right). \tag{10.61}$$

x1n5

This is a functional equation similar to the Rodrigues formula for Hermite polynomials. This is clarified by the following theorem

Theorem 10.5 *Hermite polynomials can be expressed as follows*

$$H_n(y) \;=\; \exp\, \left(\, \frac{y^2}{2}\, \right) \left(\, y \;-\; \frac{d}{dy}\, \right)^n \exp\, \left(\, -\, \frac{y^2}{2}\, \right). \tag{10.62}$$

x1Hpol

We accept this theorem without proof (which is not difficult, when one uses the Rodrigues formula for Hermite polynomials). Changing the variable $y = x\sqrt{\lambda}$, we can easily show that eq.(10.61 leads to the expression

$$\varphi_n(x) \;=\; \left(\, \frac{\lambda}{\pi}\, \right)^{1/4} \sqrt{\frac{1}{2^n\, n!}}\, \exp\, \left(\, -\frac{\lambda x^2}{2}\, \right)\, H_n(x\sqrt{\lambda}), \tag{10.63}$$

x1n6

which, together with notation introduced in (10.54) exactly reproduces the standard wave functions of the n-th energy eigenstate of the quantum-mechanical harmonic oscillator.

* *

Chapter 11

Density operator

ac:do

11.1 Introductory remarks

According to the principles of quantum mechanics full information about the physical system is contained in the time-dependent state $|\,\psi(t)\,\rangle$ which is a normalized vector from certain Hilbert space. To each physical quantity there corresponds a Hermitian operator $\hat{A}$. The expectation value of the observable A is then given in Schrödinger picture as

$$\langle\, A\,\rangle_t = \langle\, \psi(t)\,|\, A\,|\,\psi(t)\,\rangle \tag{11.1}$$ do1

This statement can be checked only by performing the measurement of observable A on the ensemble of systems, each prepared in the quantum-mechanical state $|\,\psi\,\rangle$). In case of the measurements done on one system only we cannot predict the result with certainty. We note that the average in (11.1) depends parametrically on time, so it evolves in time.

Let us assume that the considered system possesses a Hamiltonian, for which we can find the eigenstates and eigenvalues (energies)

$$H\,|\,\varphi_n\,\rangle = E_n\,|\,\varphi_n\,\rangle, \tag{11.2}$$ do2

where the states $|\,\varphi_n\,\rangle$ are orthonormal and complete, that is

$$\langle\,\varphi_m\,|\,\varphi_n\,\rangle = \delta_{mn}, \qquad \sum_n\, |\,\varphi_n\,\rangle\langle\,\varphi_n\,| = 1. \tag{11.3}$$ do3

Then, any state of our system can be expanded in the basis provided by the eigenstates of the Hamiltonian, and we have

$$|\,\psi(t)\,\rangle = \sum_n\, C_n(t)\,|\,\varphi_n\,\rangle, \tag{11.4}$$ do4

with time-dependent expansion coefficients. The norm conservation results in the requirement

$$\sum_n\, |\,C_n(t)\,|^2 = 1, \qquad \text{for any instant}\ \ t. \tag{11.5}$$ do5

Let us now compute the expectation value of the observable A. We insert expansions (11.4) into Eq.(11.1) and by standard calculation we get

$$\langle\, A\,\rangle_t = \sum_{m,n}\, C_n^*(t)\, C_m(t)\, A_{nm}, \tag{11.6}$$ do6

where we denoted the matrix element $A_{nm} = \langle \varphi_n | A | \varphi_m \rangle$. We see that the average value $\langle A \rangle_t$ is bilinear in eigenstates $| \varphi_n \rangle$. It is a very important feature of quantum mechanics which, among other things, accounts for interference phenomena, characteristic for quantum description.

In many practical experiments we do not deal with single entities as atoms. Usually we have some ensemble of atoms and molecules. Then we understand the necessity of the description in the language of statistical physics. We measure some average characteristics of the ensemble of atoms, or molecules. In such a case we do not have exact information about quantum state of each atom within the ensemble. This leads to the concept of density operator. We will also discuss elsewhere that a system interacting with the surroundings (an open system) must be described with the aid of density operator. Hence we proceed to introduce this concept.

11.2 The basic concept of density operator

We will try to introduce the idea of the density operator in a simple and intuitive manner. To this end, let us consider a system consisting of N atoms (subsystems) numbered by an index i. Let us assume that the i-th atom is in the quantum state $| \psi^{(i)} \rangle$. The quantum-mechanical average of the observable A for this particle is $\langle A \rangle = \langle \psi^{(i)} | A | \psi^{(i)} \rangle$. The statistical average over the ensemble of the particles is given as

$$\overline{\langle A \rangle} = \frac{1}{N} \sum_{i=1}^{N} \langle \psi^{(i)} | A | \psi^{(i)} \rangle, \tag{11.7}$$ do7

where we have two kinds of averaging: the quantum-mechanical expressed by the matrix element, and statistical – over the ensemble. Constructing the second one we assumed that atoms are equivalent, each contributes in the same manner to the total average. Hence each atom is accounted for with the weight factor $1/N$. Clearly, each atomic state $| \psi^{(i)} \rangle$ can be expanded as in (11.4), that is we have

$$| \psi^{(i)} \rangle = \sum_n C_n^{(i)} | \varphi_n \rangle, \qquad C_n^{(i)} = \langle \varphi_n | \psi^{(i)} \rangle \qquad \sum_n \left| C_n^{(i)} \right|^2 = 1, \tag{11.8}$$ do8

Similarly as we obtained (11.6), we now expand states $| \psi^{(i)} \rangle$ as above, and compute the average defined in (11.7). Thus we get

$$\langle A \rangle = \sum_{m,n} \left(\frac{1}{N} \sum_{i=1}^{N} C_n^{(i)*} C_m^{(i)} \right) A_{nm}, \tag{11.9}$$ do9

where we dropped the time argument. The obtained expression involving two kinds of averaging can be rewritten as follows. We define a new matrix (note the change sequence of factors)

$$\rho_{mn} = \frac{1}{N} \sum_{i=1}^{N} C_m^{(i)} C_n^{(i)*} = \overline{C_m^{(i)} C_n^{(i)*}}. \tag{11.10}$$ do10

We note that the statistical information about the considered ensemble is reflected by this matrix. It is worth noting, that due to the conditions imposed upon coefficients $C_n^{(i)}$ imply that

$$\mathrm{Tr}\,\{\,\rho\,\} = \sum_n\ \rho_{nn} = \frac{1}{N}\sum_{i=1}^{N}\sum_n\ C_n^{(i)}\,C_n^{(i)*} = \frac{1}{N}\sum_{i=1}^{N} 1 = 1. \tag{11.11}$$ do11

This important result is called normalization of the density operator.

Relation (11.9) can be reexpressed with the aid of the introduced matrix

$$\langle\, A\,\rangle = \sum_{m,n}\ \rho_{mn}\,A_{nm} = \sum_m\ \,(\,\rho\,A\,)_{mm} = \mathrm{Tr}\,\{\,\rho\,A\,\}\,, \tag{11.12}$$ do12

where we use the rules of matrix multiplication. Evidently, the average value of the unit operator is equal 1. Eq.(11.12) for $A = 1$ gives

$$\langle\, 1\,\rangle = \sum_{m,n}\ \rho_{mn}\,\langle\,\varphi_n\,|\,1\,|\,\varphi_m\,\rangle = \sum_{m,n}\ \rho_{mn}\,\delta_{nm} = \mathrm{Tr}\,\{\,\rho\,\} = 1 \tag{11.13}$$ do13

as expected due to the normalization of the density operator.

The matrix ρ_{mn} is expressed by the expansion coefficients $C_n^{(i)}$ obtained in the energy representation (see (11.8)). Nevertheless, relation (11.12) indicates, that the average of an observable A is computed via the trace. We know that the trace of any operator is independent of the particular basis chosen in the Hilbert space. This suggest that operator ρ has more general sense, its representation by (11.10) is only one of the possible expansions.

Defining the density operator in terms of the state of the system (independently of the particular basis in the Hilbert space) we can write

$$\rho = \frac{1}{N}\sum_{i=1}^{N}\ |\,\psi^{(i)}\,\rangle\langle\,\psi^{(i)}\,|. \tag{11.14}$$ do14

We see that statistical information is still present in this expression. We have to show that this definition is equivalent to (11.10). Indeed, in energy representation we have

$$\langle\,\varphi_m\,|\,\rho\,|\,\varphi_n\,\rangle = \frac{1}{N}\sum_{i=1}^{N}\ \langle\,\varphi_m\,|\,\psi^{(i)}\,\rangle\langle\,\psi^{(i)}\,|\,\varphi_n\,\rangle = \frac{1}{N}\sum_{i=1}^{N}\ C_m^{(i)}\,C_n^{(i)\,*}, \tag{11.15}$$ do15

which clearly reproduces the previous definition (11.10).

We adopt (11.14) as the intuitive definition of the density operator. It includes the statistical information (in this case equivalence reflected by the factor $1/N$) about the subsystems constituting the whole one.

11.3 Some generalizations

We now proceed to generalize the introduced concept of the density operator. There are no restrictions on states $|\,\psi^{(i)}\,\rangle$. In general, they can be nonorthogonal (although it is

inconvenient), some of them may be the same (some atoms may be in the same quantum states), etc. Therefore, we generalize the definition (11.14) as follows

$$\rho = \sum_{\alpha} \, | \, \psi^{(\alpha)} \, \rangle \, P(\alpha) \, \langle \, \psi^{(\alpha)} \, | . \tag{11.16}$$ do16

In this case we do not sum over the atoms in the ensemble, but over the multiplicity of states which are accessible to the constituents of the ensemble. We require that

$$\sum_{\alpha} \, P(\alpha) \; = \; 1, \tag{11.17}$$ do17

which is necessary to preserve the statistical interpretation of $P(\alpha)$ as the probability of encountering the state $| \, \psi^{(\alpha)} \, \rangle$. In the following we will examine and discuss such an interpretation.

11.3.1 Projection operators

We write a projection operator on (normalized) state $| \, \chi \, \rangle$ as

$$\mathbf{P}_{\chi} = | \, \chi \, \rangle \langle \, \chi \, | , \tag{11.18}$$ do18

because $\mathbf{P}_{\chi} | \, \psi \, \rangle = | \, \chi \, \rangle \langle \, \chi \, | \, \psi \, \rangle$ which is a component of $| \, \psi \, \rangle$ in the direction of $| \, \chi \, \rangle$. It is straightforward to show that projection operator is idempotent, that is

$$\mathbf{P}_{\chi}^2 = | \, \chi \, \rangle \langle \, \chi \, | \, \chi \, \rangle \langle \, \chi \, | = | \, \chi \, \rangle \langle \, \chi \, | = \mathbf{P}_{\chi}. \tag{11.19}$$ do19

Expectation value of the projector $\mathbf{P}_{\chi}$ when the system is described by the state $| \, \psi \, \rangle$ is

$$\langle \, \mathbf{P}_{\chi} \, \rangle = \langle \, \psi \, | \, \mathbf{P}_{\chi} \, | \, \psi \, \rangle = \langle \, \psi \, | \, \chi \, \rangle \langle \, \chi \, | \, \psi \, \rangle = \langle \, \chi \, | \, \psi \, \rangle^* \langle \, \chi \, | \, \psi \, \rangle = | \langle \, \chi \, | \, \psi \, \rangle |^2. \tag{11.20}$$ do20

So it is the probability of finding the system in state $| \, \chi \, \rangle$ (while the system is prepared in state $| \, \psi \, \rangle$). We can say that it is the probability that state $| \, \chi \, \rangle$ is populated.

11.3.2 Application to density operator

Let us now consider the system described by the density operator ρ. According to (11.12) The expectation value of the observable A is given by the trace over the product $\rho \, A$. We recall that the trace is invariant with respect to the choice of the basis in which it is computed. Thus, it is unimportant which basis we employ. We will use the energy basis defined in (11.2). so, let us compute the expectation value of the projector $\hat{\pi}$

$$\begin{aligned} \overline{\langle \, \mathbf{P}_{\chi} \, \rangle} \; &= \; \mathrm{Tr} \, \{ \mathbf{P}_{\chi} \rho \} = \sum_{n} \, \langle \, \varphi_n \, | \, \chi \, \rangle \langle \, \chi \, | \, \rho \, | \, \varphi_n \, \rangle = \sum_{n} \, \langle \, \chi \, | \, \rho \, | \, \varphi_n \, \rangle \langle \, \varphi_n \, | \, \chi \, \rangle \\ &= \; \langle \, \chi \, | \, \rho \, | \, \chi \, \rangle, \end{aligned} \tag{11.21}$$

where we have used the completeness of states $| \, \varphi_n \, \rangle$. Eq. (11.21) tells us that the probability of finding the system, which is described by the density operator ρ, in state $| \, \chi \, \rangle$ is given just by the diagonal element of the density operator in the given state.

Now we use the definition (11.16) to find the probability of finding the system in state $|\,\psi^{(\beta)}\,\rangle$ – one of the states defining the density operator. Due to the discussed interpretation, we can use (11.21) with $|\,\chi\,\rangle$ replaced by $|\,\psi^{(\beta)}\,\rangle$. Then, we obtain

$$\begin{aligned}\langle\,\psi^{(\beta)}\,|\,\rho\,|\,\psi^{(\beta)}\,\rangle &= \sum_\alpha \langle\,\psi^{(\beta)}\,|\,\psi^{(\alpha)}\,\rangle\,P(\alpha)\,\langle\,\psi^{(\alpha)}\,|\,\psi^{(\beta)}\,\rangle \\ &= \sum_\alpha P(\alpha)\,\left|\langle\,\psi^{(\beta)}\,|\,\psi^{(\alpha)}\,\rangle\right|^2. \end{aligned} \tag{11.22}$$

If states $|\,\psi^{(\alpha)}\,\rangle$ are not orthonormal, there is no simple relation between populations (probabilities) $\langle\,\psi^{(\beta)}\,|\,\rho\,|\,\psi^{(\beta)}\,\rangle$ and statistical weights $P(\alpha)$. On the other hand, when states $|\,\psi^{(\alpha)}\,\rangle$ are orthonormal, then eq.(11.22) yields

$$\langle\,\psi^{(\beta)}\,|\,\rho\,|\,\psi^{(\beta)}\,\rangle = \sum_\alpha \delta_{\beta\alpha}\,P(\alpha) = P(\beta). \tag{11.23}$$ do23

We conclude, that $P(\alpha)$ can be interpreted as the probability of finding the system in state $|\,\psi^{(\alpha)}\,\rangle$ if these states (defining the density operator) are orthonormal. Frequently, $P(\alpha)$ is called the population of state $|\,\psi^{(\alpha)}\,\rangle$. If states $|\,\psi^{(\alpha)}\,\rangle$ are not orthogonal, then $P(\alpha)$ is the function (see (11.22)) which tells us with what statistical weight the state $|\,\psi^{(\alpha)}\,\rangle$ is represented in the ensemble specified by the density operator.

11.4 Properties of the density operator

The fundamental reason for the introduction of density operator is that when a system is not ideally prepared, we may describe its state as a statistical distribution over state vectors. Then, we can describe the state by specifying the probabilities w_i that the system is in the state vector $|\,i\,\rangle$. We write

$$\rho = \sum_i |\,i\,\rangle\,w_i\,\langle\,i\,|. \tag{11.24}$$ do24

By definition the density operator is Hermitian, and as such can be diagonalized, thus it can be written as above. The states $|\,i\,\rangle$ are then orthonormal and form a basis. Moreover the physical sense of the coefficient w_i follows from the given discussion – it is the population of state $|\,i\,\rangle$, or in other words, the probability of finding the system in state $|\,i\,\rangle$. We stress, that in the present context we do not specify the meaning of the states $|\,i\,\rangle$. They may refer to very different physical situations.

Having defined the density operator, we recall that the expectation value of an observable A is simply the classical average of the expectation values corresponding to each of the state vectors. So, the averaging procedure leads to the expectation value of the observable A

$$\begin{aligned}\langle\,A\,\rangle &= \mathrm{Tr}\left\{\hat{A}\rho\right\} = \sum_j \langle\,j\,|\,\hat{A}\rho\,|\,j\,\rangle = \sum_{i,j}\langle\,j\,|\,i\,\rangle w_i\langle\,i\,|\,\hat{A}\,|\,j\,\rangle \\ &= \sum_{i,j}\delta_{ij}w_i\langle\,i\,|\,\hat{A}\,|\,j\,\rangle = \sum_i w_i\langle\,i\,|\,\hat{A}\,|\,i\,\rangle. \end{aligned} \tag{11.25}$$

The trace is invariant with respect to the choice of the basis, so we have taken the most convenient one to compute it

Since the density operator is Hermitian, we know that w_i are real. We want to make sure that they are nonnegative. To do so, let us consider the projector $\hat{\pi}_k = |\,k\,\rangle\langle\,k\,|$ where state $|\,k\,\rangle$ belongs to the set forming the density operator as in (11.24). Then, we have

$$0 \;\geq\; \langle\,\mathbf{P}_k\,\rangle \;=\; \mathrm{Tr}\,\{\,\mathbf{P}_k\,\rho\,\} \;=\; \sum_j \langle\,j\,|\,\mathbf{P}_k\,\rho\,|\,j\,\rangle \;=\; \sum_j \langle\,j\,|\,k\,\rangle\langle\,k\,|\,\rho\,|\,j\,\rangle$$

$$= \sum_{j,i} \langle\,j\,|\,k\,\rangle\langle\,k\,|\,i\,\rangle\,w_i\,\langle\,i\,|\,j\,\rangle \;=\; \sum_{j,i} \delta_{jk}\,\delta_{ki}\,w_i\,\delta_{ij} \;=\; \sum_i \delta_{ik}\,w_i \;=\; w_k. \tag{11.26}$$

So coefficient w_i are indeed nonnegative. We already know that the density operator must be normalized, in the sense that

$$\mathrm{Tr}\,\{\,\rho\,\} \;=\; \sum_i w_i \;=\; 1. \tag{11.27}$$ do27

Since we have the conditions

$$w_i \geq 0, \qquad\qquad \sum_i w_i = 1, \tag{11.28}$$ do28

we conclude that the coefficients w_i can indeed be interpreted as probabilities of finding the system in states $|\,i\,\rangle$.

In many practically interesting cases we do not know exactly the state of the system. We are unable to give the full wave vector $|\,\psi(t)\,\rangle$. The only thing we can do, is to give the probability w_i, that our system is in the state $|\,i\,\rangle$. Then we describe the system with the density operator. This is connected with complicated phase relationships which are usually unknown. Hence we have to deal with incoherent mixture of states $|\,i\,\rangle$ each of which appears with certain statistical weight. This is the reason why computing the expectation value of the observable A we first have to find the quantum averages $\langle\,i\,|\,A\,|\,i\,\rangle$ and then average over the distribution w_i. This clearly leads to (11.25). Such a incoherent mixture of states is called a mixed state in contrast to the situation when the state vector $|\,\psi(t)\,\rangle$ carries all information. The latter situation – described by a state vector is called a pure state.

Lemma 11.1 *Assume that the set of numbers* $\{\,w_i\,\}$ *satisfies the conditions* $w_i \geq 0$, *and* $\sum_i\; w_i = 1$. *Then, we have* do29

1. $$\sum_i w_i^2 \leq 1 \tag{11.29a}$$

2. $$\sum_i w_i^2 = 1 \quad \textit{if, and only if} \quad w_i = \delta_{ik} \quad \textit{for certain index} \quad k. \tag{11.29b}$$

Proof. From our assumption it follows that

$$1 = \Big(\sum_i\; w_i\Big)\Big(\sum_j\; w_j\Big) = \sum_{i,j} w_i\,w_j = \sum_i\; w_i^2 \;+\; \sum_{i\neq j} w_i\,w_j. \tag{11.30}$$ do30

The second sum contains products of nonnegative numbers, so it is nonnegative. The first sum must be smaller or equal one. (11.29a) is thus proved.

Thesis (11.29b) means that the second sum in (11.30) is zero. If even two numbers, say w_i and w_j are nonzero, the second sum is greater than zero. The second sum can be zero if, and only if, just only one of the numbers w_k is nonzero. Then due to imposed conditions, this single nonzero number must be equal to 1. This shows the second part of the lemma. ■

This lemma is useful when proving the following fact. If the system is in the mixed state, then at least two of the probabilities w_i are nonzero. Then we have

$$\begin{aligned} \mathrm{Tr}\,\{\,\rho^2\,\} &= \sum_k \langle\, k \,|\, \rho^2 \,|\, k \,\rangle = \sum_{i,j,k} \langle\, k \,|\, i \,\rangle\, w_i \,\langle\, i \,|\, j \,\rangle\, w_j \,\langle\, j \,|\, k \,\rangle \\ &= \sum_{i,j,k} \delta_{ik}\,\delta_{ij}\,\delta_{jk}\, w_i\, w_j = \sum_{j,k} \delta_{kj} w_k\, w_j = \sum_k w_k^2 < 1, \end{aligned} \tag{11.31}$$

as it follows from the lemma for at least two w_i being nonzero.

When the system is in the pure state, then we can say that it is in state $|\, j \,\rangle$ with probability $w_i = \delta_{ij}$. Lemma ensures that in such a case we have $\mathrm{Tr}\,\{\,\rho^2\,\} = 1$. We conclude that the trace of the square of the density operator gives the criterion whether the system is in the mixed or pure state.

11.5 Equation of motion for density operator

Let some physical system be described by the density operator ρ. We know that the expectation value of an observable A may, in general, be time-dependent. In the Schrödinger picture the operators are time-independent, hence the time dependence of the average must be reflected in the time dependence of the density operator, so that we have

$$\langle\, A \,\rangle_t = \mathrm{Tr}\,\{\,\rho(t)\, A\,\}. \tag{11.32}$$ do32

Thus, in order to be able to make physical predictions we need an equation of motion for the density operator. The argumentation leading to such an equation can be as follows. The physical contents of the Schrödinger picture must be the same as that of the Heisenberg picture. The density operator is defined as the mixture of the projection on a certain set of states. In the Heisenberg picture the states are time independent, hence we may expect that in this picture the density operator is defined by the initial state of the system. The time dependence is shifted to the operators and the average (11.32) can be compared to the same average but computed in the Heisenberg picture

$$\langle\, A \,\rangle_t = \mathrm{Tr}\,\{\,\rho(t)\, A_S\,\} = \langle\, A_H(t) \,\rangle = \mathrm{Tr}\,\{\,\rho(t_0)\, A_H(t)\,\}. \tag{11.33}$$ do33

We know that in the Heisenberg picture the operators evolve as

$$A_H(t) = \mathbf{U}^\dagger(t,t_0)\, A_S\, \mathbf{U}(t,t_0), \tag{11.34}$$ do34

where $\mathbf{U}(t,t_0)$ is the evolution operator

$$\mathbf{U}(t,t_0) = \exp\left(-\frac{i}{\hbar}\, H\,(t-t_0)\right) \tag{11.35}$$ do35

with H being the Hamiltonian of the considered system. In (11.35) the hamiltonian is taken to be time-independent. There is, however, no problem to extend the theory to case with $H = H(t)$. Introducing (11.35) into (11.30) we get

$$\langle A \rangle_t \;=\; \mathrm{Tr}\,\{\,\rho(t)\,A_S\,\} \;=\; \mathrm{Tr}\,\{\,\rho(t_0)\;\mathbf{U}^\dagger(t,t_0)\,A_S\;\mathbf{U}(t,t_0)\,\} \tag{11.36}$$ do36

Invoking the cyclic property of the trace we immediately get

$$\mathrm{Tr}\,\{\,\rho(t)\,A_S\,\} \;=\; \mathrm{Tr}\,\{\;\mathbf{U}(t,t_0)\,\rho(t_0)\;\mathbf{U}^\dagger(t,t_0)\,A_S\,\}, \tag{11.37}$$ do37

and thus we can write

$$\rho(t) \;=\; \mathbf{U}(t,t_0)\,\rho(t_0)\;\mathbf{U}^\dagger(t,t_0). \tag{11.38}$$ do38

This result gives the sought time dependence of the density operator. By simple differentiation we can obtain the equation of motion for density operator

$$\begin{aligned} i\hbar\,\frac{\partial}{\partial t}\,\rho(t) \;&=\; \left(i\hbar\,\frac{\partial}{\partial t}\;\mathbf{U}(t,t_0)\right)\,\rho(t_0)\;\mathbf{U}^\dagger(t,t_0) \\ &\qquad -\;\mathbf{U}(t,t_0)\,\rho(t_0)\;\left(-i\hbar\,\frac{\partial}{\partial t}\;\mathbf{U}^\dagger(t,t_0)\right). \end{aligned} \tag{11.39}$$

The evolution operator satisfies Schrödinger equation, hence (11.39) is equivalent to

$$\begin{aligned} i\hbar\,\frac{\partial}{\partial t}\,\rho(t) \;&=\; H\;\mathbf{U}(t,t_0)\,\rho(t_0)\;\mathbf{U}^\dagger(t,t_0) \;-\; \mathbf{U}(t,t_0)\,\rho(t_0)\,H\;\mathbf{U}^\dagger(t,t_0) \\ &=\; H\,\rho(t) \;-\; \rho(t)\,H, \end{aligned} \tag{11.40}$$

Since the hamiltonian commutes with evolution operator and where in the last step we have used eq.(11.38) for time dependent density operator. The obtained equation of motion (called von Neumann equation) for the density operator is, thus, of the form

$$i\hbar\,\frac{\partial}{\partial t}\,\rho = [\,H,\;\rho\,] \tag{11.41}$$ do41

Von Neumann equation for the density operator (mixed state) is the equivalent of the Schrödinger equation for the state vector (pure state). It should be stressed that von Neumann equation correspond to the Schrödinger picture where the observables are time-independent. In the Heisenberg picture we have (11.33) where the density operator is specified by initial conditions and is time-independent.

11.6 Density operator for open system

The formalism of the density operator is especially useful for description of the open system. By an open system we understand a system consisting of two parts. The first part is labelled by $\mathcal{A}$ and the observations (measurements) we make, concern only this part of the total system. The second part, labelled by $\mathcal{B}$, is the surrounding which may exchange energy with the subsystem $\mathcal{A}$. Thus, the subsystem $\mathcal{B}$ is a heat reservoir, such as frequently discussed in the context of statistical mechanics. System $\mathcal{A}$ may, for example, corresponds to a vapor cell with some gas, while $\mathcal{B}$ is the surroundings which may exchange the heat with the gas (across the cell walls). Another example is an atom immersed in the radiation field.

The heat bath $\mathcal{B}$ is considered to be much larger than the system of interest $\mathcal{A}$. That is, the number of degrees of freedom of the bath is much larger. In many cases it is possible to assume that the bath is always in thermal equilibrium. Here, we discuss only the main features of reservoir. In practical applications one usually needs to specify the properties of system $\mathcal{B}$ in more detail.

In general, the state of the joint system $\mathcal{A}+\mathcal{B}$ is described by a density operator ρ_{AB}. Let us, however, assume that the situation is simpler and that the Joint system is in a pure state, given by a vector $|\,\Psi\,\rangle$ This state can always be expanded on an orthonormal basis of states $\{|\,\xi_n\,\rangle\}$ of $\mathcal{B}$

$$|\,\Psi\,\rangle = \sum_n\, C_n\,|\,\psi_n\,\rangle\otimes|\,\xi_n\,\rangle, \tag{11.42}$$ do42

where the $|\,\psi_n\,\rangle$ are normalized (but not necessarily orthogonal) states of subsystem $\mathcal{A}$. The coefficients C_n are the probability amplitudes that the bath $\mathcal{B}$ is in its basis state $|\,\xi_n\,\rangle$, which correlates with the normalized state $|\,\psi_n\,\rangle$ of the subsystem $\mathcal{S}$. The normalization of the joint state $|\,\Psi\,\rangle$ is as follows

$$\begin{aligned} 1 &= \langle\,\Psi\,|\,\Psi\,\rangle = \sum_{m,n}\Big(\,\langle\,\psi_m\,|\otimes\langle\,\psi_m\,|\,C_m^*\Big)\Big(C_n\,|\,\psi_n\,\rangle\otimes|\,\xi_n\,\rangle\,\Big) \\ &= \sum_m\sum_n\, C_m^*\,C_n\,\langle\,\xi_m\,|\,\xi_n\,\rangle\,\langle\,\psi_m\,|\,\psi_n\,\rangle = \sum_m\sum_n\, C_m^*\,C_n\,\delta_{mn}\,\langle\,\psi_m\,|\,\psi_n\,\rangle \\ &= \sum_m\,\,|\,C_m\,|^2\,\,\langle\,\psi_m\,|\,\psi_m\,\rangle = \sum_m\,\,|\,C_m\,|^2\,. \end{aligned} \tag{11.43}$$

Performing this computation we note that the states of the bath, that is states $|\,\xi_n\,\rangle$ and the states $|\,\psi_n\,\rangle$ of subsystem $\mathcal{S}$ are independent what is indicated by a tensor product. Hence, we take separate scalar products, corresponding to two different Hilbert spaces. We again stress, that states $|\,\psi_n\,\rangle$ of $\mathcal{A}$ are only normalized, no assumption is made on their orthogonality. Finally, the result (11.43) shows that interpretation of coefficients C_n as probability amplitudes is indeed correct.

Let us now consider a measurement of an observable $A\otimes\hat{\mathbf{1}}_B$ performed on subsystem $\mathcal{A}$ only. By such a measurement we understand that the operator A operates only on states of $\mathcal{A}$. The expectation value of A, due to orthonormality of the basis states $\{\,|\,\xi_n\,\rangle\,\}$, can be then found to be

$$\langle\,A\,\rangle = \langle\,\Psi\,|\,A\,|\,\Psi\,\rangle = \sum_n\,\,|C_n|^2\,\,\langle\,\psi_n\,|\,A\,|\,\psi_n\,\rangle. \tag{11.44}$$ do44

This relation is obviously equivalent to

$$\langle A \rangle = \mathrm{Tr}_{AB} \left\{ \rho_{AB} A \otimes \hat{\mathbf{1}}_B \right\}, \tag{11.45}$$ do45

with $\rho_{AB} = |\Psi\rangle\langle\Psi|$ being the density operator for the joint (total) system $\mathcal{S}+\mathcal{B}$, while Tr_{AB} indicates that we take the trace with respect to the states of both subsystems. The density operator ρ_{AB} contains information on both parts of the whole system. However, we are not interested in the heat reservoir. Therefore, we define the reduced density operator ρ_A which contains data only on the relevant subsystem $\mathcal{A}$. We define ρ_A as

$$\rho_A = \mathrm{Tr}_B \{ \rho_{AB} \} = \mathrm{Tr}_B \{ |\Psi\rangle\langle\Psi| \}. \tag{11.46}$$ do46

Then, using (11.42) we calculate the trace with respect to the basis vectors $\{|\xi_k\rangle\}$ of the subsystem $\mathcal{B}$. We get

$$\begin{aligned}
\rho_A &= \mathrm{Tr}_B \left\{ \sum_{m,n} C_n |\psi_n\rangle \otimes |\xi_n\rangle\langle\xi_m| \otimes \langle\psi_m| C_m^* \right\} \\
&= \sum_{k,m,n} C_m^* C_n \langle\xi_k| \Big(|\psi_n\rangle \otimes |\xi_n\rangle\langle\xi_m| \otimes \langle\psi_m| \Big) |\xi_k\rangle \\
&= \sum_{k,m,n} C_m^* C_n |\psi_n\rangle\langle\xi_k|\xi_n\rangle\langle\xi_m|\xi_k\rangle\langle\psi_m| \;=\; \sum_{k,m,n} C_m^* C_n |\psi_n\rangle \delta_{kn}\delta_{mk} \langle\psi_m| \\
&= \sum_{m,n} C_m^* C_n |\psi_n\rangle \delta_{mn} \langle\psi_m| \\
&= \sum_n |\psi_n\rangle |C_n|^2 \langle\psi_n|.
\end{aligned} \tag{11.47}$$

The advantage of the reduced density operator is that in order to find expectation value of the observable A concerning the subsystem $\mathcal{A}$ only, we can write

$$\langle A \rangle = \mathrm{Tr}_A \{ \rho_A A \}, \tag{11.48}$$ do48

where Tr_A indicates that we compute the trace only with respect to the states of the subsystem $\mathcal{A}$. To find the trace in (11.48) we introduce a basis $\{|\varphi_a\rangle\}$ in the Hilbert space of states of the subsystem $\mathcal{A}$. Then, we have

$$\begin{aligned}
\langle A \rangle &= \mathrm{Tr}_A \{ \rho_A A \} = \sum_a \langle\varphi_a| A \rho_A |\varphi_a\rangle \\
&= \sum_a \sum_n \langle\varphi_a| A |\psi_n\rangle |C_n|^2 \langle\psi_n|\varphi_a\rangle \\
&= \sum_a \sum_n |C_n|^2 \langle\psi_n|\varphi_a\rangle\langle\varphi_a| A |\psi_n\rangle \\
&= \sum_n |C_n|^2 \langle\psi_n| A |\psi_n\rangle
\end{aligned} \tag{11.49}$$

Comparison of (11.49) and (11.44) shows that the reduced density operator is indeed sufficient to find necessary information about measurements on subsystem $\mathcal{A}$ only. The structure of the density operator ρ_A as in (11.47) is similar to that given in Eq.(11.15).

The difference is that the statistical probabilities are now replaced by quantum-mechanical probabilities $|\,C_n\,|^2$. We recall that the amplitudes C_n are the probability amplitudes that the reservoir $\mathcal{B}$ is in its basis state $|\,\xi_n\,\rangle$, which correlates with the normalized state $|\,\psi_n\,\rangle$ of the observed subsystem $\mathcal{S}$ which is of interest.

The discussed case concerns a pure state $|\,\Psi\,\rangle$ of the joint system. Similar considerations can be also done for a more general case, when the joint system is in the mixed state. It is, however, worth noting that even in this simple case the description of the relevant subsystem $\mathcal{S}$ must be done with density operator. Although the joint system is in the pure state, the subsystem is in the mixed state described by the reduced density operator ρ_A which is defined in eq.(11.47). Therefore, to describe subsystem $\mathcal{A}$ only we need reduced density matrix ρ_A. The only exception occurs, when the joint system happens to be in state for which $C_n = \delta_{nk}$, that is when all terms except one in combination (11.42) are zeroes.

11.7 Evolution of the reduced density operator

11.7.1 Introductory remarks

We are interested in the evolution of the subsystem $\mathcal{A}$ which is coupled to the heat reservoir $\mathcal{B}$. This evolution cannot be described by the von Neumann equation for the subsystem $\mathcal{A}$ alone due to the influence of the interaction with $\mathcal{B}$. Therefore, we must start studying the evolution of reduced density operator ρ_A with the evolution of the whole system $\mathcal{A}+\mathcal{B}$, which is assumed to be closed. The total density operator ρ_{AB} obeys the von Neumann equation (11.41), where the total Hamiltonian of the combined system can be separated as

$$H = H_0 + V_{AB}, \qquad \text{with} \qquad H_0 = H_A \otimes \hat{\mathbf{1}}_B + \hat{\mathbf{1}}_A \otimes H_B, \tag{11.50}$$ do50

where H_A and H_A describe the free evolution of subsystems $\mathcal{A}$ and $\mathcal{B}$, whereas V_{AB} is their interaction Hamiltonian. We note that the Hamiltonian H_A operates only on states $|\,\psi_n\,\rangle$ of the subsystem $\mathcal{A}$, while H_B only on the state vectors $|\,\xi_n\,\rangle$ of the reservoir $\mathcal{B}$. The von Neumann equation for the total system reads

$$i\hbar\,\frac{d}{dt}\;\rho_{AB}(t) = [\,H,\;\rho_{AB}(t)\,] \tag{11.51}$$ do51

This is our starting point for finding the evolution equation for the reduced density operator for the system of interest $\rho_A = \mathrm{Tr}_B\{\rho_{AB}\}$.

11.7.2 Transformation to interaction picture and formal integration

The main advantage of the interaction picture is that the free time evolution (due to free Hamiltonian H_0) is transformed away. The remaining time evolution is entirely due to the interaction. Therefore we take the full density operator $\rho_{AB}(t)$ in the Schrödinger picture and we transform it to the interaction picture

$$\widetilde{\varrho}_{AB}(t) = e^{iH_0 t/\hbar}\;\rho_{s+b}(t)\;e^{-iH_0 t/\hbar}, \tag{11.52}$$ do52

or equivalently

$$\rho_{AB}(t) = e^{-iH_0 t/\hbar}\, \widetilde{\varrho}_{AB}(t)\, e^{iH_0 t/\hbar}, \tag{11.53}$$ do53

where tilde denotes the interaction picture.

Before proceeding further with the problem of evolution, let us note that the definition (11.46) of the reduced density operator implies (in the Schrödinger picture)

$$\rho_A(t) = \mathrm{Tr}_b \left\{ e^{-i(H_A\otimes H_B)t/\hbar}\, \widetilde{\varrho}_{AB}(t)\, e^{i(H_A\otimes H_B)t/\hbar} \right\}. \tag{11.54}$$ do54

It is not obvious that we can simply use the cyclic property of the trace. However, we can. The reason is that $\mathcal{A}$ variables are not affected by Tr_B. Free Hamiltonians H_A and H_B act in two different Hilbert spaces, so they commute, hence we can write

$$e^{\pm i(H_A\otimes H_B)t/\hbar} = e^{\pm iH_A t/\hbar} \otimes e^{\pm H_B t/\hbar}. \tag{11.55}$$ do55

In (11.54) we compute the trace with respect to reservoir variables only, hence due to (11.55) we can write

$$\rho_A(t) = e^{-iH_A t/\hbar}\, \mathrm{Tr}_B \left\{ e^{-iH_B t/\hbar}\, \widetilde{\varrho}_{AB}(t)\, e^{iH_B t/\hbar} \right\} e^{iH_A t/\hbar}. \tag{11.56}$$ do56

Using the cyclic property of the trace, we obtain

$$e^{iH_A t/\hbar}\, \rho_A(t)\, e^{-iH_A t/\hbar} = \mathrm{Tr}_b \left\{ \widetilde{\varrho}_{AB}(t) \right\}. \tag{11.57}$$ do57

We easily see that the left-hand side represents the reduced density operator in the interaction picture (since it depends solely on the variables of the subsystem $\mathcal{A}$), we can say that the variables of reservoir "are traced out" So we have

$$\widetilde{\varrho}_A(t) = \mathrm{Tr}_B \left\{ \widetilde{\varrho}_{AB}(t) \right\}. \tag{11.58}$$ do58

Hence the relation (11.46) is formally identical to (11.58). The connection between the reduced density operator and the total one is the same in both pictures.

Now, we transform the von Neumann equation (11.51) into the interaction picture. We insert (11.52) into the lhs, and we use (11.50) in the rhs. By differentiation we get

$$\begin{aligned} i\hbar \Big\{ \left(-\frac{i}{\hbar} H_0 \right) e^{-iH_0 t/\hbar}\, \widetilde{\varrho}_{AB}(t)\, e^{iH_0 t/\hbar} \;+\; e^{-iH_0 t/\hbar} \left(\frac{d}{dt}\, \widetilde{\varrho}_{AB}(t) \right) e^{iH_0 t/\hbar} \\ + e^{-iH_0 t/\hbar}\, \widetilde{\varrho}_{AB}(t) \left(\frac{i}{\hbar} H_0 \right) e^{iH_0 t/\hbar} \Big\} = \\ = \;\; (\, H_0 + V_{AB}\,)\, e^{-iH_0 t/\hbar}\, \widetilde{\varrho}_{AB}(t)\, e^{iH_0 t/\hbar} \;-\; e^{-iH_0 t/\hbar}\, \widetilde{\varrho}_{AB}(t)\, e^{iH_0 t/\hbar} (\, H_0 + V_{AB}) \end{aligned} \tag{11.59}$$ do51 do52 do50

Since H_0 obviously commutes with exponential operators the terms containing H_0 cancel out. Then, we multiply this equation by $e^{iH_0 t/\hbar}$ at the left and by $e^{-iH_0 t/\hbar}$ at the right. Hence, we get

$$i\hbar\, \frac{d}{dt}\, \widetilde{\varrho}_{AB}(t) \;=\; e^{iH_0 t/\hbar}\, V_{AB}\, e^{-iH_0 t/\hbar}\, \widetilde{\varrho}_{AB}(t) \;-\; \widetilde{\varrho}_{AB}(t)\, e^{iH_0 t/\hbar}\, V_{AB}\, e^{-iH_0 t/\hbar}. \tag{11.60}$$ do60

Thus, and we arrive at

$$\frac{d}{dt}\ \widetilde{\varrho}_{AB}(t)\ =\ \frac{1}{i\hbar}\ \Big[\ \widetilde{V}_{AB}(t),\ \widetilde{\varrho}_{AB}(t)\ \Big]\,, \tag{11.61}$$ do61

where $\widetilde{V}_{AB}(t)$ is the interaction hamiltonian in the interaction picture

$$\widetilde{V}_{AB}(t)\ =\ e^{iH_0t/\hbar}\,V_{AB}\,e^{-iH_0t/\hbar}. \tag{11.62}$$ do62

Equation (11.61) is the interaction picture version of the von Neumann equation for the density operator of the full system $\mathcal{A}+\mathcal{B}$. We shall investigate it further to extract evolution equation for the reduced density operator $\widetilde{\varrho}_A$ for the subsystem of interest.

In the next step we formally integrate the von Neumann equation (11.61). This yields

$$\widetilde{\varrho}_{AB}(t)\ =\ \widetilde{\varrho}_{AB}(t_0)\ +\ \frac{1}{i\hbar}\int_{t_0}^{t}dt_1\ \Big[\ \widetilde{V}_{AB}(t_1),\ \widetilde{\varrho}_{AB}(t_1)\ \Big]\,, \tag{11.63}$$ do63

where $\widetilde{\varrho}_{AB}(t_0)$ is the initial condition.

The result of the iteration is the substituted into the von Neumann equation, and we get

$$\begin{aligned}\frac{d}{dt}\ \widetilde{\varrho}_{AB}(t)\ &=\ \frac{1}{i\hbar}\ \Big[\ \widetilde{V}_{AB}(t),\ \widetilde{\varrho}_{AB}(t_0)\ \Big]\\ &\quad+\ \left(\frac{1}{i\hbar}\right)^2\int_{t_0}^{t}dt_1\Big[\ \widetilde{V}_{AB}(t),\ \big[\ \widetilde{V}_{AB}(t_1),\ \widetilde{\varrho}_{AB}(t_1)\ \big]\Big].\end{aligned} \tag{11.64}$$

Taking the trace Tr_B which commutes with time derivative, we obtain an equation for the reduced density operator

$$\begin{aligned}\frac{d}{dt}\ \widetilde{\varrho}_{A}(t)\ &=\ \frac{1}{i\hbar}\,\mathrm{Tr}_B\Big\{\big[\ \widetilde{V}_{AB}(t),\ \widetilde{\varrho}_{AB}(t_0)\ \big]\Big\}\\ &\quad+\ \left(\frac{1}{i\hbar}\right)^2\int_{t_0}^{t}dt_1\ \mathrm{Tr}_B\Big\{\Big[\ \widetilde{V}_{AB}(t),\ \big[\ \widetilde{V}_{AB}(t_1),\ \widetilde{\varrho}_{AB}(t_1)\ \big]\Big]\Big\}.\end{aligned} \tag{11.65}$$

This is exact equation. However, to get useful information we must introduce several simplifying assumptions which will yield a tractable and closed equation for $\rho_A(t)$. This is so, because right-hand side of (11.65) still contains the full density operator $\widetilde{\varrho}_{AB}(t_1)$.

Let us note that there is also another another possibility to analyze von Neumann equation (11.61). Relation (11.63) can be treated as the first iteration. Then we rewrite it as

$$\widetilde{\varrho}_{AB}(t_1)\ =\ \widetilde{\varrho}_{AB}(t_0)\ +\ \frac{1}{i\hbar}\int_{t_0}^{t_1}dt_2\ \Big[\ \widetilde{V}_{AB}(t_2),\ \widetilde{\varrho}_{AB}(t_2)\ \Big]\,. \tag{11.66}$$ do66

Next, we insert (11.66) again into (11.63) and we obtain

$$\begin{aligned}\frac{d}{dt}\ \widetilde{\varrho}_{AB}(t)\ &=\ \widetilde{\varrho}_{AB}(t_0)\ +\ \frac{1}{i\hbar}\ \Big[\ \widetilde{V}_{AB}(t),\ \widetilde{\varrho}_{AB}(t_0)\ \Big]\\ &\quad+\ \left(\frac{1}{i\hbar}\right)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\Big[\ \widetilde{V}_{AB}(t_1),\ \big[\ \widetilde{V}_{AB}(t_2),\ \widetilde{\varrho}_{AB}(t_2)\ \big]\Big].\end{aligned} \tag{11.67}$$

We can apply this procedure once more. We put t_2 in (11.66) instead of t_1 and insert it into (11.67) and we get

$$\begin{aligned}\frac{d}{dt}\,\widetilde{\varrho}_{AB}(t) &= \widetilde{\varrho}_{AB}(t_0) + \frac{1}{i\hbar}\Big[\,\widetilde{V}_{AB}(t),\,\widetilde{\varrho}_{AB}(t_0)\,\Big] \\ &+ \left(\frac{1}{i\hbar}\right)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\Big[\,\widetilde{V}_{AB}(t_1),\,\big[\,\widetilde{V}_{AB}(t_2),\,\widetilde{\varrho}_{AB}(t_0)\,\big]\Big] \\ &+ \left(\frac{1}{i\hbar}\right)^3\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\int_{t_0}^{t_2}dt_3\Big[\,V_{AB}(t_1),\Big[\,\widetilde{V}_{AB}(t_2),\,\big[\,\widetilde{V}_{AB}(t_3),\,\widetilde{\varrho}_{AB}(t_3)\,\big]\Big]\Big]\end{aligned} \tag{11.68}$$

This third-order equation is clearly exact. The iteration procedure can be carried out farther to fourth, fifth orders and so on. It can be truncated, for example at the second order, then Eq.(11.67) is taken as a second order approximation to the exact von Neumann equation and it is used in practical calculations.

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Chapter 12

Master Equation

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12.1 Evolution of the reduced density operator

12.1.1 Introductory remarks

We consider a physical system which consists of two parts $\mathcal{A}$ and $\mathcal{B}$. We are interested only in what happens in part $\mathcal{A}$ which usually is much smaller than part $\mathcal{B}$, which we will call a reservoir (environment). We will assume that the whole systemy, that $\mathcal{A}+\mathcal{B}$ is closed. The total hamiltonian can be written as

$$H_{AB} = H_0 + V_{AB}, \tag{12.1}$$ me01a

where H_0 is the free-evolution hamiltonian

$$H_0 \;=\; H_A \otimes \mathbf{1}_B \;+\; \mathbf{1}_A \otimes H_B, \tag{12.2}$$ me01b

where H_A and H_B describe the free, independent evolution of each of the subsystems $\mathcal{A}$ and $\mathcal{B}$. V_{AB} is the hamiltonian describing the interaction between two parts. Some additional assumptions concerning both subsystems will be introduced when necessary.

As it is well-known, the interaction between two (sub)systems usually leads to mixed states, even if the initial state is a pure one. Therefore, investigating the joint system $\mathcal{A}+\mathcal{B}$ we will use the density operator $\rho_{AB}(t)$. On the other hand, the interesting (relevant) subsystem $\mathcal{A}$ is then described by the reduced density operator

$$\rho_A(t) = \mathrm{Tr}_B\{\rho_{AB}(t)\}. \tag{12.3}$$ me03

Evolution of the state ρ_{AB} of the whole system $\mathcal{A}+\mathcal{B}$ is governed by von Neumann equation

$$i\hbar\,\frac{d}{dt}\;\rho_{AB}(t) = \big[\, H_{AB},\, \rho_{AB}(t)\,\big], \tag{12.4}$$ me04

which, in the interaction picture is of the form

$$\frac{d}{dt}\;\widetilde{\varrho}_{AB}(t) \;=\; \frac{1}{i\hbar}\,\big[\,\widetilde{V}_{AB}(t),\,\widetilde{\varrho}_{AB}(t)\,\big], \tag{12.5}$$ me05

where, we obviously denoted

$$\widetilde{\varrho}_{AB}(t) \;=\; e^{iH_0t/\hbar}\,\rho_{AB}(t)\,e^{-iH_0t/\hbar}, \qquad \widetilde{V}_{AB}(t) \;=\; e^{iH_0t/\hbar}\,V_{AB}\,e^{-iH_0t/\hbar}, \tag{12.6}$$ me06

with H_0 given in Eq.(12.2). Reduction of the density operator (as in (12.3)) is preserved in the interaction picture

$$\widetilde{\varrho}_A(t) \;=\; \mathrm{Tr}_B\{\widetilde{\varrho}_{AB}(t)\}. \tag{12.7}$$

Additional information on interaction picture can be found in auxiliary sections.

So we start with von Neumann equation (12.5). Formal integration yields the following expression

$$\widetilde{\varrho}_{AB}(t+\Delta t) \;=\; \widetilde{\varrho}_{AB}(t) \;+\; \frac{1}{i\hbar}\int_t^{t+\Delta t} dt_1\,\big[\,\widetilde{V}_{AB}(t_1),\,\widetilde{\varrho}_{AB}(t_1)\,\big], \tag{12.8}$$

which gives the density operator at a later moment $t+\Delta t$, while the initial one at a moment t is assumed to be known. Iterating further and denoting

$$\Delta\widetilde{\varrho}_{AB}(t) \;=\; \widetilde{\varrho}_{AB}(t+\Delta t) \;-\; \widetilde{\varrho}_{AB}(t), \tag{12.9}$$

we obtain

$$\begin{aligned}\Delta\widetilde{\varrho}_{AB}(t) \;=\;& \left(\frac{1}{i\hbar}\right)\int_t^{t+\Delta t} dt_1\,\big[\,\widetilde{V}_{AB}(t_1),\,\widetilde{\varrho}_{AB}(t)\,\big] \\ &+\;\left(\frac{1}{i\hbar}\right)^2\int_t^{t+\Delta t} dt_1\int_t^{t_1} dt_2\,\big[\,\widetilde{V}_{AB}(t_1),\,\big[\,\widetilde{V}_{AB}(t_2),\,\widetilde{\varrho}_{AB}(t)\,\big] \\ &+\;\left(\frac{1}{i\hbar}\right)^3\int_t^{t+\Delta t} dt_1\int_t^{t_1} dt_2\int_t^{t_2} dt_3\,\big[\,\widetilde{V}_{AB}(t_1),\,\big[\,\widetilde{V}_{AB}(t_2),\big[\,\widetilde{V}_{AB}(t_3)\,\widetilde{\varrho}_{AB}(t_3)\,\big]\end{aligned} \tag{12.10}$$

Higher order iterations will contain fourfold, etc., integrals and commutators. Let us note that in the last term we have time ordering $t+\Delta t \geq t_1 \geq t_2 \geq t_3 \geq t$. The above equation is rigorous, no approximations have been made.

12.1.2 Weak-coupling approximation

Weak-coupling approximation consists in retaining the terms up to the second order in interaction hamiltonian. Higher order terms are then neglected. Thus, we remain with

$$\begin{aligned}\Delta\widetilde{\varrho}_{AB}(t) \;=\;& \left(\frac{1}{i\hbar}\right)\int_t^{t+\Delta t} dt_1\,\big[\,\widetilde{V}_{AB}(t_1),\,\widetilde{\varrho}_{AB}(t)\,\big] \\ &+\left(\frac{1}{i\hbar}\right)^2\int_t^{t+\Delta t} dt_1\int_t^{t_1} dt_2\,\big[\,\widetilde{V}_{AB}(t_1),\,\big[\,\widetilde{V}_{AB}(t_2),\,\widetilde{\varrho}_{AB}(t)\,\big].\end{aligned} \tag{12.11}$$

Alternatively, we can say that the obtained equation is valid in the second-order perturbation theory. Such an approximation requires a justification. The necessary justification will be presented in the auxiliary sections, now we focus on further steps of the derivation.

Reduction of the operator $\widetilde{\varrho}_{AB}(t)$ poses no difficulties. Tracing over the reservoir variables (subsystem $\mathcal{B}$) we obtain

$$\Delta\widetilde{\varrho}_A(t) \;=\; \left(\frac{1}{i\hbar}\right)\int_t^{t+\Delta t} dt_1\ \mathrm{Tr}_B\big[\,\widetilde{V}_{AB}(t_1),\ \widetilde{\varrho}_{AB}(t)\,\big]$$
$$+\ \left(\frac{1}{i\hbar}\right)^2\int_t^{t+\Delta t} dt_1\int_t^{t_1} dt_2\ \mathrm{Tr}_B\big[\,\widetilde{V}_{AB}(t_1),\ \big[\,\widetilde{V}_{AB}(t_2),\ \widetilde{\varrho}_{AB}(t)\,\big]. \qquad (12.12)$$

This expression has certain drawback. The point is that the commutators contain full density operator $\widetilde{\varrho}_{AB}(t)$, and not the interesting (relevant) reduced one $\widetilde{\varrho}_A(t)$. To proceed, we need some more assumptions and approximations.

One more remark seems to be in place. Subsequant iterations leading to Eq. (12.10) are rigorous. In equation (12.12) – which is approximate – there occurs the operator $\rho_{AB}(t)$, taken at the initial moment. The last term in the exact equation (12.10) contains $\widetilde{\varrho}_{AB}$ for moments earlier than the current moment $t+\Delta t$, but later than the initial instant t. This means that we neglect the influence of the "history" on the present moment. We shall return to the discussion of this point.

12.1.3 Neglecting the intial correlatios

The key role in our consideration is played by the assumption that there are to distinct time scales. The first one is specified by time τ_B – typical time during which the internal correlations in the reservoir $\mathcal{B}$ exist. This will discussed in more detail later. Here we will only say that time τ_B is such a time, that when it elapses, the state of the resrevoir is practically idependent of is initial state. The second time scale is provide by time T_A. It is a time which characterises evolution (changes) of the operator $\widetilde{\varrho}_A(t)$ which is due to the interaction with resrvoir, and which may be specified by the relation

$$\frac{\Delta\widetilde{\varrho}_A(t)}{\Delta t}\ \sim\ \frac{1}{T_A}\,\widetilde{\varrho}_A(t). \qquad (12.13)$$

Time T_A may be called the characteristic relaxation time of subsystem ukadu $\mathcal{A}$. Let us note that we are speaking about interaction – the interaction picture we employ is thus, particularly useful. We make no statements about the rate of the free evolutions of ρ_A (in the Schrödinger picture), which is governed by hamiltonian H_A. Usually, the characteristic times of free evolution (the times of the order of $\tau_A \sim \langle H_A\rangle_A/\hbar$) are typically much shorter that T_A describing the interaction between subsystems.

Now we assume that the introduced time scale satisfy the requirement

$$\tau_B \ll \Delta t \ll T_A. \qquad (12.14)$$

We have a fast scale (small τ_B) determining the decay of correlations within the reservoir and the second – much slower – scale defined by relatively long relaxation time T_A, characterizing the interaction between the two parts of the entire physical system. This

may be phrased differently. We have assumed that the interaction is weak. Let V denote the average "strength" of this interaction. Uncertainty principle states that

$$VT_A \sim \hbar \quad \Longrightarrow \quad T_A \sim \frac{\hbar}{V}. \tag{12.15}$$ me19

The condition $\tau_B \ll T_A$ implies that

$$\tau_B \ll T_A \sim \frac{\hbar}{V} \quad \Longrightarrow \quad \frac{V\tau_B}{\hbar} \ll 1. \tag{12.16}$$ me20

Still in other words we can say that spectral widths are the reciprocals of characteristic times, so the condition $\tau_B \ll T_A$ means that the spectral width of the reservoir must be much larger than the spectral width of the interaction between subsystem $\mathcal{A}$ with reservoir. Further discussion and justification of our approximations is postponed to other section. Here we focus on the derivation of the master equation.

The adopted assumption $\tau_B \ll T_A$ allows us to make the following approximation. Initial density operator for the whole system $\mathcal{A}+\mathcal{B}$ can always be written as

$$\widetilde{\varrho}_{AB}(t) \;=\; \widetilde{\varrho}_A(t) \otimes \widetilde{\varrho}_B(t) \;+\; \widetilde{\varrho}_{corel}(t), \tag{12.17}$$ me21

where $\widetilde{\varrho}_A(t)$ and $\widetilde{\varrho}_B(t)$ are the initial reduced density operators for two subsystems. The state of the whole system consists of a factorizable part $\widetilde{\varrho}_A(t) \otimes \widetilde{\varrho}_B(t)$ and the entangled part $\widetilde{\varrho}_{corel}(t)$, which describes the correlations between the subsystems and which are due to the interaction. Equation (12.12) gives us the change $\Delta\widetilde{\varrho}_A(t) = \widetilde{\varrho}_A(t+\Delta t) - \widetilde{\varrho}_A(t)$, hence informs us about changes occuring in te time interval Δt. Assumption that $\tau_B \ll \Delta t$ allows us to neglect the mentioned correlations. As previously, we postpone the discusion for later sections. At present, we assume that

me16x

$$\widetilde{\varrho}_{AB}(t) \;\approx\; \widetilde{\varrho}_A(t) \otimes \widetilde{\varrho}_B(t). \tag{12.18}$$ me23

By assumption the reservoir (environment) is very large, it correlation time is very short, so the resrvoir's relaxation is very fast. We may say that before any significant changes occur in subsystem $\mathcal{A}$, the resevoir would have enough time to reach thermodynamic equilibrium. As it is known from statistical physics such state is given as

$$\bar{\sigma}_B = \sum_z p(z) |\, z\,\rangle\langle\, z\,| \qquad \text{where} \qquad p(z) = \frac{1}{\mathbb{Z}} \exp\left(-\frac{E_z}{k_B T}\right). \tag{12.19}$$ me23b

The quantity Z is a partition sum

$$\mathbb{Z} \;=\; \sum_z \exp\left(-\frac{E_z}{k_B T}\right). \tag{12.20}$$ me23c

States $|\, z\,\rangle$ are the eigenstates of the reservoir hamiltonian and they satisfy the relation $H_B\,|\, z\,\rangle = E_z|\, z\,\rangle$. At thermodynamic equilibrium the system does not change its state. It means that the density operator $\bar{\sigma}_B$ satisfies the requirement

$$\big[\, \bar{\sigma}_B,\; H_B \,\big] \;=\; 0, \tag{12.21}$$ me23d

so we can say that operator $\bar{\sigma}_B$ is stationary – does not change in time. Obviously the states $|\, z\,\rangle$ are common eigenstates of $\bar{\sigma}_B$ and H_B. This commutation relation also ensures that the reduced density operator of the reservoir is equal to $\bar{\sigma}_B$ both in Schrödinger and interaction pictures. Hence, operator $\widetilde{\varrho}_B(t)$ appearing in Eq.(12.18) is simply replaced by $\bar{\sigma}_B$. Therefore, in Eq.(12.12) we make the replacement $\widetilde{\varrho}_{AB} = \widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B$. So we have now

$$\Delta\widetilde{\varrho}_A(t) \;=\; \left(\frac{1}{i\hbar}\right) \int_t^{t+\Delta t} dt_1 \; \mathrm{Tr}_B\big[\, \widetilde{V}_{AB}(t_1),\; \widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B \,\big]$$
$$+ \left(\frac{1}{i\hbar}\right)^2 \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \; \mathrm{Tr}_B\big[\, \widetilde{V}_{AB}(t_1),\; \big[\, \widetilde{V}_{AB}(t_2),\; \widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B \,\big], \qquad (12.22)$$

which will be analyzed further.

12.2 Interaction hamiltonian and its properties

12.2.1 The form of $\widetilde{V}_{AB}(t)$

Our next assumption concerns the shape of the interaction hamiltonian which will be taken as

$$V_{AB} \;=\; \sum_\alpha \; A_\alpha \otimes X_\alpha \;=\; \sum_\alpha \; A_\alpha^\dagger \otimes X_\alpha^\dagger, \qquad (12.23)$$ me30

where A_α are operators which act in the space of the states of subsystem $\mathcal{A}$, while operators X_α correspond to space of the reservoir's states. Operators appearing in the definition (12.23) nedd not be hermitian (each one separately) The hamiltonian V_{AB} must ber hermitian. That is why we have written the second equality. We can say that to each nonhermitian term $A_\alpha \otimes X_\alpha$ corresponds the term $A_\alpha^\dagger \otimes X_\alpha^\dagger$, and the latter appears in the sum V_{AB}, but with another number. In auxiliary sections we will show that it is not any significant limitation. It is only important that the whole hamiltonian V_{AB} must be hermitian.

Operators A_α i X_α act in different spaces so they are independent and commute. In the interaction picture we immediately have

$$\widetilde{V}_{AB}(t) \;=\; \sum_\alpha \; \widetilde{A}_\alpha(t) \otimes \widetilde{X}_\alpha(t) \;=\; \sum_\alpha \; \widetilde{A}_\alpha^\dagger(t) \otimes \widetilde{X}_\alpha^\dagger(t), \qquad (12.24)$$ me31

with

$$\widetilde{A}_\alpha(t) \;=\; e^{iH_A t/\hbar}\, A_\alpha\, e^{-iH_A t/\hbar}, \qquad \widetilde{X}_\alpha(t) \;=\; e^{iH_B t/\hbar}\, X_\alpha\, e^{-iH_B t/\hbar}. \qquad (12.25)$$ me32

Rules of hermitian conjugation imply that

$$\widetilde{A}_\alpha^\dagger(t) \;=\; e^{iH_A t/\hbar}\, A_\alpha^\dagger\, e^{-iH_A t/\hbar}, \qquad \widetilde{X}_\alpha^\dagger(t) \;=\; e^{iH_B t/\hbar}\, X_\alpha^\dagger\, e^{-iH_B t/\hbar}, \qquad (12.26)$$ me33

So the conjugate operators transform to interaction picture in the exactly the same manner as the initial ones.

We now make one more assuption about reservoir. We have already assumed that $\widetilde{\varrho}_B(t) \approx \bar{\sigma}_B$. Here, we assume that in the Schrödinger picture

$$\langle X_\alpha \rangle_B \equiv \mathrm{Tr}_B \{ X_\alpha \rho_B(t) \} = \mathrm{Tr}_B \{ X_\alpha \bar{\sigma}_B \} = 0. \tag{12.27}$$ me37

This assumption easily transform to interaction picture

$$\begin{aligned} \langle \widetilde{X}_\alpha(t) \rangle_B &= \mathrm{Tr}_B \left\{ e^{iH_B t/\hbar} X_\alpha e^{-iH_B t/\hbar} \bar{\sigma}_B \right\} \\ &= \mathrm{Tr}_B \left\{ X_\alpha e^{-iH_B t/\hbar} \bar{\sigma}_B e^{iH_B t/\hbar} \right\} = \mathrm{Tr}_B \{ X_\alpha \bar{\sigma}_B \} = 0, \end{aligned} \tag{12.28}$$

which follows due to cyclic property of trace and to (12.27). This is rather a simplification and not a restrictive assumption. This will be clarified and explained in auxiliary sections. Relation (12.27) (leading to (12.28)) aloows us to see that the first term in the ME (12.22) is, in fact, zero. Indeed

$$\begin{aligned} \mathrm{Tr}_B \big[\widetilde{V}_{AB}(t_1), \ \widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B \big] &= \mathrm{Tr}_B \big[\sum_\alpha \widetilde{A}_\alpha(t_1) \otimes \widetilde{X}_\alpha(t_1), \ \widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B \big] \\ &= \sum_\alpha \big[\widetilde{A}_\alpha(t_1) \widetilde{\varrho}_A(t) \, \mathrm{Tr}_B \big(\widetilde{X}_\alpha(t_1) \bar{\sigma}_B \big) - \widetilde{\varrho}_A \widetilde{A}_\alpha(t_1) \, \mathrm{Tr}_B \big(\bar{\sigma}_B \widetilde{X}_\alpha(t_1) \big) \big] \\ &= 0. \end{aligned} \tag{12.29}$$

Both traces are equal (cyclic property), nevertheless this expression need not be zero, because operators of the $\mathcal{A}$ system need not commute. If requirement (12.27) is not fulfiled then the above average may not vanish. Assumption (12.27) and its consequence (12.28) fortunately give zero, and the first term of Eq.(12.22) vanishes and we remain with the master equation

$$\Delta \widetilde{\varrho}_A(t) = \left(\frac{1}{i\hbar} \right)^2 \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \, \mathrm{Tr}_B \Big[\widetilde{V}_{AB}(t_1), \ \big[\widetilde{V}_{AB}(t_2), \ \widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B \big] \Big]. \tag{12.30}$$ me41a

Expanding the commutators is simple. Moreover, one easily notices that there are two pairs of hermitian conjugates. Hence we have

$$\begin{aligned} \frac{\Delta \widetilde{\varrho}_A(t)}{\Delta t} = \frac{1}{\hbar^2 \Delta t} \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \, \mathrm{Tr}_B \Big\{ & \widetilde{V}_{AB}(t_2) \big(\widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B \big) \widetilde{V}_{AB}(t_1) \\ & - \widetilde{V}_{AB}(t_1) \widetilde{V}_{AB}(t_2) \big(\widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B \big) \Big\} + \mathbb{H}.\mathbb{C}. \end{aligned} \tag{12.31}$$

We can now use hamiltonian (12.24) and perform futher transformations in (12.31). It can be, however, shown that this equation does not guarantee that the positivity of the density operator $\widetilde{\varrho}_A(t)$ is preserved. It appears that the so-called secular approximation is necessary. To perform it effectively it is worth to present the interaction hamiltonian in a somewhat different form.

12.2.2 Operators $A_\alpha(\Omega)$

Let us write the hamiltonian of the subsystem $\mathcal{A}$ as

$$H_A = \sum_a \hbar\omega_a | a \rangle\langle a |. \tag{12.32}$$ me44

States $|\,a\,\rangle$ constitute the complete and orthonormal basis in the space of states of the subsystem $\mathcal{A}$. The eigenfrequencies ω_a may or may no be degenerate. We allow $\omega_a = \omega_b$ for $a \neq b$. At present it suffices that we distinguish different kets $|\,a\,\rangle$ solely by their "number a. Now, we define the operators $A_\alpha(\Omega)$ via the following relation

$$A_\alpha(\Omega) = \sum_{a,b} \delta(\omega_{ba} - \Omega)\,|\,a\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,b\,|. \tag{12.33}$$ me45

This representation may be called the decomposition of operator A_α into eigenprojectors of hamiltonian H_A. Delta $\delta(\omega_{ba} - \Omega)$ is of the Kronecker type, thus

$$\delta(\omega_{ba} - \Omega) = \begin{cases} 0 & \text{for} \quad \Omega_{ba} \neq \Omega, \\ 1 & \text{for} \quad \Omega_{ba} = \Omega_{ba}, \end{cases} \tag{12.34}$$ me46

In our considerations we allow for nonhermitian operators A_α. Hence, definition (12.33) me45 is augmented by the following one

$$A^\dagger_\alpha(\Omega) = \sum_{a,b} \delta(\omega_{ba} - \Omega)\,|\,b\,\rangle\langle\,b\,|\,A^\dagger_\alpha\,|\,a\,\rangle\langle\,a\,| = \sum_{a,b} \delta(\omega_{ab} - \Omega)\,|\,a\,\rangle\langle\,a\,|\,A^\dagger_\alpha\,|\,b\,\rangle\langle\,b\,|, \tag{12.35}$$ me47

because it is always allowed the interchange the summation indices $a \leftrightarrow b$. we stress that $A_\alpha(\Omega)$ contains Bohr frequancy ω_{ba}, while in $A^\dagger_\alpha(\Omega)$ we have $\omega_{ab} = -\omega_{ba}$. The following relation seems to be quite obvious

$$\sum_{\Omega} \delta(\omega_{kn} - \Omega) = 1. \tag{12.36}$$ me48

As a consequence we we obtain

$$\sum_{\Omega} A_\alpha(\Omega) = A_\alpha. \tag{12.37}$$ me49

Indeed, from definition (12.33) me45 and relation (12.36) me48 we get

$$\begin{aligned} \sum_{\Omega} A_\alpha(\Omega) &= \sum_{\Omega} \sum_{a,b} \delta(\omega_{ba} - \Omega)\,|\,a\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,b\,| \\ &= \sum_{a,b} |\,a\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,b\,| = \mathbf{1}A_\alpha\mathbf{1} = A_\alpha. \end{aligned} \tag{12.38}$$

Relation (12.37) me49 implies that the interaction hamiltonian can be written as (in Schrödinger picture)

$$V_{AB} = \sum_\alpha A_\alpha \otimes X_\alpha = \sum_{\Omega} \sum_\alpha A_\alpha(\Omega) \otimes X_\alpha. \tag{12.39}$$ me51

Similarly as above we show that

$$\sum_{\Omega} A^\dagger_\alpha(\Omega) = A^\dagger_\alpha, \tag{12.40}$$ me52

and

$$V_{AB} = V^\dagger_{AB} = \sum_{\Omega} \sum_\alpha A^\dagger_\alpha(\Omega) \otimes X^\dagger_\alpha. \tag{12.41}$$ me53

Using definition (12.33) we find the operator $\widetilde{A}_j(\Omega)$ in the interaction picture

$$\widetilde{A}_\alpha(\Omega) \;=\; e^{iH_At/\hbar}\, A_\alpha(\Omega)\, e^{-iH_At/\hbar} \;=\; e^{-i\Omega t}\, A_\alpha(\Omega). \tag{12.42}$$

Certainly, by hermitian conjugation

$$\widetilde{A}^\dagger_\alpha(\Omega) \;=\; e^{iH_At/\hbar}\, A^\dagger_\alpha(\Omega)\, e^{-iH_At/\hbar} \;=\; e^{i\Omega t}\, A^\dagger_\alpha(\Omega). \tag{12.43}$$

Linking expressions (12.39) and (12.42) we write the interaction hamiltonian in the interaction picture

$$\widetilde{V}_{AB}(t) = \sum_\Omega \sum_\alpha e^{-i\Omega t}\, A_\alpha(\Omega) \otimes \widetilde{X}_\alpha(t). \tag{12.44}$$

Equally well we can also write

$$\widetilde{V}_{AB}(t) = \widetilde{V}^\dagger_{AB}(t) = \sum_\Omega \sum_\alpha e^{i\Omega t}\, A^\dagger_\alpha(\Omega) \otimes \widetilde{X}^\dagger_\alpha(t). \tag{12.45}$$

Before starting to analyze ME (12.31), let us notice that operators $A_\alpha(\Omega)$ possess some intresting properties. For exaple, the following commutation relations hold

$$\big[\, H_A,\; A_\alpha(\Omega)\,\big] \;=\; -\hbar\Omega A_\alpha(\Omega), \tag{12.46a}$$

$$\big[\, H_A,\; A^\dagger_\alpha(\Omega)\,\big] \;=\; \hbar\Omega A^\dagger_\alpha(\Omega), \tag{12.46b}$$

$$\big[\, H_A,\; A^\dagger_\alpha(\Omega) A_\beta(\Omega)\,\big] \;=\; 0. \tag{12.46c}$$

The proofs wil be given in auxiliary sections.

12.2.3 Further analysis of master equation

We return to master equation (12.31). Interaction hamiltonian $\widetilde{V}_{AB}(t_2)$ is taken as in (12.44), while $\widetilde{V}_{AB}(t_1)$ is represented according to (12.45). This gives

$$\begin{aligned}\frac{\Delta\, \widetilde{\varrho}_A(t)}{\Delta t} \;=\; \frac{1}{\hbar^2\, \Delta t} \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \sum_{\alpha,\beta} \sum_{\Omega,\Omega'} \mathrm{Tr}_B \Big\{ \\ e^{-i\Omega t_2} A_\beta(\Omega) \otimes \widetilde{X}_\beta(t_2) \big[\widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B\big] e^{i\Omega' t_1} A^\dagger_\alpha(\Omega') \otimes \widetilde{X}^\dagger_\alpha(t_1) \\ - \; e^{i\Omega' t_1} A^\dagger_\alpha(\Omega') \otimes \widetilde{X}^\dagger_\alpha(t_1) \big[e^{-i\Omega t_2} A_\beta(\Omega) \otimes \widetilde{X}_\beta(t_2)\big] \widetilde{\varrho}_A(t) \otimes \bar{\sigma}_B \Big\} \;+\; \mathbb{H}.\mathbb{C}.\end{aligned} \tag{12.47}$$

Performing tensor products we remember that partial trace is computed only with respect to reservoir variables. Moreover we note that these traces are the same (cyclic property). Therefore we denote

$$\bar{G}_{\alpha\beta}(t_1 - t_2) \;=\; \mathrm{Tr}_B \Big\{\, \widetilde{X}^\dagger_\alpha(t_1)\, \widetilde{X}_\beta(t_2)\, \bar{\sigma}_B \,\Big\}. \tag{12.48}$$

Finally we rewrite the arguments of the exponentials as $i\Omega' t_1 - i\Omega t_2 = i(\Omega' - \Omega)t_1 + i\Omega(t_1 - t_2)$. Thus Eq.(12.47) becomes

$$\begin{aligned}\frac{\Delta\, \widetilde{\varrho}_A(t)}{\Delta t} \;=\; \frac{1}{\hbar^2\, \Delta t} \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \sum_{\alpha,\beta} \sum_{\Omega,\Omega'} e^{i(\Omega'-\Omega)t_1}\; e^{i\Omega(t_1-t_2)} \bar{G}_{\alpha\beta}(t_1 - t_2) \\ \times \Big[\, A_\beta(\Omega) \widetilde{\varrho}_A(t) A^\dagger_\alpha(\Omega') \;-\; A^\dagger_\alpha(\Omega') A_\beta(\Omega) \widetilde{\varrho}_A(t) \Big] \;+\; \mathbb{H}.\mathbb{C}.\end{aligned} \tag{12.49}$$

The quantity $\bar{G}_{\alpha\beta}(t_1 - t_2)$ is called the correlation function of the reservoir. We will briefly discuss its properties.

12.2.4 Correlation functions $\bar{G}_{\alpha\beta}$

Let us focus for a while on the functions defined by the right hand side of Eq.(12.48), they are

$$G_{\alpha\beta}(t_1,t_2) \;=\; \mathrm{Tr}_B\left\{\widetilde{X}^\dagger_\alpha(t_1)\,\widetilde{X}_\beta(t_2)\,\bar{\sigma}_B\right\}. \tag{12.50}$$ me65a

These are the function of two variables and it is not *a priori* clear that they are function only of the difference $\tau = t_1 - t_2$. Before proving this fact, let us note that

$$G^*_{\alpha\beta}(t_1,t_2) \;=\; G_{\beta\alpha}(t_2,t_1). \tag{12.51}$$ me65b

To prove it, we use relation $\mathrm{Tr}^*_B\{A\} = \mathrm{Tr}_B\{A^\dagger\}$, so that the definition (12.50) gives

$$G^*_{\alpha\beta}(t_1,t_2) \;=\; \mathrm{Tr}_B\left\{\bar{\sigma}_B\widetilde{X}^\dagger_\beta(t_2)\,\widetilde{X}_\alpha(t_1)\right\} \;=\; \mathrm{Tr}_B\left\{\widetilde{X}^\dagger_\beta(t_2)\,\widetilde{X}_\alpha(t_1)\,\bar{\sigma}_B\right\} \;=\; G_{\beta\alpha}(t_2,t_1), \tag{12.52}$$ me65c

Where in the second step we have used the cyclic property of trace.

Now we will show that the function $G_{jk}(t_1,t_2)$ is indeed a function of the difference of its arguments. The key role plays the fact that the state of the reservoir (density operator $\bar{\sigma}_B$) is stationary (does not change in time). Explicitly using the interaction picture we get

$$G_{\alpha\beta}(t_1,t_2) \;=\; \mathrm{Tr}_B\left\{\left(e^{iH_Bt_1/\hbar}\,X^\dagger_\alpha\,e^{-iH_Bt_1/\hbar}\right)\left(e^{iH_Bt_2/\hbar}\,X_\beta\,e^{-iH_Bt_2/\hbar}\right)\bar{\sigma}_B\right\}. \tag{12.53}$$ me65d

The trace is cyclic and $\bar{\sigma}_B$ commutes with hamiltonianem H_B so we conclude that

$$\begin{aligned} G_{jk}(t_1,t_2) \;&=\; \mathrm{Tr}_B\left\{\,e^{iH_B(t_1-t_2)/\hbar}\,X^\dagger_\alpha\,e^{-iH_B(t_1-t_2)/\hbar}\,X_\beta\,\bar{\sigma}_B\,\right\} \\ &=\; \mathrm{Tr}_B\left\{\,\widetilde{X}^\dagger_\alpha(t_1-t_2)\,\widetilde{X}_\beta(0)\,\bar{\sigma}_B\,\right\} \;=\; \bar{G}_{\alpha\beta}(\tau=t_1-t_2), \end{aligned} \tag{12.54}$$

for two moments of time $t_1 > t_2$. Reservoir's correlation function effectively depends only on one variable. This fact is denoted by a bar over the symbol od correlation function. Thus we write

$$G_{\alpha\beta}(t_1,t_2) \;=\; \bar{G}_{\alpha\beta}(\tau) \;=\; \mathrm{Tr}_B\left\{\,\widetilde{X}^\dagger_\alpha(\tau)\,X_\beta\,\bar{\sigma}_B\,\right\} \tag{12.55}$$ me65f

Such correlation functions are called stationary. In this case stationarity Stacjonarno means invariance with respect to time translation. Indeed

$$\bar{G}_{\alpha\beta}(t_1+T,t_2+T) \;=\; \bar{G}_{\alpha\beta}\big((t_1+T)-(t_2+T)\big) \;=\; \bar{G}_{\alpha\beta}(t_1-t_2). \tag{12.56}$$ me65g

Stationarity of the correlation functions is a straightforward consequence of the reservoir's density operator $\bar{\sigma}_B$.

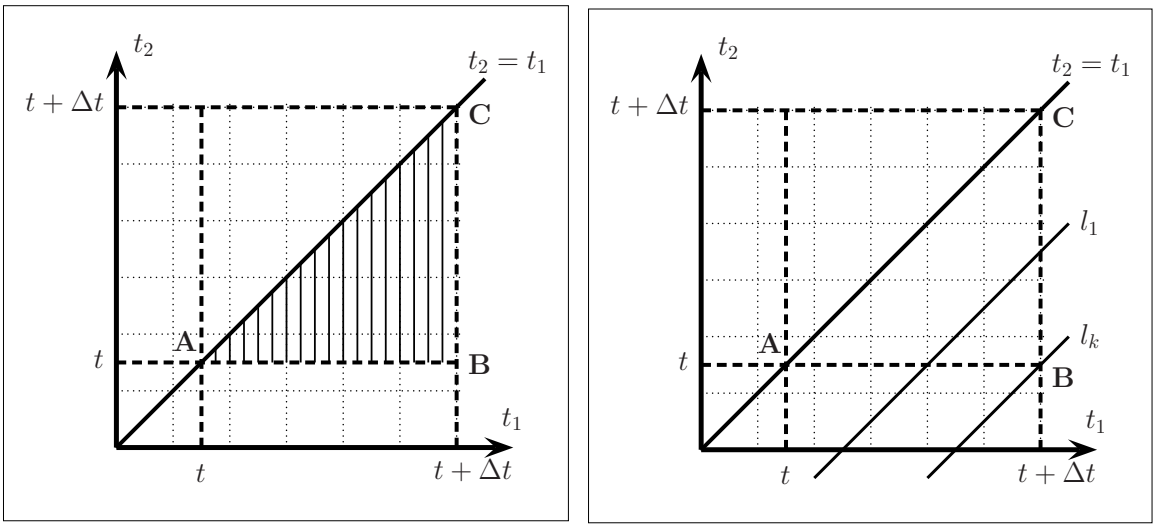

Fig. 12.1: Left figure presents the integration region in the double integral in Eq.(12.49). Right figure illustrates the change to new variables $\tau = t_1 - t_2$ and t_1. Other explanantions are to be found in the text. xmerys01

12.3 Discusion of times

12.3.1 Limits of the integrals and Markov approximation

In master equation (12.49) one integrates over the triangle ABC which is shown in picture 12.1. First one computes the integral over dt_2 in the range from t to t_1, This is indicated by thin vertical lines (at left). Next one sums such contributions by integrating over dt_1 from t to $t + \Delta t$. The integrand in (12.49) contains correlation functions of the reservoir which depend on the difference $\tau = t_1 - t_2$. We stress that we always have $t_1 \geq t_2$, so that $\tau \geq 0$. The integration over the triangle can be performed in another manner.

Let us consider the geometry. Along the diagonal AC we have $t_1 = t_2$, so $\tau = t_1 - t_2 = 0$. The straight line l_1 has (in t_1 and t_2 variables) the equation $t_2 = t_1 - \tau$, where τ is fixed, since $(-\tau)$ is the coordinate t_2 of the point where the discussed line intersects the axis t_2. Then, for the line l_k (passing through the point B) τ is also fixed (by the same argument, as in the case of line l_1). On l_k, at the point B we have $t_1 = t + \Delta t$ oraz $t_2 = t$. Thus at that point (B) (and on the line l_k) we have $\tau = \Delta t$. Parametr τ specifies the skew straight lines (parallel to the diagonal AC) and passing through triangle ABC. Integration over the triangle ABC is now done as follows. We fix $\tau \in (0, \Delta t)$ and we move along the segment A'C' (see Fig.12.2). Variable t_1 runs in the interval from $t + \tau$ to $t + \Delta t$. So, first we integrate over dt_1 from $t + \tau$ to $t + \Delta t$ (along the segment A'C'). Next we integrate over $d\tau$ from zero to Δt. In this manner we sum the contributions from all skew segments covering the triangle ABC. Therefore, we can write

$$\int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \;=\; \int_0^{\Delta t} d\tau \int_{t+\tau}^{t+\Delta t} dt_1, \qquad (12.57)$$ me70

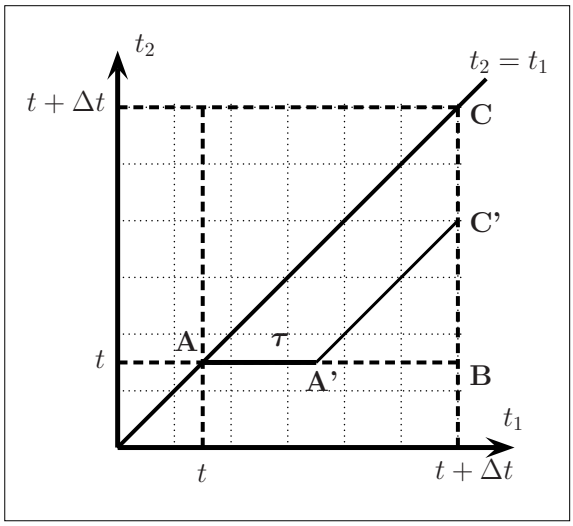

Fig. 12.2: Illlustration of the change of integration variables in equation (12.49), Transformation to new variables $\tau = t_1 - t_2$ i t_1. Other explanations – in the text. xmerys02

while we remember that $\tau = t_1 - t_2$ (or $t_2 = t_1 - \tau$).

Due to the discussed change of integration variables instead of expression (12.49) we get

$$\frac{\Delta\,\widetilde{\varrho}_A(t)}{\Delta t} \;=\; \frac{1}{\hbar^2\,\Delta t}\int\limits_0^{\Delta t} d\tau \int\limits_{t+\tau}^{t+\Delta t} dt_1 \sum_{\alpha,\beta}\sum_{\Omega,\Omega'} e^{i(\Omega'-\Omega)t_1}\; e^{i\Omega\tau}\bar{G}_{\alpha\beta}(\tau)$$
$$\times\Big[\,A_\beta(\Omega)\widetilde{\varrho}_A(t)A^\dagger_\alpha(\Omega')\;-\;A^\dagger_\alpha(\Omega')A_\beta(\Omega)\widetilde{\varrho}_A(t)\Big]\;+\;\mathbb{H}.\mathbb{C}., \quad (12.58)$$

which should be further analyzed and discussed.

First of all we recall that the considered time intervals satisfy the requirement $\Delta t \gg \tau_B$, which will be discussed in detail later. If it is true, then the main contribution to the integral over $d\tau$ in Eq.(12.58) will come from the region in the neighborhood of $0 \le \tau < \tau_B \ll \Delta t$. Geometrically, this corresponds to a narrow belt which is parallel to the diagonal AC and lies just below it. It follows from the fact that outside this region the reservoir's correlation functions practically vanish (decay to zero). Therefore, we will not make any serious error moving the upper limit of integration over $d\tau$ to infinity. Moreover, since only small τ's contribute significantly, the lower limit of the integral over dt_1 may be approximated simply by t, so only a small "inital" region will be neglected. With this approximations equation (12.58) yields

$$\frac{\Delta\,\widetilde{\varrho}_A(t)}{\Delta t} \;=\; \frac{1}{\hbar^2\,\Delta t}\sum_{\Omega,\Omega'}\sum_{\alpha,\beta}\int_0^{\infty} d\tau\; e^{i\Omega\tau}\bar{G}_{\alpha\beta}(\tau)\int\limits_{t}^{t+\Delta t} dt_1\; e^{i(\Omega'-\Omega)t_1}$$
$$\times\Big[\,A_\beta(\Omega)\widetilde{\varrho}_A(t)A^\dagger_\alpha(\Omega')\;-\;A^\dagger_\alpha(\Omega')A_\beta(\Omega)\widetilde{\varrho}_A(t)\Big]\;+\;\mathbb{H}.\mathbb{C}. \quad (12.59)$$

me73 Introducing the quantities

$$J(\Omega' - \Omega) \;=\; \frac{1}{\Delta t}\int\limits_{t}^{t+\Delta t} dt_1 \;\exp\big[\, i(\Omega' - \Omega)t_1 \,\big], \tag{12.60a}$$

$$W_{\alpha\beta}(\Omega) \;=\; \int_0^\infty d\tau\; e^{i\Omega\tau}\; \bar{G}_{\alpha\beta}(\tau) = \int_0^\infty d\tau\; e^{i\Omega\tau}\, \mathrm{Tr}_{\,B}\big\{\widetilde{X}^\dagger_\alpha(\tau)\, X_\beta \bar{\sigma}_B\big\}, \tag{12.60b}$$

we rewrite Eq.(me72 12.59) as follows

$$\frac{\Delta\, \widetilde{\varrho}_A(t)}{\Delta t} \;=\; \frac{1}{\hbar^2}\sum_{\Omega,\Omega'}\sum_{\alpha,\beta} J(\Omega' - \Omega) W_{\alpha\beta}(\Omega) \times\Big[\, A_\beta(\Omega)\widetilde{\varrho}_A(t)A^\dagger_\alpha(\Omega') \;-\; A^\dagger_\alpha(\Omega')A_\beta(\Omega)\widetilde{\varrho}_A(t)\Big] \;+\; \mathbb{H}.\mathbb{C}. \tag{12.61}$$

This equation specifies the rate of change of the reduced density operator $\widetilde{\varrho}_A(t)$ within the time interval $(t, t+\Delta t)$. The quotient $\Delta\widetilde{\varrho}_A(t)/\Delta t$ can be traeted as an averaging

$$\frac{\Delta\, \widetilde{\varrho}_A(t)}{\Delta t} \;=\; \frac{\widetilde{\varrho}_A(t+\Delta t) - \widetilde{\varrho}_A(t)}{\Delta t} \;=\; \frac{1}{\Delta t}\int_t^{t+\Delta t} dt_1\; \frac{d\,\widetilde{\varrho}_A(t_1)}{dt_1}. \tag{12.62}$$ me75

This averaging results in smoothing all very rapid changes of $\widetilde{\varrho}_A(t)$ which may occur during the interval $(t,\; t+\Delta t)$. In principle we should account for such rapid changes. We do not do that because right hand side of Eq.(me74 12.61) contains $\widetilde{\varrho}_A(t)$, while the left hand side represent the smoothed rate of change. This rate depends on the density operator $\widetilde{\varrho}_A$ in past , that is at the moment when the smoothed evolution was started. So our next approximation consists in replacing the Smoothed rate by a usual derivative In other words the variation at an instant t (that is the derivative $d\widetilde{\varrho}_A(t)/dt$) is connected with the value of $\widetilde{\varrho}_A(t)$ at the very same instant. This approximation allows us to use a usual derivative at the left hand side of (me74 12.61). This approximation sometimes is called a markovian one since it connects the variations of some physical quantity with its value at the same instant, independently from the values which this quantity had at earlier moments. We can say that markovian approximation consists in neglecting the influence of the history of the physical on its current state which fully determines the presently occurring changes. In some literature sources this approximation is also called the coarse-graining one, because small and rapid fluctuactions are neglected when the evolution is investigated on a much longer time scale specified by Δt.

With all the discussed approximation our master equation (me74 12.61) becomes

$$\frac{d}{dt}\;\widetilde{\varrho}_A(t) \;=\; \frac{1}{\hbar^2}\sum_{\Omega,\Omega'}\sum_{\alpha,\beta} J(\Omega' - \Omega) W_{\alpha\beta}(\Omega) \times\Big[\, A_\beta(\Omega)\widetilde{\varrho}_A(t)A^\dagger_\alpha(\Omega') \;-\; A^\dagger_\alpha(\Omega')A_\beta(\Omega)\widetilde{\varrho}_A(t)\Big] \;+\; \mathbb{H}.\mathbb{C}. \tag{12.63}$$

12.3.2 Schrödinger picture

At this stage we return to the Schrödinger picture and we insert

$$\widetilde{\varrho}_A(t) \;=\; e^{iH_A t/\hbar}\, \rho_A(t)\, e^{-iH_A t/\hbar}. \tag{12.64}$$ me77

When computing the derivative at the left hand side we reproduce the free evolution term. Thus, we get

$$
\begin{aligned}
& e^{iH_At/\hbar}\left(\frac{d}{dt}\,\rho_A(t)\right)e^{-iH_At/\hbar} \;= \\
&\quad = -\,\frac{i}{\hbar}\,e^{iH_At/\hbar}\big[\,H_A,\;\rho_A(t)\,\big]e^{-iH_At/\hbar} \\
&\qquad + \Big\{\,\frac{1}{\hbar^2}\sum_{\Omega,\Omega'}\sum_{\alpha,\beta}J(\Omega'-\Omega)W_{\alpha\beta}(\Omega)\Big[\,A_\beta(\Omega)\,e^{iH_At/\hbar}\,\rho_A(t)\,e^{-iH_At/\hbar}A^\dagger_\alpha(\Omega') \\
&\qquad\quad - A^\dagger_\alpha(\Omega')A_\beta(\Omega)e^{iH_At/\hbar}\,\rho_A(t)\,e^{-iH_At/\hbar}\Big]\;+\;\mathbb{H}.\mathbb{C}\;\Big\}. \qquad (12.65)
\end{aligned}
$$

Multiplying on the left by $e^{-iH_At/\hbar}$ and on the right by $e^{iH_At/\hbar}$, we use relation (12.42) and (12.43) (for negative times). This yields

$$
\begin{aligned}
\frac{d}{dt}\,\rho_A(t) \;&= -\,\frac{i}{\hbar}\big[\,H_A,\;\rho_A(t)\,\big] + \Big\{\,\frac{1}{\hbar^2}\sum_{\Omega,\Omega'}\sum_{\alpha,\beta}J(\Omega'-\Omega)W_{\alpha\beta}(\Omega)\;e^{i(\Omega-\Omega')t} \\
&\qquad \times\Big[\,A_\beta(\Omega)\rho_A(t)A^\dagger_\alpha(\Omega')\;-\;A^\dagger_\alpha(\Omega')A_\beta(\Omega)\rho_A(t)\,\Big]\;+\;\mathbb{H}.\mathbb{C}\;\Big\}. \qquad (12.66)
\end{aligned}
$$

12.3.3 Integral $J(\Omega'-\Omega)$ and secular approximation

Our master equation contains the integral $J(\Omega'-\Omega)$ defined in (12.60a). Its computation is straightforward. Denoting temporarily tymczasowo $x=\Omega'-\Omega$ we get

$$
\begin{aligned}
J(x) \;&=\; \int_t^{t+\Delta t} dt_1\;\frac{e^{ixt_1}}{\Delta t} \;=\; \left(\frac{1}{\Delta t}\right)\frac{e^{ixt_1}}{ix}\,\Big|_t^{t+\Delta t} \;=\; \left(\frac{1}{\Delta t}\right)\frac{e^{ix(t+\Delta t)}-e^{ixt}}{ix} \\
&=\; e^{ixt+ix\Delta t/2}\;\frac{e^{ix\Delta t/2}-e^{-ix\Delta t/2}}{ix\Delta t} \;=\; e^{ixt+ix\Delta t/2}\;\frac{\sin\left(\frac{x\Delta t}{2}\right)}{\left(\frac{x\Delta t}{2}\right)} \\
&=\; e^{ixt}\;F(x), \qquad (12.67)
\end{aligned}
$$

Where we have introduced a function specified by

$$
F(x) \;=\; e^{ix\Delta t/2}\;\frac{\sin\left(\frac{x\Delta t}{2}\right)}{\left(\frac{x\Delta t}{2}\right)}. \qquad (12.68)
$$

Due to the obtained results we can write

$$
J(\Omega'-\Omega) \;=\; e^{i(\Omega'-\Omega)t}\,F(\Omega'-\Omega). \qquad (12.69)
$$

Inserting the computed integral into(12.66) we note that the exponential factor cancels out. Hence

$$
\begin{aligned}
\frac{d}{dt}\,\rho_A(t) \;&=\; -\;\frac{i}{\hbar}\,\big[\,H_A,\;\rho_A(t)\,\big] + \Big\{\,\frac{1}{\hbar^2}\sum_{\Omega',\Omega}\sum_{\alpha,\beta}F(\Omega'-\Omega)W_{\alpha\beta}(\Omega) \\
&\qquad \times\Big[\,A_\beta(\Omega)\,\rho_A(t)\,A^\dagger_\alpha(\Omega)\;-\;A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)\,\rho_A(t)\,\Big]\;+\;\mathbb{H}.\mathbb{C}\;\Big\}. \qquad (12.70)
\end{aligned}
$$

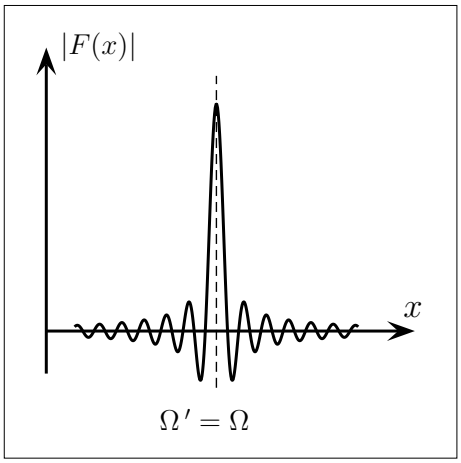

Fig. 12.3: The graph of the modulus of the function $F(\Omega'-\Omega)$ which appears in (12.70). If the time Δt is sufficiently large then the graph has a sharp maximum for $\Omega' = \Omega$. xmerys03

The sense of function $F(\Omega' - \Omega)$ which appears in (12.70) must be now carefully considere. It is easy to see that function $|F(x)|$ has a sharp maximum for $x = \Omega' - \Omega = 0$, where it is equal tu unity.
Zeroes of this function corresppond to

$$\tfrac{1}{2}x\Delta t = n\pi \qquad \Longrightarrow \qquad x = \frac{2n\pi}{\Delta t}. \tag{12.71}$$ me89

If the time Δt is sufficiently long then the central maximum is very narrow. The quaestion is what does it mean "sufficiently long time". Let us consider two possibilities.

1. If $x = \left|\Omega' - \Omega\right| \ll (\Delta t)^{-1}$, the argument of function $|F(x)|$ is very close to zero, her valu is practically one.
2. If $x = \left|\Omega' - \Omega\right| \gg (\Delta t)^{-1}$ (Bohr frequencies are significantly different) then $|F(x)|$ is close to zero.

We conclude that the terms at the right hand side of master equation (12.70) containing the operator products $A^\dagger_\alpha(\Omega')\, A_\beta(\Omega)$, for which $\left|\Omega' - \Omega\right| \gg (\Delta t)^{-1}$ practically do not contribute to the evolution of the density operator $\rho_A(t)$ which appears in the left hand side. According to the first possibility above, significant contribution comes only from such couplings that operators $A_\alpha(\Omega')$ and $A_\beta(\Omega)$ have practically equal corresponding Bohr frequencies.

As we know time T_A is a characteristic relaxation time in subsystem $\mathcal{A}$ due to interaction with reservoir. All the time we take the estimate $\Delta t \ll T_A$ holds (We discuss it later). It can be argued that the terms in master equation (12.70), in which $|\Omega' - \Omega| \sim (\Delta t)^{-1}$ also give very small contributions, so that they can be neglected. As a result of all these approximations, we may say that only those terms in right hand side of master equation (12.70) contribute significantly for which $\left|\Omega' - \Omega\right| = 0$. Such an approximation is called the secular one. It allows us to replace the function $F(\Omega' - \Omega)$ by the Kronecker delta $\delta(\Omega' - \Omega)$ defined as in (12.34). It reminds us that only the terms satysfying the requirement $(\Omega = \Omega)$ give nonzero contribution. Due to all these arguments our master equation

attains the form

$$\frac{d}{dt}\,\rho_A(t) \;=\; -\,\frac{i}{\hbar}\,\big[\,H_A,\;\rho_A(t)\,\big] \;+\; \Big\{\,\frac{1}{\hbar^2}\sum_{\alpha,\beta}\sum_{\Omega',\Omega}\delta(\Omega'-\Omega)\,W_{\alpha\beta}(\Omega) \times\Big[\,A_\beta(\Omega)\,\rho_A(t)\,A^\dagger_\alpha(\Omega')\;-\;A^\dagger_\alpha(\Omega')\,A_\beta(\Omega)\,\rho_A(t)\,\Big] \;+\; \mathbb{H}.\mathbb{C}\,\Big\}. \quad (12.72)$$

The presence of the discussed Kronecker delta simplifies one of the summations, which gives

$$\frac{d}{dt}\,\rho_A(t) \;=-\,\frac{i}{\hbar}\big[H_A,\;\rho_A(t)\big] + \Big\{\,\frac{1}{\hbar^2}\sum_{\alpha,\beta}\sum_{\Omega}W_{\alpha\beta}(\Omega)\Big[A_\beta(\Omega)\rho_A(t)A^\dagger_\alpha(\Omega)\;-\;A^\dagger_\alpha(\Omega)A_\beta(\Omega)\rho_A(t)\Big]+\mathbb{H}.\mathbb{C}\,\Big\} \quad (12.73)$$

The fundamental part of the microscopic derivation of the master equation is finished. We shall perform some transformations which have important, but rather cosmetic character. We want to transform master equation into the so-called standard form. All other discussions are, as mentioned many times, are left to auxiliary sections.

12.4 Standard form

12.4.1 Introduction

Standard form is important, because it can be shown (in a complicated and difficult mathematical manner) that this form guarantees prservation of hermiticity, normalization and, first of all, the positivity of the reduced density operator. If our master equation (12.73) can be brought into the standard form then we can be sure that all the necessary properties of the density operator of subsystem $\mathcal{A}$ are indeed preserved. Obviously, the first term in the right hand side of equation (12.73) describers the unitary evolution, hence we shall concentrate only on the second term. Writing explicitly the hermitian conjugates, we have

$$\frac{d}{dt}\,\rho_A(t)\Big|_{d.} \;=\; \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}W_{\alpha\beta}(\Omega)\Big[\,A_\beta(\Omega)\rho_A(t)A^\dagger_\alpha(\Omega)\;-\;A^\dagger_\alpha(\Omega)A_\beta(\Omega)\rho_A(t)\,\Big] + \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}W^*_{\alpha\beta}(\Omega)\Big[\,A_\alpha(\Omega)\rho_A(t)A^\dagger_\beta(\Omega)\;-\;\rho_A(t)A^\dagger_\beta(\Omega)A_\alpha(\Omega)\Big], \quad (12.74)$$

because operator $\rho_A(t)$ is hermitian (the proof that hermiticity is preserved will be presented in auxiliary sections). In the second term we interchange the summation indices $j \leftrightarrow k$ which gives

$$\frac{d}{dt}\,\rho_A(t)\Big|_{d.} \;=\; \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}W_{\alpha\beta}(\Omega)\Big[\,A_\beta(\Omega)\rho_A(t)A^\dagger_\alpha(\Omega)\;-\;A^\dagger_\alpha(\Omega)A_\beta(\Omega)\rho_A(t)\,\Big] + \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}W^*_{\beta\alpha}(\Omega)\Big[\,A_\beta(\Omega)\rho_A(t)A^\dagger_\alpha(\Omega)\;-\;\rho_A(t)A^\dagger_\alpha(\Omega)A_\beta(\Omega)\Big], \quad (12.75)$$

12.4.2 New notation

me97 For further convenience we introduce the following notation

$$\Gamma_{\alpha\beta}(\Omega) \;=\; W_{\alpha\beta}(\Omega) \;+\; W^*_{\beta\alpha}(\Omega), \tag{12.76a}$$

$$\Delta_{\alpha\beta}(\Omega) \;=\; \frac{1}{2i}\big[W_{\alpha\beta}(\Omega) \;-\; W^*_{\beta\alpha}(\Omega)\big]. \tag{12.76b}$$

The matrix $\Gamma_{\alpha\beta}(\Omega)$ is hermitian and positively defined. The proof of the latter fact is difficult so it will be given later. Hermiticity of $\Gamma_{\alpha\beta}$ follows directly from the definition (12.76a). Indeed, we have

$$\Gamma^*_{\alpha\beta}(\Omega) \;=\; W^*_{\alpha\beta}(\Omega) \;+\; W_{\beta\alpha}(\Omega) \;=\; \Gamma_{\beta\alpha}(\Omega). \tag{12.77}$$ me98

The second matrix $\Delta_{\alpha\beta}(\Omega)$ is also hermitian. From (12.76b) it follows that

$$\Delta^*_{\alpha\beta}(\Omega) = -\frac{1}{2i}\big[W^*_{\alpha\beta}(\Omega) - W_{\beta\alpha}(\Omega)\big] = \frac{1}{2i}\big[W_{\beta\alpha}(\Omega) - W^*_{\alpha\beta}(\Omega)\big] = \Delta_{\beta\alpha}(\Omega). \tag{12.78}$$ me100

Let us focus on the method of computation of elements $\Gamma_{\alpha\beta}(\Omega)$. As it will be shown, elements $\Delta_{\alpha\beta}(\Omega)$ are less important (they will be considered in auxiliary sections). To find $\Gamma_{\alpha\beta}$ we need quantities $W^*_{\beta\alpha}$. Conjugating definition (12.60b) we find that

$$\begin{aligned} W^*_{\beta\alpha}(\Omega) \;&=\; \left(\int_0^\infty d\tau\; e^{i\Omega\tau}\; \mathrm{Tr}_B\big\{\widetilde{X}^\dagger_\beta(\tau) X_\alpha \bar\sigma_B\big\}\right)^* \\ &=\; \int_0^\infty d\tau\; e^{-i\Omega\tau}\; \mathrm{Tr}_B\big\{X^\dagger_\alpha \widetilde{X}_\beta(\tau)\bar\sigma_B\big\} \\ &=\; \int_0^\infty d\tau\; e^{-i\Omega\tau}\; \mathrm{Tr}_B\big\{e^{-iH_B\tau/\hbar} X^\dagger_\alpha e^{iH_B\tau/\hbar} X_\beta \bar\sigma_B\big\}, \end{aligned} \tag{12.79}$$

where we used relations (12.21), (12.26) and cyclic property of trace. Changing the integration variable $\tau \to -\tau$, we have

$$W^*_{\beta\alpha}(\Omega) = \int_{-\infty}^0 d\tau\; e^{i\Omega\tau}\; \mathrm{Tr}_B\big\{\widetilde{X}^\dagger_\alpha(\tau) X_\beta \bar\sigma_B\big\}. \tag{12.80}$$ me101d

The integrand is identical identical as in (12.60b), Only the integration limits are different. Combining both formulas, we get

$$\Gamma_{\alpha\beta}(\Omega) = \int_{-\infty}^\infty d\tau\; e^{i\Omega\tau}\; \mathrm{Tr}_B\big\{\widetilde{X}^\dagger_\alpha(\tau) X_\beta \bar\sigma_B\big\} = \int_{-\infty}^\infty d\tau\; e^{i\Omega\tau} \bar G_{\alpha\beta}(\tau). \tag{12.81}$$ me101g

The elements $\Gamma_{\alpha\beta}(\Omega)$ are the Fourier transforms of the corresponding correlation function of the reservoir.

Matrix $\Delta_{\alpha\beta}(\Omega)$ does not have such a simple representation. From the definition (12.76b) and the second relation in (12.79)

$$\Delta_{\alpha\beta}(\Omega) = \frac{1}{2i}\Big[\int_0^\infty d\tau\; e^{i\Omega\tau}\; \mathrm{Tr}_B\big\{\widetilde{X}^\dagger_\alpha(\tau) X_\beta \bar\sigma_B\big\} \;-\; \int_0^\infty d\tau\; e^{-i\Omega\tau}\; \mathrm{Tr}_B\big\{X^\dagger_\alpha \widetilde{X}_\beta(\tau)\bar\sigma_B\big\}\Big]. \tag{12.82}$$ me101h

12.4.3 Standard form

Inverting relations (12.76) we express elements $W_{\alpha\beta}$ via $\Gamma_{\alpha\beta}$ and $\Delta_{\alpha\beta}$. After simple regrouping of the terms in Eq.(12.75) we get

$$\frac{d}{dt}\ \rho_A(t)\Big|_{d.} = \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}\ \Gamma_{\alpha\beta}(\Omega)\ \Big\{\ A_\beta(\Omega)\ \rho_A(t)\ A^\dagger_\alpha(\Omega) - \tfrac{1}{2}\ \Big[A^\dagger_\alpha(\Omega)\ A_\beta(\Omega),\ \rho_A(t)\Big]_+ - i\Delta_{\alpha\beta}(\Omega)\Big[A^\dagger_\alpha(\Omega)A_\beta(\Omega),\ \rho_A(t)\Big]\ \Big\}. \tag{12.83}$$

me102d

Let us note that the last term is a commutator, so we denote

$$H_{LS} = \frac{1}{\hbar}\sum_{\Omega}\sum_{\alpha,\beta}\Delta_{\alpha\beta}(\Omega)A^\dagger_\alpha(\Omega)A_\beta(\Omega). \tag{12.84}$$

me103

Taking into account hermiticity of matrix $\Delta_{\alpha\beta}(\omega)$ and changing the names of the summation indices we can easily show that the operator H_{LS} is hermitian. Returning to full master equation, that is to Eq.(12.73), we conclude that the term containing H_{LS} in (12.83) can be connected with the free hamiltonian term. In this manner connecting Eqs.(12.73) and (12.83) we finally have

$$\frac{d}{dt}\ \rho_A(t) = -\frac{i}{\hbar}\big[H_A + H_{LS},\ \rho_A(t)\big] + \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}\ \Gamma_{\alpha\beta}(\Omega)\ \Big\{\ A_\beta(\Omega)\ \rho_A(t)\ A^\dagger_\alpha(\Omega) - \tfrac{1}{2}\ \big[A^\dagger_\alpha(\Omega)\ A_\beta(\Omega),\ \rho_A(t)\big]_+\Big\}, \tag{12.85}$$

me106

which coincides exactly with the standard form of the evolution equation for the reduced density operator $rho_A(t)$ which describes the state of the subsystem $\mathcal{A}$ interacting with reservoir $\mathcal{B}$. This allows us to be sure that hermiticity, normalization and positivity of the operator $\rho_A(t)$ is indeed ensured. Finally let us remark that operator H_{LS} which gives a contribution to the hamiltonian (unitary) evolution, usually produces small shifts of the eigenenergies of the subsystem $\mathcal{A}$. That is why, in many practical applications, this term is simply omitted. This explains our previous remark that matrix $\Delta_{\alpha\beta}$ is less important than $\Gamma_{\alpha\beta}$. Obviously one can construct operator H_{LS} and investigate its influence on the unperturbed energy levels of the subsystem $\mathcal{A}$. Small energy shifts of eigenenergies of subsystem $\mathcal{A}$ are qualitatively similar to the well-known Lamb shifts, which explains the employed notation.

The obtained master equation (12.85) is an operator one. In practice, we frequently need an equation of motion for the matrix elements of the reduced density operator $\rho_A(t)$. It seems to be natural to use the energy representation, that is to consider matrix elements of $\rho_A(t)$ calculated in the basis $\{|\,a\,\rangle\}$ of the eigenstates of the free hamiltonian H_A (see Eq.(12.32)). This will be done in the next section.

12.4.4 Energy representation

When analyzing master equation in the basis of the eigenstates of free hamiltonian We must be careful. The reason is that the the commutator in (12.85) contains an additional

term, namely the Lamb-shift hamiltonian. One may argue that this changes the hamiltonian and a new basis should be found (a basis in which $H_A + H_{LS}$ is diagonal). We will, however, proceed in the spirit of the perturbative approach. We will treat H_{LS} as a small perturbation which, at most, will yield small energy shifts. Therefore, the set $\{|\,A\,\rangle\}$ of eigenstates of the unperturbed hamiltonian H_A can be used as complete and orthonormal basis. Working within this scheme we can easily construct master equation (equation of motion) for matrix elements of the density operator for subsystem $\mathcal{A}$. We will suppress the index A since it should lead to no misunderstanding. Taking matrix elements $\rho_{ab}(t) = \langle\, a\,|\,\rho_A(t)\,|\,b\,\rangle$ and expanding the anticommutator term we obtain

$$\begin{aligned}\frac{d}{dt}\ \rho_{ab}(t) = &-\ \frac{i}{\hbar}\langle\, a\,|\big[H_A + H_{LS},\ \rho(t)\big]|\,b\,\rangle \\ &+\ \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}\Gamma_{\alpha\beta}(\Omega)\,\Big\{\,\langle\, a\,|A_\beta(\Omega)\,\rho(t)\,A^\dagger_\alpha(\Omega)|\,b\,\rangle \\ &-\tfrac{1}{2}\,\langle\, a\,|A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)\,\rho(t)|\,b\,\rangle - \tfrac{1}{2}\,\langle\, a\,|\rho(t)\,A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)|\,b\,\rangle\Big\}. \qquad (12.86)\end{aligned}$$

me112

The second term – last three ones – will be called a dissipative one and we will concentrate on its form. First we use expressions (12.33), (12.35) for operators $A_\alpha(\Omega)$ and $A^\dagger_\alpha(\Omega)$. Then we consider three matrix elements. Necessary computations in the basis of eigenstates of free hamiltonian H_A are simple though a bit tedious, in some cases a suitable changes of summation indices is necessary. The result of these calculations is as follows

me117

$$\begin{aligned}&\langle\, a\,|A_\beta(\Omega)\,\rho(t)\,A^\dagger_\alpha(\Omega)|\,b\,\rangle = \\ &\qquad = \sum_{m,n}\delta(\omega_{ma}-\Omega)\,\delta(\omega_{nb}-\Omega)\langle\, a\,|\,A_\beta\,|\,m\,\rangle\langle\, n\,|\,A^\dagger_\alpha\,|\,b\,\rangle\,\rho_{mn}(t), \qquad (12.87a)\end{aligned}$$

$$\begin{aligned}&\langle\, a\,|A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)\,\rho(t)|\,b\,\rangle = \\ &\qquad = \sum_{m,n}\delta(\omega_{an}-\Omega)\,\delta(\omega_{mn}-\Omega)\langle\, a\,|\,A^\dagger_\alpha\,|\,n\,\rangle\langle\, n\,|\,A_\beta\,|\,m\,\rangle\,\rho_{mb}(t), \qquad (12.87b)\end{aligned}$$

$$\begin{aligned}&\langle\, a\,|\rho(t)\,A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)|\,b\,\rangle = \\ &\qquad = \sum_{m,n}\delta(\omega_{mn}-\Omega)\,\delta(\omega_{bn}-\Omega)\langle\, m\,|\,A^\dagger_\alpha\,|\,n\,\rangle\langle\, n\,|\,A_\beta\,|\,b\,\rangle\,\rho_{am}(t). \qquad (12.87c)\end{aligned}$$

The computed matrix elements are plugged into equation (12.86) and perform summation over frequency Ω. After some regrouping we find that

$$\begin{aligned}\frac{d}{dt}\ \rho_{ab}(t)\Big|_{d.} = \frac{1}{\hbar^2}\sum_{\alpha,\beta}\sum_{m,n}\Big\{&\Gamma_{\alpha\beta}(\omega_{ma})\,\delta(\omega_{nb}-\omega_{ma})\langle\, a\,|\,A_\beta\,|\,m\,\rangle\langle\, b\,|\,A_\alpha\,|\,n\,\rangle^*\,\rho_{mn}(t) \\ &-\tfrac{1}{2}\,\Gamma_{\alpha\beta}(\omega_{an})\,\delta(\omega_{mn}-\omega_{an})\langle\, n\,|\,A_\beta\,|\,m\,\rangle\langle\, n\,|\,A_\alpha\,|\,a\,\rangle^*\,\rho_{mb}(t) \\ &-\tfrac{1}{2}\,\Gamma_{\alpha\beta}(\omega_{mn})\,\delta(\omega_{bn}-\omega_{mn})\langle\, n\,|\,A_\beta\,|\,b\,\rangle\langle\, n\,|\,A_\alpha\,|\,m\,\rangle^*\,\rho_{am}(t)\Big\} \qquad (12.88)\end{aligned}$$

This expression is transformed further. In the first term we use the evenness of Kronecker delta, while the presence of the deltas in the second and third term allows us to change arguments in the elements of matrix $\Gamma_{\alpha\beta}$. Next, we denote

$$K(am,bn) \;=\; \frac{1}{\hbar^2}\sum_{\alpha,\beta}\Gamma_{\alpha\beta}(\omega_{ma})\langle\, a\,|\,A_\beta\,|\,m\,\rangle\langle\, b\,|\,A_\alpha\,|\,n\,\rangle^*, \tag{12.89}$$ me119

Due to these facts we write formula (12.88) as me118b

$$\begin{aligned}\frac{d}{dt}\;\rho_{ab}(t)\Big|_{d.} \;=\; &\sum_{m,n}\delta(\omega_{ma}-\omega_{nb})\;K(am,bn)\;\rho_{mn}(t)\\ &-\tfrac{1}{2}\sum_{m,n}\delta(\omega_{mn}-\omega_{an})\;K(nm,na)\;\rho_{mb}(t)\\ &-\tfrac{1}{2}\sum_{m,n}\delta(\omega_{bn}-\omega_{mn})\;K(nb,nm)\;\rho_{am}(t).\end{aligned} \tag{12.90}$$

Let us note the specific symmetry of this expression. Further analysis depends on whether the eigenfrequencies of the hamiltonian H_A are degenerate or not. We also note that Kronecker delats in the second and third terms are correspondingly given as $\delta(\omega_{mn}-\omega_{an}) = \delta(\omega_{ma})$ and $\delta(\omega_{bn}-\omega_{mn}) = \delta(\omega_{bm})$, which allows one to perform summation over n. However, one has to be careful because eigenfrequencies ω_n can be degenerate.

12.4.5 Degenerate eigenfrequencies

Let us write the hamiltonian of the considered system $\mathcal{A}$ in the following form

$$H_A = \sum_N \hbar\omega_N \sum_{n=1}^{g_N} |\,Nn\,\rangle\langle\,Nn\,|, \tag{12.91}$$ me130

where N is the main quantum number which distinguishes energy levels (energy multiplets), while $n = 1, 2, \ldots, g_N$ are subsidiary quantum numbers. Is is obvious that $\omega_N \neq \omega_M$ for $N \neq M$. Certainly the nondegenerate case follows immediately and it corresponds to $g_N \equiv 1$, then subsidiary quantum numbers are unnecessary and can be simply supressed.

In the degenerate case single indices appearing in equation (12.90) must be replaced by corresponding pairs, for example $a \to Aa$. Equation (12.90) is now rewritten as me120 me120

$$\begin{aligned}\frac{d}{dt}\;\rho_{AaBb}(t)\Big|_{d.} \;=\; &\sum_{Mm}\sum_{Nn}\delta(\omega_{MA}-\omega_{NB})\;K(AaMm,BbNn)\;\rho_{MmNn}(t)\\ &-\tfrac{1}{2}\sum_{Mm}\sum_{Nn}\delta(\omega_{MN}-\omega_{AN})\;K(NnMm,NnAa)\;\rho_{MmBb}(t)\\ &-\tfrac{1}{2}\sum_{Mm}\sum_{Nn}\delta(\omega_{BN}-\omega_{MN})\;K(NnBb,NnMm)\;\rho_{AaMm}(t).\end{aligned} \tag{12.92}$$

One immediately sees that $\delta(\omega_{MN}-\omega_{AN}) = \delta(\omega_{MA}) = \delta_{MA}$ and similarly $\delta(\omega_{BN}-\omega_{MN}) = \delta_{MB}$, where the last deltas are the simple Kronecker ones. The sum over M in the second

term is trivial. We put $M = A$ and we "land within multiplet A", hence we change $m = a''$. Analogously, in the second term $M = B$ oraz $m = b''$. Therefore, we have

$$\frac{d}{dt}\ \rho_{AaBb}(t)\Big|_{d.} = \sum_{Mm}\sum_{Nn} \delta(\omega_{MA} - \omega_{NB})\ K(AaMm, BbNn)\ \rho_{MmNn}(t) - \tfrac{1}{2}\sum_{Nn}\sum_{a''} K(NnAa'', NnAa)\ \rho_{Aa''Bb}(t) - \tfrac{1}{2}\sum_{Nn}\sum_{b''} K(NnBb, NnBb'')\ \rho_{AaBb''}(t). \tag{12.93}$$

In two last terms matrix elements do not depend on quantum numers Nn, hence we can denote

$$\kappa(Aa, Bb) = \sum_{Nn} K(NnAa, NnBb). \tag{12.94}$$ me133

This allows us to write equation (12.94) in the form

$$\frac{d}{dt}\ \rho_{AaBb}(t)\Big|_{d.} = \sum_{Mm}\sum_{Nn} \delta(\omega_{MA} - \omega_{NB})\ K(AaMm, BbNn)\ \rho_{MmNn}(t) - \tfrac{1}{2}\sum_{a''}\kappa(Aa'', Aa)\ \rho_{Aa''Bb}(t)\ -\ \tfrac{1}{2}\sum_{b''}\kappa(Bb, Bb'')\ \rho_{AaBb''}(t). \tag{12.95}$$

Obviously fro the nondegenerate case "small" indices play no role – they can be supressed. Then, instead of equation (12.95) we get

$$\frac{d}{dt}\ \rho_{AB}(t)\Big|_{d.} = \sum_{M}\sum_{N} \delta(\omega_{MA} - \omega_{NB})\ K(AM, BN)\ \rho_{MN}(t) - \tfrac{1}{2}\Big[\ \kappa(A, A) + \kappa(B, B)\ \Big]\ \rho_{AB}(t), \tag{12.96}$$

which is a nondegenerate analog of (12.95).

12.5 Auxiliary sections

12.5.1 Preservation of normalization

Any density operator, so also the reduced one for subsystem $\mathcal{A}$ must be normalized: $\mathrm{Tr}_A\{\rho_A(t)\} = 1$. This requirement has a simple consequence

$$\frac{d}{dt}\,\mathrm{Tr}_A\{\rho_A(t)\} = \mathrm{Tr}_A\left\{\frac{d\,\rho_A(t)}{dt}\right\} = 0. \tag{12.97}$$ mea02

Clearly the hamiltonian part (the commutator) preserves the trace, which follows from cyclic property. Hence we must check the second – dissipative part of our ME. One may ask at which stage of our derivation such a check should be made. In principle this can be done at any stage. In this section we shall do so twice. Once for standard form (12.85), and the for ME (12.95) in the energy basis.

Standard form

Taking ME in its standard form (12.85) we need to compute the following trace

$$t_S = \mathrm{Tr}_A\Big\{\sum_{\Omega}\sum_{\alpha,\beta}\Big[\,\Gamma_{\alpha\beta}(\Omega)\,A_\beta(\Omega)\,\rho_A(t)\,A^\dagger_\alpha(\Omega) - \tfrac{1}{2}\,\Gamma_{\alpha\beta}(\Omega)\,A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)\,\rho_A(t) - \tfrac{1}{2}\,\Gamma_{\alpha\beta}(\Omega)\,\rho_A(t)\,A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)\Big]\Big\}, \tag{12.98}$$

and show that it vanishes, ie., $t_S = 0$. The trace is s linear operation. so then

$$t_S = \sum_{\Omega}\sum_{\alpha,\beta}\Big[\,\Gamma_{\alpha\beta}(\Omega)\,\mathrm{Tr}_A\Big\{A_\beta(\Omega)\,\rho_A(t)\,A^\dagger_\alpha(\Omega)\Big\} - \tfrac{1}{2}\,\Gamma_{\alpha\beta}(\Omega)\,\mathrm{Tr}_A\Big\{A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)\,\rho_A(t)\Big\} - \tfrac{1}{2}\,\Gamma_{\alpha\beta}(\Omega)\,\mathrm{Tr}_A\Big\{\rho_A(t)\,A^\dagger_\alpha(\Omega)\,A_\beta(\Omega)\Big\}\Big]. \tag{12.99}$$

Cyclic property allows to see that all three traces are equal. Therefore, $t_S = 0$ and we conclude that preservation of the normalization for ME in the standard form is proved.

ME in energy basis

In this case we check the trace preservation for Eq.(12.95). Thus we must put $Bb = Aa$ (and consequently, in the last term we change $b'' \to a''$). We need to compute

$$\begin{aligned} t_S &= \sum_{Aa}\frac{d}{dt}\,\rho_{AaAa}(t)\Big|_{d.} = \sum_{Aa}\sum_{Mm,Nn}\delta(\omega_{AM}-\omega_{AN})\,K(AaMm,AaNn)\,\rho_{MmNn}(t) \\ &\quad - \tfrac{1}{2}\sum_{Aa}\sum_{a''}\kappa(Aa'',Aa)\,\rho_{Aa''Aa}(t) \\ &\quad - \tfrac{1}{2}\sum_{Aa}\sum_{a''}\kappa(Aa,Aa'')\,\rho_{AaAa''}(t). \end{aligned} \tag{12.100}$$

In the first term we have $\delta(\omega_{AM}-\omega_{AN}) == \delta(\omega_{NM}) = \delta_{NM},$. hence, $M = N$ oraz $n = m'$. We now find

$$\begin{aligned} t_S &= \sum_{Aa}\sum_{Mm,m'}K(AaMm,AaMm')\,\rho_{MmMm'}(t) \\ &\quad - \tfrac{1}{2}\sum_{Aa}\sum_{a''}\kappa(Aa'',Aa)\,\rho_{Aa''Aa}(t) - \tfrac{1}{2}\sum_{Aa}\sum_{a''}\kappa(Aa,Aa'')\,\rho_{AaAa''}(t). \end{aligned} \tag{12.101}$$

In the first term we use definition of the parameter κ (see (12.94)). In the second one we notice that indices a oraz a'' concern the same multiplet A, so the summation range is also the same. We can interchange $a \to a''$ and obtain

$$\begin{aligned} t_S &= \sum_{Mm,m'}\kappa(Mm,Mm')\,\rho_{MmMm'}(t) \\ &\quad - \tfrac{1}{2}\sum_{Aa}\sum_{a''}\kappa(Aa,Aa'')\,\rho_{AaAa''}(t) - \tfrac{1}{2}\sum_{Aa}\sum_{a''}\kappa(Aa,Aa'')\,\rho_{AaAa''}(t). \end{aligned} \tag{12.102}$$

The second and third terms are identical and cancel out with the first one (names of summation indices are irrelevant). We have shown that in the energetic basis the trace of the reduced density operator for subsystem $\mathcal{A}$ is preserved In other words the derived ME preserves normalization.

12.5.2 Hermiticity of the reduced density operator

The nect necessary property of any density operator is its hermiticity. If the equation of motion for $\rho_A^\dagger(t)$ is identical with the similar equatin for $\rho_A(t)$, then the same equations must yield the same solutions, this means that $\rho_A^\dagger(t) = \rho_A(t)$ – hermiticity of the reduced density operator for subsystem $\mathcal{A}$. Free evolution is given by the hamiltonian term $(-i/\hbar)\,[H_A + H_{LS},\ \rho_A(t)\ ]$ which poses no problems due to the commutator properties. One need to investigate the dissipative part of ME. Bada wic trzeba pozosta, dyssypatywn cz uzyskanego ME. As in the previous section we perform such a check for Me in standard form and for the one in energy basis.

Standard form

We take the hermitian conjugate of the dissipative part of ME

$$\frac{d}{dt}\ \rho_A^\dagger(t)\Big|_{d.} = +\ \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}\Big\{\ \Gamma^*_{\alpha\beta}(\Omega)\ A_\alpha(\Omega)\ \rho_A^\dagger(t)\ A_\beta(\Omega) - \ \tfrac{1}{2}\,\Gamma^*_{\alpha\beta}(\Omega)\ \big[A^\dagger_\beta(\Omega)\ A_\alpha(\Omega),\ \rho_A^\dagger(t)\big]_+\Big\}, \tag{12.103}$$

because conjugate anticommutator is equal to the anticommutator of conjugated operators. We know (see (12.77)) that matrix $\Gamma_{\alpha\beta}$ is hermitian. Interchanging the indices $\alpha \leftrightarrow \beta$ we get

$$\frac{d}{dt}\ \rho_A^\dagger(t))\Big|_{d.} = +\ \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}\Big\{\ \Gamma_{\alpha\beta}(\Omega)\ A_\beta(\Omega)\ \rho_A^\dagger(t)\ A_\alpha(\Omega) - \ \tfrac{1}{2}\,\Gamma_{\alpha\beta}(\Omega)\ \big[A^\dagger_\alpha(\Omega)\ A_\beta(\Omega),\ \rho_A^\dagger(t)\big]_+\Big\}, \tag{12.104}$$

We see that the equation of motion for $\rho_A^\dagger$ is identical with standard form (12.85) of ME. Thus, $\rho_A^\dagger = \rho_A$ – hermiticity is preserved.

ME in energetic basis

Hermiticity of the density operator means that $\rho_{AaBb} = \rho^*_{BbAa}$. It entails, that the equation of motion for the element ρ^*_{BbAa} must be the same as for ρ_{AaBb}. We say that we investigate an equation of motion for $\rho^*_{BbAa} = \langle\, Bb\,|\,\rho\,|\,Aa\,\rangle^* = \langle\, Aa\,|\,\rho^\dagger\,|\,Bb\,\rangle$. So the equation of motion for $(\rho^\dagger)_{AaBb}$ must be the same as for ρ_{AaBb}. Starting from ME (12.95) we look for a corresponding equation for ρ^*_{BbAa}. First we need to change the indices in (12.95) (remebering that corresponding changes must be made for summation indices in all terms) and then we perform complex conjugation. In this manner we find

$$\frac{d}{dt}\ \rho^*_{BbAa}(t)\Big|_{d.} = \sum_{Mm}\sum_{Nn}\ \delta(\omega_{MB}-\omega_{NA})\ K^*(BbMm, AaNn)\ \rho^*_{MmNn}(t) - \ \tfrac{1}{2}\sum_{b''}\kappa^*(Bb'', Bb)\ \rho^*_{Bb''Aa}(t)\ -\ \tfrac{1}{2}\sum_{a''}\kappa^*(Aa, Aa'')\ \rho^*_{BbAa''}(t) \tag{12.105}$$

Next, we need to consider the conjugated quantities K^* and κ^*. By definition (12.89)

$$\delta(\omega_{MA}-\omega_{NB})K(AaMm, BbNn)\ = \ = \ \frac{1}{\hbar^2}\sum_{\alpha,\beta}\Gamma_{\alpha\beta}(\omega_{MA})\langle\, Aa\,|\,A_\beta\,|\,Mm\,\rangle\langle\, Bb\,|\,A_\alpha\,|\,Nn\,\rangle^*. \tag{12.106}$$

We take complex conjugates, use hermiticity of matrix $\Gamma_{\alpha\beta}$ and we notice that the presence of the Kronecker delta allows to change the argument in Γ. Interchanging the summation indices $\alpha \leftrightarrow \beta$ we have

$$\delta(\omega_{MA}-\omega_{NB})K^*(AaMm,BbNn) \;=\; \\ =\; \frac{1}{\hbar^2}\sum_{\alpha,\beta}\Gamma_{\alpha\beta}(\omega_{NB})\langle\, Bb\,|\,A_\beta\,|\,Nn\,\rangle\langle\, Aa\,|\,A_\alpha\,|\,Mm\,\rangle^*. \tag{12.107}$$

Comparing this relation with definition (12.89) we see that

$$\delta(\omega_{MA}-\omega_{NB})K^*(AaMm,BbNn) \;=\; \delta(\omega_{MA}-\omega_{NB})K(BbNn,AaMm). \tag{12.108}$$ meb06

We consider the parameter $\kappa^*(Aa'',Aa)$. In the above relation we substitute $Aa \to Nn$, $Mm \to Aa''$, $Bb \to Nn$ and $Nn \to Aa$. Then

$$\delta(\omega_{AN}-\omega_{AN})K^*(NnAa'',NnAa) \;=\; \delta(\omega_{AN}-\omega_{AN})K(NnAa,NnAa''). \tag{12.109}$$ meb08

Obviously Kronecker deltas are equal to one, so they are unimportant. Using this result in the definition (12.94) of the parametr κ we get

$$\kappa^*(Aa'',Aa) \;=\; \sum_{Nn}K^*(NnAa'',NnAa) \;=\; \sum_{Nn}K(NnAa,NnAa'') \;=\; \kappa^*(Aa,Aa''). \tag{12.110}$$ meb10

Returning to the analysis of formula (12.105) we use the proven relations (12.108) i (12.110). At the same time, in the first term in the right hand side we interchange the summation indices $Mm \leftrightarrow Nn$. Moreover we recall that Kronecker delta is even. Thus, we have

$$\frac{d}{dt}\;\rho^*_{BbAa}(t)\Big|_{d.} \;=\; \sum_{Mm}\sum_{Nn}\delta(\omega_{MA}-\omega_{NB})\;K(AaMm,BbNn)\;\rho^*_{NnMm}(t) \\ -\;\tfrac{1}{2}\sum_{b''}\kappa(Bb,Bb'')\;\rho^*_{Bb''Aa}(t) \;-\; \tfrac{1}{2}\sum_{a''}\kappa(Aa'',Aa)\;\rho^*_{BbAa''}(t) \tag{12.111}$$

Comparing this result with Eq.(12.95) we find that when in (12.95) we replace ρ_{AaBb} by ρ^*_{BbAa} (consequently in all the terms) then we will arrive at (12.111). To see thais better recall that $\rho^*_{BbAa} = (\rho^\dagger)_{AaBb}$ and rewrite (12.111) in the form

$$\frac{d}{dt}\;\left[\rho^\dagger(t)\right]_{AaBb}(t)\Big|_{d.} \;=\; \sum_{Mm}\sum_{Nn}\delta(\omega_{MA}-\omega_{NB})\;K(AaMm,BbNn)\;\left[\rho^\dagger(t)\right]_{MmNn} \\ -\;\tfrac{1}{2}\sum_{b''}\kappa(Bb,Bb'')\;\left[\rho^\dagger(t)\right]_{AaBb''} \;-\; \tfrac{1}{2}\sum_{a''}\kappa(Aa'',Aa)\;\left[\rho^\dagger(t)\right]_{Aa''Bb} \tag{12.112}$$

This equation is formally identical with Eq.(12.95), hence $\rho = \rho^\dagger$, what we intended to show. Our ME preserve hermiticity of the reduced density operator of subsystem $\mathcal{A}$.

12.5.3 Transformation to interaction picture

In this section we consider the derivation of Eq. (12.5), the von Neumann equation in the interaction picture. Moreover, we will show that the reduction of the density operator is invariant with respect to the choice of the picture. We will also consider the transformation from Schrödingera picture to the interaction one. For clarity, we will use somewhat simplified notation, We consider an equation of motion

$$i\hbar \frac{d}{dt}\ \rho(t) = \big[\ H_0 + V,\ \rho(t)\ \big]. \tag{12.113}$$

Let us perform the transformation

$$\widetilde{\varrho}(t)\ =\ e^{iH_0t/\hbar}\,\rho(t)\,e^{-iH_0t/\hbar}, \tag{12.114}$$

which can be easily inverted, to yield

$$\rho(t) = e^{-iH_0t/\hbar}\,\widetilde{\varrho}(t)\,e^{iH_0t/\hbar}. \tag{12.115}$$

Inserting this relation into Eq.(12.113) we get

$$\begin{aligned} i\hbar\Big\{ &\left(-\frac{i}{\hbar}\,H_0\right) e^{-iH_0t/\hbar}\,\widetilde{\varrho}(t)\,e^{iH_0t/\hbar} \\ &+\ e^{-iH_0t/\hbar}\left(\frac{d}{dt}\ \widetilde{\varrho}(t)\right) e^{iH_0t/\hbar} \\ &\qquad +e^{-iH_0t/\hbar}\,\widetilde{\varrho}(t)\left(\frac{i}{\hbar}\,H_0\right)e^{iH_0t/\hbar}\Big\} \\ =\ &(\ H_0+V\ )\,e^{-iH_0t/\hbar}\,\widetilde{\varrho}(t)\,e^{iH_0t/\hbar}\ -\ e^{-iH_0t/\hbar}\,\widetilde{\varrho}(t)\,e^{iH_0t/\hbar}\,(\ H_0+V\ ). \end{aligned} \tag{12.116}$$

We see that the terms containing H_0 at both sides cancel out. As a result we are left with

$$\begin{aligned} i\hbar\,e^{-iH_0t/\hbar}&\left(\frac{d}{dt}\ \widetilde{\varrho}(t)\right) e^{iH_0t/\hbar} \\ &=\ V\,e^{-iH_0t/\hbar}\,\widetilde{\varrho}(t)\,e^{iH_0t/\hbar}\ -\ e^{-iH_0t/\hbar}\,\widetilde{\varrho}(t)\,e^{iH_0t/\hbar}\,V. \end{aligned} \tag{12.117}$$

Multiplying at the left by $e^{iH_0t/\hbar}$ and at the right by $e^{-iH_0t/\hbar}$ we get

$$i\hbar\,\frac{d}{dt}\ \widetilde{\varrho}(t)\ =\ e^{iH_0t/\hbar}\,V\,e^{-iH_0t/\hbar}\,\widetilde{\varrho}(t)\ \ -\ \widetilde{\varrho}(t)\,e^{iH_0t/\hbar}\,V\,e^{-iH_0t/\hbar}. \tag{12.118}$$

Interaction operator is here transformed in an exactly the same way as specified in Eq. (12.114). So we define

$$\widetilde{V}(t)\ =\ e^{iH_0t/\hbar}\,V\,e^{-iH_0t/\hbar}, \tag{12.119}$$

which allows us to write Eq. (12.118) as

$$i\hbar\,\frac{d}{dt}\ \widetilde{\varrho}(t)\ =\ \big[\ \widetilde{V}(t),\ \widetilde{\varrho}(t)\ \big]. \tag{12.120}$$

Transformation (12.114) or (12.119) can be applied to any operator. We stress that we made no assumptions concerning neither the structure of the space in which the operators act nor the structure of the operator space. Transformation from A to $\widetilde{A}(t) = e^{iH_0t/\hbar}\ A\ e^{-iH_0t/\hbar}$, is called the transformation from Schrödinger picture to interaction one. The free evolution is "transformed out" only the influence of interaction remains. This explains the adopted terminology.

Before proceeding further, let us note that the definition of the reduced density operator and the definition (12.114) of the transformation to the interaction picture imply that the operator $\rho_A(t)$ is expressed as

$$\rho_A(t) \ = \ \mathrm{Tr}_B\{\rho_{AB}(t)\} \ = \ \mathrm{Tr}_B\left\{\, e^{-iH_0t/\hbar}\ \widetilde{\varrho}_{AB}(t)\ e^{iH_0t/\hbar}\,\right\}. \tag{12.121}$$ mec09

We note that the free evolution of each of the subsystems written as

$$|\,\varphi_A(0)\,\rangle \otimes |\,\psi_B(0)\,\rangle \longrightarrow |\,\varphi_A(t)\,\rangle \otimes |\,\psi_B(t)\,\rangle, \tag{12.122}$$ mec10a

can be expressed with the aid of the operator

$$\exp\left(-\frac{i}{\hbar}H_0t\right) \ = \ \exp\left(-\frac{i}{\hbar}H_At\right) \otimes \exp\left(-\frac{i}{\hbar}H_Bt\right), \tag{12.123}$$ mec10b

because both hamiltonians are fully independent and commute. In Eq.(12.121) we compute the trace only over reservoir variables, so we can write

$$\rho_A(t) = e^{-iH_At/\hbar}\,\mathrm{Tr}_B\left\{\, e^{-iH_Bt/\hbar}\ \widetilde{\varrho}_{AB}(t)\ e^{iH_Bt/\hbar}\,\right\} e^{iH_At/\hbar}. \tag{12.124}$$ mec11

Cyclic property of the trace yields

$$e^{iH_At/\hbar}\ \rho_A(t)\ e^{-iH_At/\hbar} \ = \ \mathrm{Tr}_B\left\{\ \widetilde{\varrho}_{AB}(t)\ \right\}. \tag{12.125}$$ mec12

Left hand side represents the reduced density operator in the interaction picture (it depends solely on the variables of the subsystem $\mathcal{A}$). Hence, we have

$$\widetilde{\varrho}_A(t) \ = \ \mathrm{Tr}_B\left\{\ \widetilde{\varrho}_{AB}(t)\ \right\}. \tag{12.126}$$ mec13

This relation is formally identical with the definition of the reduced density operator in the Schrödinger picture. The relation between the reduced density and the total one is the same in both pictures. In other words, reduction of the operatora $\rho_A(t) = \mathrm{Tr}_B\left\{\ \rho_{AB}(t)\ \right\}$, is invariant with respect to the change of the pictures.

12.5.4 Two time scales and consequences

Order of magnitude of time T_A

The key role in our considerations is played by the assumption that (12.14), to jest warunek

$$\tau_B \ll \Delta t \ll T_A. \tag{12.127}$$ med01

In other words we assume that there exist two, quite distinst, time scales. Firstly, let us try to estimate the time T_A which characterizes the evolution of system $\mathcal{A}$ which is due to the interaction with reservoir. To find such an estimate we use Eq. (12.30), that is

$$\Delta\,\widetilde{\varrho}_A(t) \;=\; \left(\frac{1}{i\hbar}\right)^2 \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2\; \mathrm{Tr}_B\Big[\,\widetilde{V}_{AB}(t_1),\;\big[\,\widetilde{V}_{AB}(t_2),\;\widetilde{\varrho}_A(t)\otimes\bar{\sigma}_B\,\big]\Big]\,. \quad (12.128)$$

where we employed the discussed properties of the resevoir. We also recall that the main contribution to the integrals comes from a thin belt (of width τ_B lying below the diagonal $t_1 = t_2$. This allows us to estimate the integrand in the following way

$$\mathrm{Tr}_B\Big[\,\widetilde{V}_{AB}(t_1),\;\big[\,\widetilde{V}_{AB}(t_2),\;\widetilde{\varrho}_A(t)\otimes\bar{\sigma}_B\,\big]\Big] \;\sim\; \widetilde{\varrho}_A\,\mathrm{Tr}_B\Big\{\,\widetilde{V}^2\bar{\sigma}_B\,\Big\} \;=\; V^2\widetilde{\varrho}_A. \quad (12.129)$$

Hence, left hand side of Eq.(12.128) is estimated by

$$\frac{\Delta\widetilde{\varrho}_A}{\Delta t} \;\sim\; \frac{1}{\hbar^2}\,\tau_B\,V^2\widetilde{\varrho}_A, \quad (12.130)$$

because the area of the integration region is estimated by the product $\tau_B\Delta t$ (area of the belt under the diagonal $t_1 = t_2$). Introduced parameter V characterizes the "strength" of the interaction between the reservoir and system $\mathcal{A}$. The factoe which multiplies mnocy $\widetilde{\varrho}_A$ in (12.130) has (according to (12.13)) the sense of the inverse of time T_A. Therefore, we obtain an estimate

$$\frac{1}{T_A} \;\sim\; \frac{V^2\tau_B}{\hbar^2}, \qquad \text{lub} \qquad T_A \;\sim\; \frac{\hbar^2}{V^2\tau_B}. \quad (12.131)$$

Condition for existence of two time scales

What is the condition of the existence of two time scales? The estimate of T_A given in (12.131) allows us to find such a condition. Let us look upon condition $\tau_B \ll T_A$ more carefully and introduce the estimate (12.131). This yields

$$\tau_B \ll \frac{\hbar^2}{V^2\tau_B} \qquad \Longrightarrow \qquad \frac{V\tau_B}{\hbar} \ll 1. \quad (12.132)$$

The last inequality is the sought condition of existence of two time scales. If we denote $\Omega_{AB} = V/\hbar$, then we can write $\Omega_{AB}\tau_B \ll 1$. So the interaction must be characterized by such Bohr frequency Ω_{AB} that during the time interval of magnitude of τ_B its influence on system $\mathcal{A}$ is negligibly small.

Justification of weak coupling approximation

We already mentioned (see the discussion of Eq.(12.11)), it is possible to iterate von Neumanna equation – accounting of higher order corrections would increase accuracy. We can estimate these higher order terms in the same manner as done above. For example for the third order term we have

$$\frac{\Delta\widetilde{\varrho}_A}{\Delta t}\Big|^{(3)} \;\sim\; \frac{V^3}{\hbar^3}\,\tau_B^2\,\widetilde{\varrho}_A, \quad (12.133)$$

because times t_1, t_2 oraz t_3 must be close to each other (with accuracy of the order of τ_B). Then the region of integration has volume of the order of $\tau_B^2 \Delta t$. Due to Eq.(12.131) we get

$$\left.\frac{\Delta\widetilde{\varrho}_A}{\Delta t}\right|^{(3)} \sim \frac{V\tau_B}{\hbar}\cdot\frac{1}{T_A}\,\widetilde{\varrho}_A \ll \frac{1}{T_A}\,\widetilde{\varrho}_A, \tag{12.134}$$

Since the condition (12.132) must hold. The obtained estimate shows that the third order iteration (and similarly higher ones) are indeed negligible. Obviously this holds provided the condition (12.132) holds and ensures the existence of two distinct time scales.

Neglecting ρ_{corel}

Moving from Eq.(12.11) to (12.30) we have neglected initial correlations between systems $\mathcal{A}$ and $\mathcal{B}$. These correlations built up at earlier moments $t' < t$. This corresponds to the assumption that at some earlier moment t_0 ($t_0 < t$) both systems were uncorrelated. This happens, for example, when the interaction was switched on at an instant t_0. So the correlations described by $\widetilde{\varrho}_{corel}$ need time $t - t_0$ to appear. If the correlations exist ($\varrho_{corel} \neq 0$) then averaging of the term linear in interaction (as in expression (12.29)) Would not give zero. A wic $\varrho_{corel} \neq 0$ would result in the appearance of the linear term. Moreover, this would also automatically modify the quadratic term in (12.31). Let us estimate the magnitude of this modification (which is due to earlier interaction)

$$\frac{\Delta\widetilde{\varrho}_A}{\Delta t} \sim \frac{1}{\Delta t}\left(\frac{1}{i\hbar}\right)^2 \int_{-\infty}^{t} dt_1 \int_{t}^{t+\Delta t} dt_2\, \langle\, \widetilde{V}_{AB}(t_1)\widetilde{V}_{AB}(t_2)\,\rangle_B. \tag{12.135}$$

The integrand contains correlation functions of the reservoir. Hence the integrand would be practically zero for $|t_1 - t_2| \geq \tau_B$. The integration runs effectively from $t - \tau_B$ to $t + \tau_B$. Therefore, using condition (12.131), we estimate

$$\frac{\Delta\widetilde{\varrho}_A}{\Delta t} \sim \frac{1}{\Delta t}\cdot\frac{V^2}{\hbar^2}\,\tau_B^2 = \frac{V^2\tau_B}{\hbar^2}\cdot\frac{\tau_B}{\Delta t} = \frac{1}{T_A}\cdot\frac{\tau_B}{\Delta t}, \tag{12.136}$$

as the integrals are nonzero on the interval of the length of the order of τ_B. If $\tau_B \ll \Delta t$ then the correction is small (main contribution to the evolution of $\widetilde{\varrho}_A$ is of the order of $1/T_A$, which is quite larger). The key assumption that $\tau_B \ll \Delta t$ allows us to conclude that the correlations between system $\mathcal{A}$ and $\mathcal{B}$ which were built before moment t do not significantly change the evolution of $\widetilde{\varrho}_A(t)$, their influence is restricted to the moments from a very short interval $(t, t - \tau_B)$. New correlations, within a much longer interval $(t, t + \Delta t)$, are building up and have an effect on the evolution of $\widetilde{\varrho}_A(t)$. Initial correlations have small significance and hence it is justified to neglect them.

Discussion of the secular approximation

Secular approximation consists in replacing the function $F(\Omega' - \Omega)$ (defined in (12.68)) in (12.70) by Kronecker delta, which leads to Eq.(12.72). Our discussion of this replacement does not rise any doubts when $|\Omega' - \Omega| \ll (\Delta t)^{-1}$, because then $F(\Omega' - \Omega)$ is practically unity. On the other hand for $|\Omega' - \Omega| \gg (\Delta t)^{-1}$ the function $F(\Omega' - \Omega)$ is practically zero. The only problem is to justify the neglecting of the terms for which $|\Omega' - \Omega| \sim (\Delta t)^{-1}$.

To explain this point, first use the fact that the free evolution of matrix elements ρ_{ab} is governed by

$$\frac{d}{dt}\ \rho_{ab}^{(F)}\ =\ -\ \frac{i}{\hbar}\langle\, a\,|\big[H_A,\ \rho^{(F)}\,\big]|\,b\,\rangle\ =\ -\,i\omega_{ab}\rho_{ab}^{(F)}, \tag{12.137}$$ medd01

where the small Lamb shift (due to H_{LS} is ignored. The solution is simple

$$\rho_{ab}^{(F)}(t)\ =\ e^{-i\omega_{ab}t}\rho_{ab}^{(F)}(0). \tag{12.138}$$ medd02

Now, we analyze the dissipative term which is given by (12.90). We do not discuss the nuances connected with possible degeneracies. Obviously, we can write

$$\rho_{mb}=\sum_k \delta_{bk}\rho_{mk}\qquad\text{oraz}\qquad \rho_{am}=\sum_k \delta_{ak}\rho_{km}, \tag{12.139}$$ medd04

which we use in (12.90), moreover, we interchange indices $k\leftrightarrow n$ in the second term and similarly, in the third one we first interchange $m\leftrightarrow n$ and then $k\leftrightarrow m$. The result is

$$\begin{aligned}\frac{d}{dt}\ \rho_{ab}(t)\Big|_{d.}\ =&\ \sum_{m,n}\delta(\omega_{ma}-\omega_{nb})\ K(am,bn)\ \rho_{mn}(t)\\ &-\tfrac{1}{2}\sum_{k,m,n}\delta_{bn}\,\delta(\omega_{mk}-\omega_{ak})\ K(km,ka)\ \rho_{mn}(t)\\ &-\tfrac{1}{2}\sum_{k,m,n}\delta_{am}\,\delta(\omega_{bk}-\omega_{nk})\ K(kb,kn)\ \rho_{mn}(t).\end{aligned} \tag{12.140}$$

We note that δ_{bn} implies $b=n$, and then $\omega_{nb}=0$. Therefore

$$\delta_{bn}\,\delta(\omega_{mk}-\omega_{ak})=\delta_{bn}\,\delta(\omega_{ma})=\delta_{bn}\,\delta(\omega_{ma}-\omega_{nb}), \tag{12.141}$$ medd08

since $\omega_{nb}=0$ and changes nothing. Similarly we have

$$\delta_{am}\,\delta(\omega_{bk}-\omega_{nk})=\delta_{am}\,\delta(-\omega_{nb})=\delta_{bn}\,\delta(\omega_{ma}-\omega_{nb}), \tag{12.142}$$ medd09

Finally, we note that $\delta(\omega_{ma}-\omega_{nb})=\delta(\omega_{ab}-\omega_{mn})$, because Kronecker delta is even. After hese manipulations Eq. (12.140) can be written as

$$\begin{aligned}\frac{d}{dt}\ \rho_{ab}(t)\Big|_{d.}\ =&\ \sum_{m,n}\delta(\omega_{ab}-\omega_{mn})\Big\{K(am,bn)-\tfrac{1}{2}\,\delta_{bn}\,\sum_k K(km,ka)\\ &-\tfrac{1}{2}\,\delta_{am}\,\sum_k K(kb,kn)\Big\}\,\rho_{mn}(t).\end{aligned} \tag{12.143}$$ medd07

The expression in braces is denoted as $M_{am,bn}$ and we have

$$\frac{d}{dt}\ \rho_{ab}(t)\Big|_{d.}\ =\ \sum_{m,n}\delta(\omega_{ab}-\omega_{mn})M_{am,bn}\,\rho_{mn}(t). \tag{12.144}$$ medd13

This is a specific form of ME, but useful in the discussion. However, in the degenerate case some care must be exercised and renewed considerations might be necessary.

We proceed to the discussion of conditions and/or possibilities of neglecting the terms for which $|\Omega' - \Omega| \sim (\Delta t)^{-1}$. Interaction with the reservoir certainly modifies the free evolution of $\rho_{ab}^{(S)}(t) = e^{-i\omega_{ab}t}\rho_{ab}^{(S)}(0)$ If Bohr frequencies of the oscillating elements ρ_{ab} i ρ_{mn} are such that $|\omega_{ab} - \omega_{mn}| \gg 1/T_A$, then mutual couplings between these elements are quickly averaged to zero (interfere destructively) before time T_A elapses and the influence of interaction has enough time to affect the evolution. In other words, if $|\omega_{ab} - \omega_{mn}|$ differs much from $1/T_A$ then the coupling between corresponding matrix elements will have small (weak) effect. This is the situation similar to the one encountered in perturbation theory. Namely, when the energies $|E_a - E_b| \gg V_{ab} = \langle\, a \,|\, V \,|\, b \,\rangle$ then the perturbation has small (usually negligible) effect.

Since, by assumption $T_A \gg \Delta t$ the discussed situation corresponds, in fact, to the relation $|\omega_{ab} - \omega_{cd}| \sim (\Delta t)^{-1}$. This, in turn means, that such terms have little influence on the evolution of the operator $\rho_A(t)$. Such terms are neglected while passing from Eq. (12.70) to (12.72). Thus the last of our approximations is justified.

12.5.5 $V_{AB} = V_{Ab}^{\dagger}$ – nonhermiticity of operators A_α i X_α

In our considerations we have adopted the interaction hamiltonian between the system $\mathcal{A}$ and reservoir $\mathcal{B}$ in the form $V_{AB} = \sum_\alpha A_\alpha \otimes X_\alpha$, where operators A_α and X_{alpha} does not have to be hermitian. Certainly the full interaction hamiltonian must be hermitian, so we conclude that it must contain operators A_α, X_α and their hermitian conjugates $A_\alpha^\dagger$, $X_\alpha^\dagger$. Constructing linear combinations we can always transform the hamiltonian VAB into $V_{AB} = \sum_\alpha A_\alpha^{'} \otimes X_\alpha^{'}$, where the primed operators are hermitian.

We shall illustrate this with a simple example. Let the interaction hamiltonian be of the form

$$V_{AB} \;=\; A \otimes X^\dagger \;+\; A^\dagger \otimes X, \tag{12.145}$$ mee03

where operators A oraz X are nonhermitian, while the full hamiltonian is clearly hermitian. We define new operators

$$\begin{aligned} q &= \frac{1}{\sqrt{2}}\big(A + A^\dagger\big), & Q &= \frac{1}{\sqrt{2}}\big(X + X^\dagger\big), \\ p &= \frac{i}{\sqrt{2}}\big(A - A^\dagger\big), & P &= \frac{i}{\sqrt{2}}\big(X - X^\dagger\big), \end{aligned} \tag{12.146}$$

which ar evidently hermitian. Expressing operators A, X and their conjugates we obtain

$$\begin{aligned} V_{AB} &= \tfrac{1}{2}\big(q - ip\big) \otimes \big(Q + iP\big) \;+\; \tfrac{1}{2}\big(q + ip\big) \otimes \big(Q - iP\big) \\ &= q \otimes Q \;+\; p \otimes P. \end{aligned} \tag{12.147}$$

This interaction hamiltonian is expressed as a sum of products of hermitian operators. Hence construction of the interaction hamiltonian with nonhermitian operators is allowed. One can always build necessary combinations. However, in some practical applications it is much more convenient to use nonhermitian operators than the linear combinations.

12.5.6 Vanishing average $\langle X_\alpha \rangle_B$

In the main part of the lecture we assumed that Eq.(12.27) holds, that is the average $\langle X_\alpha \rangle_B \equiv \mathrm{Tr}_B \{ X_\alpha \rho_B(t) \} = 0$. We have stated that it is not really restrictive. We will show that it is true. This is so, because we can always shift the energy scale. To see this, let us write

$$\begin{aligned} V'_{AB} &= \sum_\alpha A_\alpha \otimes \big(X_\alpha - \langle X_\alpha \rangle_B\big) \\ &= \sum_\alpha A_\alpha \otimes X_\alpha - \sum_\alpha \langle X_\alpha \rangle_B \big(A_\alpha \otimes \mathbf{1}_B\big), \end{aligned} \tag{12.148}$$

where $\langle X_\alpha \rangle_B = \mathrm{Tr}_B\{\bar{\sigma}_B X_\alpha\}$ is a number not necessarily equal to zero. Then we have

$$\langle V'_{AB} \rangle_B = \sum_\alpha A_\alpha \big(\langle X_\alpha \rangle_B - \langle X_\alpha \rangle_B\big) = 0, \tag{12.149}$$ mef2

which holds no matter whether numbers $\langle X_\alpha \rangle_B$ are zeroes or not. Full hamiltonian can then be written as

$$\begin{aligned} H_{AB} &= H_A \otimes \mathbf{1}_B + \mathbf{1}_A \otimes H_B + V_{AB} \\ &= H_A \otimes \mathbf{1}_B + \mathbf{1}_A \otimes H_B + V'_{AB} + \sum_\alpha \langle X_\alpha \rangle_B \big(A_\alpha \otimes \mathbf{1}_B\big) \\ &= \big[H_A + \sum_\alpha \langle X_\alpha \rangle_B A_\alpha\big] \otimes \mathbf{1}_B + \mathbf{1}_A \otimes H_B + V'_{AB}. \end{aligned} \tag{12.150}$$

Rescaled interaction term (the last one) has zero average (as in (12.149)). This is achieved be the redefinition of the energy scale in system $\mathcal{A}$ – via redefinition of the hamiltonian H_A. We conclude that the assumption that the averages (12.27) vanish is not really restrictive, but simplifies the computations.

12.5.7 Commutators of operators $A_\alpha(\Omega)$

In the main sections we have introduced the operators

$$A_\alpha(\Omega) = \sum_{a,b} \delta(\omega_{ba} - \Omega) \,|\, a \,\rangle\langle\, a \,|\, A_\alpha \,|\, b \,\rangle\langle\, b \,|. \tag{12.151}$$ meg01

The hamiltonian of system $\mathcal{A}$ is of the form

$$H_A = \sum_n \hbar\omega_n |\, n \,\rangle\langle\, n \,|. \tag{12.152}$$ meg02

It is not difficult to find the commutator $\big[H_A,\ A_\alpha(\Omega)\big]$. Directly from the definition we obtain

$$\begin{aligned}\big[H_A,\ A_\alpha(\Omega)\big] &= \Big[\sum_n \hbar\omega_n |\,n\,\rangle\langle\,n\,|,\ \sum_{a,b}\delta(\omega_{ba}-\Omega)\,|\,a\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,b\,|\Big]\\ &= \sum_{a,b,n}\hbar\omega_n\,\delta(\omega_{ba}-\Omega)\Big\{\delta_{na}|\,n\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,b\,| \;-\; \delta_{nb}|\,a\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,n\,|\Big\}\\ &= \sum_{a,b}\hbar(\omega_a-\omega_b)\,\delta(\omega_{ba}-\Omega)|\,a\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,b\,|\\ &= -\hbar\Omega\sum_{a,b}\delta(\omega_{ba}-\Omega)|\,a\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,b\,|\\ &= -\hbar\Omega A_\alpha(\Omega), \end{aligned}\tag{12.153}$$

which ends the calculation. Conjugation changes sign, so that

$$\big[H_A,\ A^\dagger_\alpha(\Omega)\big] \;=\; \hbar\Omega A^\dagger_\alpha(\Omega).\tag{12.154}$$ meg04

Heisenberg equation of motion follows from formula (12.153), and it is

$$i\hbar\frac{d}{dt}\,A^{(H)}_\alpha(\Omega) \;=\; \big[\,A^{(H)}_\alpha(\Omega),\ H_A\,\big] \;=\; \hbar\Omega A^{(H)}_\alpha(\Omega).\tag{12.155}$$ meg05

After integration we obtain $A^{(H)}_\alpha(\Omega)=e^{i\Omega t}A_\alpha(\Omega)$ which agrees with (12.42). Finally, we present one more relation

$$\big[\,H_A,\ A^\dagger_\alpha(\Omega)A_\beta(\Omega)\,\big] = A^\dagger_\alpha(\Omega)\big[\,H_A,\ A_\beta(\Omega)\,\big] \;+\; \big[\,H_A,\ A^\dagger_\alpha(\Omega)\,\big]A_\beta(\Omega)=0,\tag{12.156}$$ meg09

which follows immediately from the derived results.

12.5.8 Additional properties of correlation functions $\bar G_{\alpha\beta}(\tau)$

Correlation function of the reservoir was defined in (12.48) or (12.55). By assumption, reservoir hamiltonian H_B and the corresponding density operator $\bar\sigma_B$ commute, so they have a common set of complete and orthonormal eigenstates $|\,z\,\rangle$. Let us calculate the trace in (12.55) in chosen basis

$$\begin{aligned}\bar G_{\alpha\beta}(\tau) &= \mathrm{Tr}_B\Big\{\,\widetilde X_\alpha\dagger(\tau)\,X_\beta\,\bar\sigma_B\,\Big\} \;=\; \mathrm{Tr}_B\big\{e^{iH_B\tau/\hbar}\,X^\dagger_\alpha\,e^{-iH_B\tau/\hbar}\,X_\beta\,\bar\sigma_B\big\}\\ &= \sum_{z,\xi}\langle\,z\,|\,e^{iH_B\tau/\hbar}\,X^\dagger_\alpha\,e^{-iH_B\tau/\hbar}\,|\,\xi\,\rangle\langle\,\xi\,|\,X_\beta\,\bar\sigma_B\,|\,z\,\rangle\end{aligned}\tag{12.157}$$

In Eq.(12.19) we denoted the eigenvalues of $\bar\sigma_B$ by $p(z)$, hence

$$\bar G_{\alpha\beta}(\tau)=\sum_{z,\xi}p(z)\;e^{i\omega_{z\xi}\tau}\langle\,z\,|\,X^\dagger_\alpha\,|\,\xi\,\rangle\langle\,\xi\,|\,X_\beta\,|\,z\,\rangle,\tag{12.158}$$ meh03

with $\omega_z=E_z/\hbar$, and $\omega_{z\xi}=\omega_z-\omega_\xi$.

Expression (12.158) shows that the correlation function $\bar G_{\alpha\beta}(\tau)$ is a complicated superposition of functions which oscillate with Bohr frequencies $\omega_{z\xi}$. Reservoir is assumed to be large, the discussed frequencies are are densely space (quasi-continuous). If time τ is sufficiently large the oscillations interfere destructively (average out to zero). We can expect that reservoir correlation function decay quickly when time $\tau=t_1-t_2$ increases. Characteristic decay time is denoted by τ_B and assumed to be, by far, the shortest time characterising the system $\mathcal{A}+\mathcal{B}$. When $\tau>\tau_B$ the correlation may be neglected.

12.5.9 Positivity of the matrix $\Gamma_{\alpha\beta}(\Omega)$

12.5.10 Calculation of matrix elements $\Delta_{\alpha\beta}(\Omega)$

12.5.11 Evolution $\big[H_A + H_{LS},\ \rho_A(t)\big]$

12.6 Summary

In this summary we describe practical steps neede in the construction of the ME for specified physical systems.

The first step consists in precise definition of the system $\mathcal{A}$ and of the reservoir $\mathcal{B}$. We need to specify their free hamiltonians H_A and H_B and (at least sometimes) their eigenenergies and eigenstates. Then we define the interaction hamiltonian in the form

$$V_{AB} \ = \ \sum_\alpha \ A_\alpha \otimes X_\alpha \ = \ \sum_\alpha \ A_\alpha^\dagger \otimes X_\alpha^\dagger, \tag{12.159}$$ mep01

where $A_\alpha,\ X_\alpha$ are (correspondingly) operators of system $\mathcal{A}$ and reservoir. We stress that these operator do not need to be (separately) hermitian. It suffices that the full interaction hamiltonian is hermitian. We also need to specify the density operator $\bar\sigma_B$ describing the state of the reservoir. It is worth remembering that operator H_B and $\bar\sigma_B$ commute. This implies that the reservoir is in the stationary state. In the second step of ME construction we build (identify) the following operators

$$A_\alpha(\Omega) = \sum_{a,b} \delta(\omega_{ba} - \Omega)\ |\,a\,\rangle\langle\,a\,|\,A_\alpha\,|\,b\,\rangle\langle\,b\,|. \tag{12.160}$$ mep02

The following matrix elements are computed in the third step

$$W_{\alpha\beta}(\Omega) = \int_0^\infty d\tau\ e^{i\Omega\tau}\ \bar G_{\alpha\beta}(\tau) = \int_0^\infty d\tau\ e^{i\Omega\tau}\ \mathrm{Tr}_B\big\{\widetilde X_\alpha^\dagger(\tau)\, X_\beta \bar\sigma_B\big\}. \tag{12.161}$$ mep03

They are seen to be partial Fourier transform of the reservoir correlation functions. Reservoir operatora are taken in the interaction picture

$$\widetilde X_\alpha(t) \ = \ e^{iH_Bt/\hbar}\ X_\alpha\ e^{-iH_Bt/\hbar}. \tag{12.162}$$ mep04

Matrix elements $W_{\alpha\beta}(\Omega)$ are then employed to construct two hermitian matrices

$$\Gamma_{\alpha\beta}(\Omega) = W_{\alpha\beta}(\Omega)\ +\ W^*_{\beta\alpha}(\Omega), \qquad \Delta_{\alpha\beta}(\Omega) = \frac{1}{2i}\big[\,W_{\alpha\beta}(\Omega)\ -\ W^*_{\beta\alpha}(\Omega)\,\big]. \tag{12.163}$$ mep05

We note that matrix $\Gamma_{\alpha\beta}(\Omega)$ is positive-definite and can be computed directly as Fourier transform

$$\Gamma_{\alpha\beta}(\Omega) = \int_{-\infty}^\infty d\tau\ e^{i\Omega\tau}\ \mathrm{Tr}_B\big\{\widetilde X_\alpha^\dagger(\tau) X_\beta\bar\sigma_B\big\} = \int_{-\infty}^\infty d\tau\ e^{i\Omega\tau}\bar G_{\alpha\beta}(\tau). \tag{12.164}$$ mep06a

Matrix $\Gamma_{\alpha\beta}(\Omega)$, in practical applications, is more important than $\Delta_{\alpha\beta}(\Omega)$. Explanation will be given later. The separate expression for elements $\Delta_{\alpha\beta}(\Omega)$ is

$$\Delta_{\alpha\beta}(\Omega) = \frac{1}{2i}\Big[\int_0^\infty d\tau\ e^{i\Omega\tau}\ \mathrm{Tr}_B\big\{\widetilde X_\alpha^\dagger(\tau) X_\beta\bar\sigma_B\big\}\ -\ \int_0^\infty d\tau\ e^{-i\Omega\tau}\ \mathrm{Tr}_B\big\{X_\alpha^\dagger\widetilde X_\beta(\tau)\bar\sigma_B\big\}\Big].$$

(12.165) mep6b

Hence, calculation of matrix $W_{\alpha\beta}(\Omega)$ can be usually omitted

Final construction of the proper ME is the fourth and the last step. The above given quantities allow us to write the ME as

$$\frac{d}{dt}\ \rho_A(t)\ = -\frac{i}{\hbar}\big[H_A + H_{LS},\ \rho_A(t)\big] + \frac{1}{\hbar^2}\sum_{\Omega}\sum_{\alpha,\beta}\Gamma_{\alpha\beta}(\Omega)\Big\{\ A_\beta(\Omega)\,\rho_A(t)\,A^\dagger_\alpha(\Omega)\ -\ \tfrac{1}{2}\Big[A^\dagger_\alpha(\Omega)\,A_\beta(\Omega),\ \rho_A(t)\Big]_+\Big\} \quad (12.166)$$

where the so-called Lamb-shift hamiltonian H_{LS} is given as

$$H_{LS} = \frac{1}{\hbar}\sum_{\Omega}\sum_{\alpha,\beta}\Delta_{\alpha\beta}(\Omega)A^\dagger_\alpha(\Omega)A_\beta(\Omega). \quad (12.167)$$ mep08

Energy shifts of the system $\mathcal{A}$ which are due to the presence of H_{LS} in the hamiltonian part , are usually quite small and frequently negligible. This explains why the role of matrix $\Delta_{\alpha\beta}$ is usually less important than that of matrix $\Gamma_{\alpha\beta}$.

* *

Part III

APENDICIES

Appendix A

Fourier transforms

ap:ff

A.1 Time–frequency Fourier transforms

A.1.1 Definition of the pair of Fourier transforms

Time–frequency Fourier transforms are essentially one–dimensional. Therefore we define
z1ftdef a pair of Fourier transforms similarly as in the main text (see Eqs.(8.19)), and we write

$$F(\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, f(t), \tag{A.1a}$$

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\, F(\omega). \tag{A.1b}$$

z1ftform These equation can be formally written as

$$\mathcal{F}[f] = F(\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, f(t), \tag{A.2a}$$

$$\mathcal{F}^{-1}[F] = f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\, F(\omega). \tag{A.2b}$$

In the forthcoming we will briefly discuss some of the most important properties of one–dimensional (time–frequency) Fourier transforms.

A.1.2 Dirac's delta function and its Fourier transform

Let $f(t) = \delta(t)$. Then, according to definition (A.2), we note that

$$\mathcal{F}^{-1}[\delta] = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, \delta(t) = \frac{1}{\sqrt{2\pi}}, \tag{A.3}$$

z1ftdel

which, after substitution into the definition (A.1b) yields

$$\delta(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}. \tag{A.4}$$

z1delft

Relation (A.4) is best remembered in the form

$$2\pi\, \delta(t) = \int_{-\infty}^{\infty} d\omega\; e^{\pm i\omega t}. \tag{A.5}$$

z1rem

We note, that both signs are allowed in the exponential under the integral in (A.5). This is so, because we can easily replace ω by $-\omega$ in the integral in rhs of (A.4). Since both variables t and ω are mathematically equivalent, we can formally write

$$\mathcal{F}[1] = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t} = \sqrt{2\pi}\ \delta(\omega). \tag{A.6}$$

It may be worth remarking that the above relation for Dirac's delta function can be intuitively explained as follows

$$\begin{aligned} F(0) &= \lim_{\varepsilon\to 0} F(\varepsilon) = \lim_{\varepsilon\to 0} \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\varepsilon t} f(t) \\ &= \lim_{\varepsilon\to 0} \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\varepsilon t} \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\, F(\omega) \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, F(\omega) \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{-i\omega t}. \end{aligned} \tag{A.7}$$

From this we easily conclude that relation (A.5) follows immediately. This train of thought explains the above relationships between Fourier transforms of delta function and unit function.

A.1.3 Basic properties of Fourier transformation

Theorem A.1 *If function $f(t)$ is real, then the Fourier transform satisfies the relation*

$$F^*(\omega) = F(-\omega). \tag{A.8}$$

Proof. We compute the complex conjugate of the Fourier transform. From the definition (A.1a) we get

$$F^*(\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{-i\omega t}\, f(t) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i(-\omega)t}\, f(t) = F(-\omega). \tag{A.9}$$

which ends the proof. ■

Theorem A.2 *If function $f(t)$ is real, then the Fourier transform of $f(-t)$ is*

$$\mathcal{F}[f(-t)] = F(-\omega) = F^*(\omega). \tag{A.10}$$

Proof. We compute the Fourier transform as in the definition, and we get

$$\mathcal{F}[f(-t)] = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, f(-t). \tag{A.11}$$

We change the integration variable $t \to -t'$, and we obtain

$$\mathcal{F}[f(-t)] = \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, e^{-i\omega t'}\, f(t') = F(-\omega). \tag{A.12}$$

Since $F(-\omega) = F^*(\omega)$, the proof is completed. ■

z1th:freoe **Theorem A.3** *If function $f(t)$ is real and either even or odd, then the Fourier transform of $f(t)$ is also either even or odd.*

Proof. From previous theorems we have

$$\mathcal{F}[f(\pm t)] = F(\pm\omega), \tag{A.13}$$ z1freoe1

so it is obvious that the symmetry of $f(t)$ is inherited by the Fourier transform $F(\omega)$. ■

The convolution of two functions $f(t)$ and $g(t)$ is defined as

$$(f*g)(t) = \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t-t')\, g(t') = \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t')\, g(t-t'). \tag{A.14}$$ z1condef

Symmetry of the convolution summarized in the second equality, follows by a straightforward change of integration variables.

z1th:contr **Theorem A.4** *Fourier transform of the convolution is equal to the product of the transforms, that is*

$$\mathcal{F}\left[f*g\right](\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t} \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t-t')\, g(t') = F(\omega)\, G(\omega). \tag{A.15}$$ z1contr

Proof. We transform the convolution

$$\mathcal{F}\left[(f*g)\right](\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t} \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t-t')\, g(t'), \tag{A.16}$$ z1contr1

where we change the integration variables. Instead of t we take $\tau = t - t'$, while we leave t' unchanged. Thus we get

$$\begin{aligned}
\mathcal{F}\left[(f*g)\right](\omega) &= \int_{-\infty}^{\infty} \frac{d\tau}{\sqrt{2\pi}}\, e^{i\omega(\tau+t')} \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(\tau)\, g(t') \\
&= \int_{-\infty}^{\infty} \frac{d\tau}{\sqrt{2\pi}}\, e^{i\omega\tau} f(\tau) \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, e^{i\omega t'} g(t') \\
&= F(\omega)G(\omega).
\end{aligned} \tag{A.17}$$

which ends the proof. ■

z1th:prodtr z1prodtr **Theorem A.5** *A transform of a product of two functions is a convolution of transforms, that is*

$$\mathcal{F}[fg] = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, f(t)g(t) \tag{A.18a}$$

$$= \int_{-\infty}^{\infty} \frac{d\omega'}{\sqrt{2\pi}}\, F(\omega')G(\omega-\omega') \tag{A.18b}$$

$$= \int_{-\infty}^{\infty} \frac{d\omega'}{\sqrt{2\pi}}\, F(\omega-\omega')G(\omega') \;=\; \left[\, F*G \,\right](\omega). \tag{A.18c}$$

Proof. We substitute Fourier transforms of both functions according to (A.1a) into right-hand side of (A.18a), which yields

z1prtr

$$\mathcal{F}[fg] = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t} \int_{-\infty}^{\infty} \frac{d\omega'}{\sqrt{2\pi}}\, e^{-i\omega' t}\, F(\omega') \int_{-\infty}^{\infty} \frac{d\omega''}{\sqrt{2\pi}}\, e^{-i\omega'' t}\, G(\omega'') \tag{A.19a}$$

$$= \frac{1}{(2\pi)^{2/3}} \int_{-\infty}^{\infty} d\omega'\, F(\omega') \int_{-\infty}^{\infty} d\omega''\, G(\omega'') \int_{-\infty}^{\infty} dt\, e^{i(\omega-\omega'-\omega'')t}. \tag{A.19b}$$

According to Eq.(A.5) the last integral (over time) gives a factor $2\pi\delta(\omega - \omega' - \omega'')$ which we substitute, and arrive at the equation

$$\mathcal{F}[fg] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega'\, F(\omega') \int_{-\infty}^{\infty} d\omega''\, G(\omega'')\, \delta(\omega - \omega' - \omega''). \tag{A.20}$$

z1prtr2

Integration over $d\omega''$ gives the convolution as defined in (A.18b). Thus, the first part of the theorem (A.18c) is proved. The second relation (i.e., (A.18c)) may proved in two ways. The first proof follows if we integrate in (A.20) over $d\omega'$ instead of $d\omega''$. The second proof consists in the change of integration variable in (A.18b). We take $\omega'' = \omega - \omega'$. Then (A.18c) follows immediately. ■

Let us assume that certain function $f(t)$ has the property

$$\lim_{t\to\pm\infty} \frac{d^n}{dt^n} f(t) = 0. \tag{A.21}$$

z1fprop

for the integer n sufficiently large. Then we can formulate the following theorem.

z1th z1dertr **Theorem A.6** *The Fourier transform of the derivative is given as follows*

$$\mathcal{F}\left[\frac{d^n f(t)}{dt^n}\right] = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, \frac{d^n}{dt^n}\, f(t) \tag{A.22a}$$

$$= (-i\omega)^n \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, f(t) \tag{A.22b}$$

$$= (-i\omega)^n\, F(\omega). \tag{A.22c}$$

Proof. Integrating by parts in the rhs of Eq.(A.22a) sufficient number of times, we take into account property (A.21). We see that the boundary terms vanishes in each step of partial integration. Thus, we obtain Eq.(A.22b). Recognizing the transform of the function $f(t)$ we immediately obtain (A.22c), which completes the proof. ■

Finally, let us note that differentiating definition (A.1b) n times with respect to time we obtain

$$\frac{d^n}{dt^n}\, f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, (-i\omega)^n\, e^{-i\omega t}\, F(\omega). \tag{A.23}$$

z1ftdd

from which (A.22c) follows immediately.

We define norms of the functions in time and frequency domains

$$||f(t)||^2 = \int_{-\infty}^{+\infty} dt\, |f(t)|^2, \qquad ||F(\omega)||^2 = \int_{-\infty}^{+\infty} d\omega\, |F(\omega)|^2. \tag{A.24}$$

z1normdef

z1th:parth **Theorem A.7 (Parseval – Plancherel)** *The norms of the pair of Fourier transforms in time and frequency domains are equal, that is*

$$||f||^2 = ||F||^2, \tag{A.25}$$ z1parth

where function $f(t)$ and $F(\omega)$ are connected by relations (A.1). z1ftdef

Proof. We simply compute the norm in time domain

$$\begin{aligned} ||f(t)||^2 &= \int_{-\infty}^{+\infty} dt\ f(t)f^*(t) \\ &= \int_{-\infty}^{+\infty} dt \int_{-\infty}^{\infty} \frac{d\omega_1}{\sqrt{2\pi}}\ e^{-i\omega_1 t}\ F(\omega_1) \int_{-\infty}^{\infty} \frac{d\omega_2}{\sqrt{2\pi}}\ e^{i\omega_2 t}\ F^*(\omega_2) \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega_1 \int_{-\infty}^{+\infty} d\omega_2\ F(\omega_1)\ F^*(\omega_2) \int_{-\infty}^{+\infty} dt\ e^{-i(\omega_1-\omega_2)t}. \end{aligned} \tag{A.26}$$

The time integral yields $2\pi\delta(\omega_1-\omega_2)$, as it follows from Eq.(A.5). z1rem Hence, the last integral easily gives the norm of the transform $F(\omega)$, and the theorem is proved. ■

A.1.4 Pseudo-convolution. An auxiliary integral

We define "pseudo-convolution" as

$$K_{[fg]}(t) = \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\ f(t+t')\ g^*(t'). \tag{A.27}$$ z1pscon1

We investigate some properties of this integral.

z1th:pscon1 **Theorem A.8** *Pseudo-convolution can be expressed as*

$$K_{[fg]}(t) = \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\ f(t+t')\ g^*(t') = \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\ f(t')\ g^*(t'-t). \tag{A.28}$$ z1pscon2

Proof. The proof follows by introduction of a new integration variable $t''=t+t'$. Hence $t'=t''-t$ and we obtain

$$K_{[fg]}(t) = \int_{-\infty}^{\infty} \frac{dt''}{\sqrt{2\pi}}\ f(t'')\ g^*(t''-t), \tag{A.29}$$ z1pscon3

which completes the proof. ■

The expression (A.28) z1pscon2 for the pseudo-convolution should be compared to the definition (A.14) z1condef for convolution.

z1th:pscon2 **Theorem A.9** *Fourier transform of the pseudo-convolution is given as*

$$\mathcal{K}_{[fg]}(\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\ e^{i\omega t}\ K_{[fg]}(t) = F(\omega)\ G^*(\omega), \tag{A.30}$$ z1pscon4

so it is the same as for true convolution.

Proof. The proof follows by direct calculation from the definition

$$\mathcal{K}_{[fg]}(\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t} \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t+t')\, g^*(t') = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dt\, dt'}{2\pi}\, e^{i\omega t}\, f(t+t')\, g^*(t'). \tag{A.31}$$

Inserting Fourier transforms for functions $f(t)$ and $g^*(t)$ we get

$$\mathcal{K}_{[fg]}(\omega) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dt\, dt'}{2\pi}\, e^{i\omega t} \int_{-\infty}^{\infty} \frac{d\omega'}{\sqrt{2\pi}} e^{-i\omega'(t+t')}\, F(\omega') \int_{-\infty}^{\infty} \frac{d\omega''}{\sqrt{2\pi}} e^{i\omega''t'}\, G^*(\omega'')$$
$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{d\omega'\, d\omega''}{2\pi}\, F(\omega')\, G^*(\omega'') \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{-i(\omega-\omega')t} \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, e^{i(\omega''-\omega')t'} \tag{A.32}$$

Employing fourier transforms of the delta function (z1rem A.5), we obtain

$$\mathcal{K}_{[fg]}(\omega) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{d\omega'\, d\omega''}{2\pi}\, F(\omega')\, G^*(\omega'')\, \sqrt{2\pi}\, \delta(\omega-\omega')\, \sqrt{2\pi}\, \delta(\omega''-\omega') = \int_{-\infty}^{\infty} d\omega'\, F(\omega')\, G^*(\omega')\, \delta(\omega-\omega') \;=\; F(\omega)\, G^*(\omega) \tag{A.33}$$

which completes the proof. ■

We summarize the results of this subsection by writing pair of Fourier transforms. Firstly, the Fourier transform of the pseudo-convolution is the product of Fourier transforms (similarly as for a true convolution), as it follows from (z1pscon7 A.33): z1pscon8

$$\int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t} \left[\int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t+t')\, g^*(t') \right] \tag{A.34a}$$
$$= \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t} \left[\int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t')\, g^*(t'-t) \right] \;=\; F(\omega)\, G^*(\omega). \tag{A.34b}$$

Similarly, the inverse transform can be written as z1pscon9

$$\int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\, F(\omega)\, G^*(\omega) \tag{A.35a}$$
$$= \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t+t')\, g^*(t') \;=\; \int_{-\infty}^{\infty} \frac{dt'}{\sqrt{2\pi}}\, f(t')\, g^*(t'-t) \tag{A.35b}$$

The last relations can be easily proved in a manner similar as above.

A.1.5 Properties of the Lorentzian curve

We define a Lorentzian as a frequency dependent function

$$L(\omega) = \frac{\Gamma/\pi}{(\omega-\omega_0)^2+\Gamma^2}, \tag{A.36}$$ z1lordef

with ω_0 and Γ being real positive parameters. We intend to compute the Fourier transform

$$l(t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\, L(\omega) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\, \frac{\Gamma/\pi}{(\omega-\omega_0)^2+\Gamma^2}. \tag{A.37}$$ z1lortr1

We separate the denominator into two factors

$$l(t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\, \frac{\Gamma/\pi}{[(\omega-\omega_0)+i\Gamma]\,[(\omega-\omega_0)-i\Gamma]}. \tag{A.38}$$ z1lortr2

The integrand has two simple poles $\omega_1 = \omega_0 - i\Gamma$ and $\omega_2 = \omega_0 + i\Gamma$. Hence, our integral becomes

$$l(t) = \frac{\Gamma}{\pi}\int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, \frac{e^{-i\omega t}}{(\omega-\omega_1)\,(\omega-\omega_2)}. \tag{A.39}$$ z1lortr3

Such an integral can be computed via the residue theory. Thus, we see that the problem of evaluation of integral (A.39) reduces to the proper choice of the integration contour.

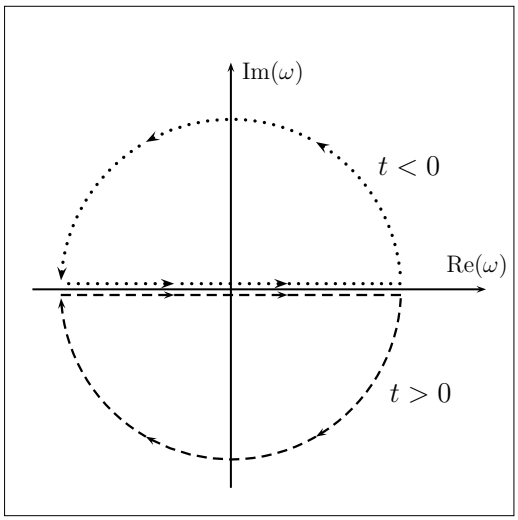

Fig. A.1: Typical integration contour for evaluation of the Fourier transforms over frequency.

Let $\omega = \alpha + i\beta$, then $e^{-i\omega t} = e^{-i(\alpha+i\beta)t} = e^{-i\alpha t+\beta t}$. Therefore we easily conclude that

- For time $t > 0$ convergence of the integral requires $\beta < 0$. This, in turn implies that ω should lie within the lower halfplane ($\mathrm{Im}(\omega) = \beta < 0$.
- On the other hand, when time $t < 0$, by the same argument of convergence we should have $\beta > 0$. So, in this case, ω should lie within the upper halfplane ($\mathrm{Im}(\omega) = \beta > 0$.

The integration contours appropriate for both case are presented in Fiq.(A.1) Jordan lemma ensures that the integrals along the arcs in lower (for $t > 0$) or upper halfplanes (for $t < 0$) tend to zero when their radius tends to infinity. The remaining integrals along the real axis reduce to the sought integrals over real axis. Hence, for time $t > 0$ we choose the contour in the lower half plane. The contour includes only one pole, namely $\omega_1 = \omega_0 - i\Gamma$. We also note that this contour has negative direction. Then by means of the residue theory we obtain

$$l(t) = -2\pi i\, \frac{1}{\sqrt{2\pi}}\, \left(\frac{\Gamma}{\pi}\right)\, \frac{e^{-i\omega_1 t}}{\omega_1-\omega_2} = \frac{1}{\sqrt{2\pi}}\, e^{-(\Gamma+i\omega_0)t}. \tag{A.40}$$ z1lortr4

Similarly, for $t < 0$ we close the contour in the upper halfplane. The contour again includes only one pole $\omega_2 = \omega_0 + i\Gamma$, and has positive direction. The residue theory yields in this case

$$l(t) = 2\pi i\, \frac{1}{\sqrt{2\pi}}\, \left(\frac{\Gamma}{\pi}\right)\, \frac{e^{-i\omega_2 t}}{\omega_2-\omega_1} = \frac{1}{\sqrt{2\pi}}\, e^{-(\Gamma-i\omega_0)|t|}, \tag{A.41}$$ z1lortr5

where we note the presence of the modulus of time in the last exponential. We can write Eqs.(A.40) and (A.41) as a single relation, in which we use the Heaviside functions to denote the corresponding time domains

$$l(t) = \frac{\theta(t)}{\sqrt{2\pi}}\, e^{-(\Gamma+i\omega_0)t} \;+\; \frac{\theta(-t)}{\sqrt{2\pi}}\, e^{(\Gamma-i\omega_0)t}, \tag{A.42}$$

z1lortr6

where the absolute value of time t is already not necessary. Combining relations (A.37) and (A.42), we finally have

z1lortr

$$\begin{aligned} l(t) \;&=\; \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, e^{-i\omega t}\, \frac{\Gamma/\pi}{(\omega-\omega_0)^2+\Gamma^2} && \text{(A.43a)}\\ &=\; \frac{1}{\sqrt{2\pi}}\, e^{-\Gamma|t|}\, e^{-i\omega_0 t}, && \text{(A.43b)}\\ &=\; \frac{\theta(t)}{\sqrt{2\pi}}\, e^{-(\Gamma+i\omega_0)t} \;+\; \frac{\theta(-t)}{\sqrt{2\pi}}\, e^{(\Gamma-i\omega_0)t}, && \text{(A.43c)} \end{aligned}$$

which completes the computation of the Fourier transform of the Lorentzian (A.36).

For pedagogical reasons it is useful to consider the inverse integral, that is the Fourier transform

$$L(\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, l(t), \tag{A.44}$$

z1lortr7

with $l(t)$ taken as in the right hand side of (A.43). Substituting $l(t)$ into Fourier integral (A.44) we obtain

$$L(\omega) = \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, \frac{\theta(t)}{\sqrt{2\pi}}\, e^{-(\Gamma+i\omega_0)t} \;+\; \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\, e^{i\omega t}\, \frac{\theta(-t)}{\sqrt{2\pi}}\, e^{(\Gamma-i\omega_0)t}. \tag{A.45}$$

z1lortr8

Simplifying, and taking into account properties of the Heaviside function, we arrive at the expression

$$L(\omega) = \frac{1}{2\pi}\int_0^{+\infty} dt\; e^{i\omega t}\; e^{-(\Gamma+i\omega_0)t} \;+\; \frac{1}{2\pi}\int_{-\infty}^{0} dt\; e^{i\omega t}\; e^{(\Gamma-i\omega_0)t}. \tag{A.46}$$

z1lortr9

In the second integral we change the integration variable $t \to -t'$, and we obtain

$$L(\omega) = \frac{1}{2\pi}\int_0^{+\infty} dt\; e^{-[\Gamma+i(\omega_0-\omega)]t} \;+\; \frac{1}{2\pi}\int_0^{+\infty} dt\; e^{-[\Gamma-i(\omega_0-\omega)]t}. \tag{A.47}$$

z1lortr10

The obtained integrals are complex conjugates, therefore we can write

$$\begin{aligned} L(\omega) &= \frac{1}{2\pi}\; 2\,\mathrm{Re}\int_0^{+\infty} dt\; e^{-[\Gamma+i(\omega_0-\omega)]t}\\ &=\; \frac{1}{\pi}\;\mathrm{Re}\,\frac{1}{\Gamma-i(\omega_0-\omega)} \;=\; \left(\frac{\Gamma}{\pi}\right)\;\frac{1}{\Gamma^2+(\omega_0-\omega)^2}. \end{aligned} \tag{A.48}$$

as it should be for the Fourier transforms $l(t)$ and $L(\omega)$.

We shall prove another extremely useful property of the Lorentzian. Let us consider an integral

$$I = \int_{-\infty}^{\infty} d\omega \; \frac{(\Gamma_1/\pi)}{(\omega-\omega_1)^2+\Gamma_1^2} \; \frac{(\Gamma_2/\pi)}{(\omega-\omega_2)^2+\Gamma_2^2}. \tag{A.49}$$ z1lor1

First, we note that this integral is proportional to the convolution of two Lorentzians. This can be shown by changing the integration variable. Instead of ω we take $\omega' = \omega - \omega_1$, and we obtain

$$I = \int_{-\infty}^{\infty} d\omega' \; \frac{(\Gamma_1/\pi)}{\omega'^2+\Gamma_1^2} \; \frac{(\Gamma_2/\pi)}{[(\omega_2-\omega_1)-\omega']^2+\Gamma_2^2}. \tag{A.50}$$ z1lor2

We see, that apart of the factor $(2\pi)^{-1/2}$, the obtained integral indeed is a convolution of two Lorentzians. Eq.(A.50) can thus, be written as

$$I = \sqrt{2\pi}\; (\, L_1 * L_2)\,(\Omega), \tag{A.51}$$ z1lor3

with $\Omega = \omega_2 - \omega_1$, and other notation following by comparison of the right hand sides of two last equations.

According to theorem (A.5) the convolution of the transforms is a transform of the product. Adopting the notation as in Eq.(A.43) to the present case we get

$$\begin{aligned} I \;&=\; \sqrt{2\pi}\; (\, L_1 * L_2)\,(\Omega) \;=\; \sqrt{2\pi}\int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\; e^{i\omega t}\; l_1(t)\, l_2(t) \\ &=\; \sqrt{2\pi}\int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\; e^{i\omega t}\; \left[\frac{\theta(t)}{\sqrt{2\pi}}\; e^{-\Gamma_1 t} \;+\; \frac{\theta(-t)}{\sqrt{2\pi}}\; e^{\Gamma_1 t}\right] \\ &\qquad\qquad \times \left[\frac{\theta(t)}{\sqrt{2\pi}}\; e^{-(\Gamma_2+i\Omega)t} \;+\; \frac{\theta(-t)}{\sqrt{2\pi}}\; e^{(\Gamma_2+i\Omega)t}\right]. \end{aligned} \tag{A.52}$$

Since $\theta(t)\,\theta(-t) = 0$, we obtain

$$I \;=\; \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi}}\; e^{i\omega t}\; \left[\frac{\theta(t)}{\sqrt{2\pi}}\; e^{-[(\Gamma_1+\Gamma_2)+i\Omega]t} \;+\; \frac{\theta(-t)}{\sqrt{2\pi}}\; e^{[(\Gamma_1+\Gamma_2)+i\Omega]t}\right]. \tag{A.53}$$ z1lor5

We recognize the Fourier transform of the Lorentzian (cf. (A.43)), and we have

$$I \;=\; \frac{(\Gamma_1+\Gamma_2)/\pi}{(\Gamma_1+\Gamma_2)^2+\Omega^2}. \tag{A.54}$$ z1lor6

Connecting equations (A.49) and (A.54) we finally have the following result

$$\int_{-\infty}^{\infty} d\omega \; \frac{(\Gamma_1/\pi)}{(\omega-\omega_1)^2+\Gamma_1^2} \; \frac{(\Gamma_2/\pi)}{(\omega-\omega_2)^2+\Gamma_2^2} \;=\; \frac{(\Gamma_1+\Gamma_2)/\pi}{(\Gamma_1+\Gamma_2)^2+(\omega_2-\omega_1)^2}, \tag{A.55}$$ z1lorf

so we can say that a convolution of two Lorentzians is proportional to a Lorentzian. This result can also be obtained by a direct computation of the integral in the left hand side of Eq.(A.55). However, usage of Fourier transforms greatly simplifies things, since direct integration is pretty complicated.

A.1.6 Sochocki formulas and related topics

Principal value of the integral

We define the principal value of the integral (shortly, principal value) by the relation

$$\mathrm{Vp}\int_{-\infty}^{\infty} dx\ \varphi(x) \;=\; \lim_{\epsilon\to 0_+}\left[\int_{-\infty}^{-\epsilon}+\int_{\epsilon}^{\infty}\right] dx\ \varphi(x), \tag{A.56}$$ sf01

which exists for some functions, and does not for some other ones. For example, function $1/x$ is divergent at $x=0$ and thus, is nonitegrable. We will show that the principal value for $\varphi(x)=1/x$ exists. Indeed

$$\begin{aligned}\mathrm{Vp}\int_{-\infty}^{\infty}\frac{dx}{x} &= \lim_{\epsilon\to 0_+}\lim_{R\to\infty}\left[\int_{-R}^{-\epsilon}\frac{dx}{x}+\int_{\epsilon}^{R}\frac{dx}{x}\right]\\ &= \lim_{\epsilon\to 0_+}\lim_{R\to\infty}\Big(\ln|x|_{-R}^{-\epsilon}\ +\ \ln|x|_{\epsilon}^{-R}\Big)\ =\ 0.\end{aligned} \tag{A.57}$$

So, the discussed principal value is well defined.

Let $\varphi(x)$ denote a differentiable function, such that $\varphi(x)=0$ for $|x|>R$ (finite support). Then, we use the concept of the principal value to define a distribution $\mathcal{P}(1/x)$ (a generalized function) as follows

$$\langle\,\mathcal{P}\frac{1}{x},\ \varphi(x)\,\rangle\ =\ \mathrm{Vp}\int_{-\infty}^{\infty}dx\ \frac{\varphi(x)}{x}\ =\ \lim_{\epsilon\to 0_+}\left[\int_{-\infty}^{-\epsilon}+\int_{\epsilon}^{\infty}\right]\ dx\ \frac{\varphi(x)}{x}. \tag{A.58}$$ sf03

The integral under the "Vp" sign is usually divergent at $x=0$. On the other hand, the last part of the above relation may give finite results because we have specified a special way of avoiding the divergence, as a result we obtain finite number, since the function $\varphi(x)$ vanishes for sufficiently large $|x|$.

Let us now transform expression (A.58) into some other form which will be useful in further developments. From (A.58) we get

$$\langle\,\mathcal{P}\frac{1}{x},\ \varphi(x)\,\rangle=\lim_{\epsilon\to 0_+}\left[\int_{-\infty}^{-\epsilon}+\int_{\epsilon}^{\infty}\right]\ dx\ \frac{\varphi(x)-\varphi(0)+\varphi(0)}{x}. \tag{A.59}$$ sf04

The quotient $[\varphi(x)-\varphi(0)]/x$ is continuous and finite at $x=0$. This follows from de L'Hospital rule and from good behavior of $\varphi(x)$. Hence, the integral of $[\varphi(x)-\varphi(0)]/x$ can be computed without any special limiting procedures. Therefore, we can write

$$\langle\,\mathcal{P}\frac{1}{x},\ \varphi(x)\,\rangle\ =\ \int_{-\infty}^{\infty}dx\ \frac{\varphi(x)-\varphi(0)}{x}\ +\ \varphi(0)\ \lim_{\epsilon\to 0_+}\left[\int_{-\infty}^{-\epsilon}\frac{dx}{x}+\int_{\epsilon}^{\infty}\frac{dx}{x}\right]. \tag{A.60}$$ sf05

The last term gives zero (see Eq.(A.57)), and we arrive at the relation

$$\langle\,\mathcal{P}\frac{1}{x},\ \varphi(x)\,\rangle\ =\ \mathrm{Vp}\int_{-\infty}^{\infty}dx\ \frac{\varphi(x)}{x}\ =\ \int_{-\infty}^{\infty}dx\ \frac{\varphi(x)-\varphi(0)}{x}. \tag{A.61}$$ sf06

This relation will appear to be useful.

Sochocki formulas

We recall that the function $\varphi(x)$ vanishes for $|x| > R$. Then we consider an integral

$$\begin{aligned}\lim_{\epsilon\to 0_+}\int_{-\infty}^{\infty} dx\ \frac{\varphi(x)}{x+i\epsilon} &= \lim_{\epsilon\to 0_+}\int_{-R}^{R} dx\ \frac{x-i\epsilon}{x^2+\epsilon^2}\ \varphi(x)\\ &= \lim_{\epsilon\to 0_+}\int_{-R}^{R} dx\ \frac{x-i\epsilon}{x^2+\epsilon^2}\ [\,\varphi(x)-\varphi(0)+\varphi(0)\,]\\ &= \varphi(0)\ \lim_{\epsilon\to 0_+}\int_{-R}^{R} dx\ \frac{x-i\epsilon}{x^2+\epsilon^2}\ +\ \lim_{\epsilon\to 0_+}\int_{-R}^{R} dx\ \frac{x-i\epsilon}{x^2+\epsilon^2}\ [\,\varphi(x)-\varphi(0)\,] \quad \text{(A.62)}\end{aligned}$$

The first integral contains an odd part (proportional to x) which does not contribute. In the second integral we take the indicated limit. Thus, we get

$$\lim_{\epsilon\to 0_+}\int_{-\infty}^{\infty} dx\ \frac{\varphi(x)}{x+i\epsilon} = -i\varphi(0)\ \lim_{\epsilon\to 0_+}\ \int_{-R}^{R} dx\ \frac{\epsilon}{x^2+\epsilon^2}\ +\ \int_{-R}^{R} dx\ \frac{\varphi(x)-\varphi(0)}{x} \quad \text{(A.63)} \quad \boxed{\texttt{sf08}}$$

The first integral is tabulated – it gives *arctg*, while the second one follows from (sf06 A.61). Since function $\varphi(x)$ vanishes beyond $|x| = R$ we obtain

$$\lim_{\epsilon\to 0_+}\int_{-\infty}^{\infty} dx\ \frac{\varphi(x)}{x+i\epsilon} = -2i\varphi(0)\ \lim_{\epsilon\to 0_+}\operatorname{arctg}\left(\frac{R}{\epsilon}\right)\ +\ \langle\,\mathcal{P}\frac{1}{x},\ \varphi(x)\,\rangle. \quad \text{(A.64)} \quad \boxed{\texttt{sf10}}$$

Taking the remaining limit is easy, and we arrive at

$$\lim_{\epsilon\to 0_+}\int_{-\infty}^{\infty} dx\ \frac{\varphi(x)}{x+i\epsilon} = -i\pi\varphi(0)\ +\ \langle\,\mathcal{P}\frac{1}{x},\ \varphi(x)\,\rangle. \quad \text{(A.65)} \quad \boxed{\texttt{sf11}}$$

The obtained relation has distributive sense. In this sense, it can be rewritten as

$$\lim_{\epsilon\to 0_+}\ \frac{1}{x+i\epsilon} = -i\pi\delta(x)\ +\ \mathcal{P}\frac{1}{x}. \quad \text{(A.66)} \quad \boxed{\texttt{sf12}}$$

Expression (sf12 A.66) must be understood as a distribution which, when applied to a function $\varphi(x)$ automatically entails relation (sf11 A.65) (with (sf05 A.60) kept in mind to explain the meaning of the last term). Relation (sf12 A.66), in its distributive sense, is called the first Sochocki formula.

The second Sochocki formula is obtained by simple complex conjugation

$$\lim_{\epsilon\to 0_+}\ \frac{1}{x-i\epsilon} = i\pi\delta(x)\ +\ \mathcal{P}\frac{1}{x}. \quad \text{(A.67)} \quad \boxed{\texttt{sf13}}$$

We stress, once again, that Sochocki formulas (sf12 A.66) and (sf13 A.67) are validin the sense of distribution (generalized functions) theory. It implies that their sense is given directly by relation (sf11 A.65). Sochocki formulas occur in some quantum-mechanical calculations. This is the reason why they are worth remembering.

Application of Sochocki formulas

Before discussing the practical applications let us transform the obtained Sochocki Formulas. First we write relation (A.66) and (A.67) as a single one

$$\lim_{\epsilon\to 0_+} \frac{1}{x \pm i\epsilon} \;=\; \mp i\pi\delta(x) \;+\; \mathcal{P}\frac{1}{x}. \tag{A.68}$$ sf16

Left hand side can be rewritten as follows

$$\lim_{\epsilon\to 0_+} \frac{1}{x \pm i\epsilon} \;=\; \lim_{\epsilon\to 0_+} \frac{1}{-i^2 x \pm i\epsilon} \;=\; \lim_{\epsilon\to 0_+} \frac{1}{\mp i(\pm ix - \epsilon)}. \tag{A.69}$$ sf17

Then, formula (A.68) gives

$$\lim_{\epsilon\to 0_+} \frac{1}{\mp i(\pm ix - \epsilon)} \;=\; \mp i\pi\delta(x) \;+\; \mathcal{P}\frac{1}{x}. \tag{A.70}$$ sf18

Multiplying both sides by $(\mp i)$ we get

$$\lim_{\epsilon\to 0_+} \frac{1}{\pm ix - \epsilon} \;=\; -\;\pi\delta(x) \;\mp\; \mathcal{P}\frac{1}{x}. \tag{A.71}$$ sf19

This is another (and useful) form of the Sochocki formulas.

In order to see the usefulness of the obtained results let us consider an integral which is encountered in some quantum-mechanical applications. It is

$$I(x) = \int_0^\infty dt\; e^{\pm ixt} = \lim_{\epsilon\to 0_+} \int_0^\infty dt\; e^{(\pm ix-\epsilon)t}. \tag{A.72}$$ sf21

The factor $e^{-\epsilon t}$ causes the integral to be convergent and allows us to compute it. The result is

$$I(x) = \lim_{\epsilon\to 0_+} \frac{e^{(\pm ix-\epsilon)t}}{\pm ix - \epsilon}\Bigg|_0^\infty = \lim_{\epsilon\to 0_+} \frac{-1}{\pm ix - \epsilon}, \tag{A.73}$$ sf22

because for $t \to \infty$ the factor $e^{-\epsilon q t}$ tends to zero. Now, comparing Eqs.(A.71) and (A.73)

$$\int_0^\infty dt\; e^{\pm ixt} \;=\; \pi\delta(x) \;\pm\; \mathcal{P}\frac{1}{x}, \tag{A.74}$$ sf23

which has to be understood in the distributive sense, as discussed above. We note that (A.74) is an analogue of the Fourier transform (A.5), that is

$$\int_{-\infty}^\infty dt\; e^{\pm ixt} \;=\; 2\pi\delta(x). \tag{A.75}$$ sf24

Let us note that from (A.74) we easily have

$$\int_0^\infty dt\; e^{ixt} \int_0^\infty dt\; e^{-ixt} \;=\; 2\pi\delta(x). \tag{A.76}$$ sf25

In the second integral we change the integration variable $t = -t'$ and we get

$$\int_0^\infty dt\; e^{ixt} \int_0^{-\infty} dt'\; e^{ixt'} \;=\; 2\pi\delta(x). \tag{A.77}$$ sf26

Reversing the integration limits in the second integral and dropping the prime we immediately see that the Fourier relation (A.75) indeed follows.

An auxiliary integral

Let us first consider an auxiliary integral

$$I(t,\gamma) = \int_{-\infty}^{\infty} d\omega \; \frac{e^{-i\omega t}}{\omega + i\gamma}, \qquad \text{with} \;\; \gamma > 0. \tag{A.78}$$ z1aint1

The integrand has the first order pole at $\omega_1 = -i\gamma$ in the lower half-plane of complex ω. Therefore, closing the contour in the upper half-plane (see Fig.(f:aintcon01 A.1)) we obtain zero, since this contour contains no poles. Closing the contour in the lower half-plane we may obtain a non-zero result. However, we must be careful. In the lower half-plane $\omega = \alpha - i|\beta|$. T hus, we have $e^{-i\omega t} = e^{-i(\alpha - i|\beta|)t} = e^{-i\alpha t - |\beta| t}$. The integral will converge if and only if the time $t > 0$. Hence, we employ the approach similar to that we used considering the Fourier transform for the Lorentzian. For time $t < 0$ we close the contour in the upper half-plane, which gives zero for the integral (see Fig.(f:aintcon01 A.1)). On the other hand, for time $t > 0$ we close the integral in the lower half plane. Noting the negative direction of the contour we compute the integral by residue theory. We use the Heaviside function which ensures that the integral vanishes for negative times, and we obtain

$$\begin{aligned} I(t,\gamma) \;&=\; \int_{-\infty}^{\infty} d\omega \; \frac{e^{-i\omega t}}{\omega + i\gamma} \;=\; \theta(t) \int_{-\infty}^{\infty} d\omega \; \frac{e^{-i\omega t}}{\omega + i\gamma} \\ &=\; \theta(t)\,(-2\pi i)\;\, e^{-it(-i\gamma)} \;=\; -\,2\pi i\;\theta(t)\;e^{-\gamma t}. \end{aligned} \tag{A.79}$$

Thus, for $\gamma > 0$ we have obtained the result

$$I(t,\gamma) \;=\; \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{\,2\pi}} \; \frac{e^{-i\omega t}}{\omega + i\gamma} \;=\; -\,i\sqrt{\,2\pi}\;\,\theta(t)\;e^{-\gamma t}. \tag{A.80}$$ z1aint3

Fourier transform of Heaviside function

From relation (z1aint3 A.80) we conclude that

$$\theta(t) \;=\; \frac{i}{\sqrt{2\pi}} \; \lim_{\epsilon \to 0_+} \; \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{\,2\pi}} \; \frac{e^{-i\omega t}}{\omega + i\epsilon}. \tag{A.81}$$ z1htr1

Hence, Fourier transform of the Heaviside function can be written as

$$\mathcal{F}[\theta(t)] \;=\; \Theta(\omega) \;=\; \frac{i}{\sqrt{2\pi}} \; \lim_{\epsilon \to 0_+} \; \frac{1}{\omega + i\epsilon}. \tag{A.82}$$ z1htr2

Employing the Sochocki formula (sf12 A.66), we get

$$\mathcal{F}[\theta(t)] \;=\; \Theta(\omega) \;=\; \frac{i}{\sqrt{2\pi}} \; \lim_{\epsilon \to 0_+} \; \frac{1}{\omega + i\epsilon} \;=\; \frac{1}{\sqrt{2\pi}} \left[\, \pi\delta(\omega) + i\mathcal{P}\frac{1}{\omega} \, \right]. \tag{A.83}$$ z1htr3

By an obvious property of Fourier transform, from relation (z1htr3 A.83) we also obtain

$$\mathcal{F}[\theta(-t)] \;=\; \Theta^*(\omega) \;=\; \frac{1}{\sqrt{2\pi}} \left[\, \pi\delta(\omega) - i\mathcal{P}\frac{1}{\omega} \, \right]. \tag{A.84}$$ z1htr4

qm:3df

A.2 Three-dimensional Fourier transformation

We shall very briefly summarize some basic facts concerning Fourier transformation. We will not be mathematically strict, and we will omit proofs of various statements or theorems. Those can be found in many mathematical handbooks.

Let us consider the function $F(\vec{\mathbf{r}})$ of the position. F may, as well depend on other variables, but we do not indicate other dependencies. The Fourier transform is defined as

$$\mathcal{F}(F)(\vec{\mathbf{k}}) = \tilde{F}(\vec{\mathbf{k}}) = \frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\; e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\; F(\vec{\mathbf{r}}). \tag{A.85}$$

z1ft1

The inverse transformation takes the form

$$\mathcal{F}^{-1}(\tilde{F})(\vec{\mathbf{r}}) = F(\vec{\mathbf{r}}) = \frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{k}}\; e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\; \tilde{F}(\vec{\mathbf{k}}). \tag{A.86}$$

z1ft2

This equation expresses $F(\vec{\mathbf{r}})$ as a superposition of plane waves with wave vector $\vec{\mathbf{k}}$.

Writing the above definitions we assume that the functions are such that the necessary integrals exist. Usually it is sufficient to assume the considered functions are square integrable or even just integrable. On the other hand, it is sometimes useful to view the Fourier transform as a certain mapping in the space of generalized functions – distributions. However, we will not go into mathematical details, we will only list some useful properties of the Fourier transforms.

z1ftd

Dirac's delta function has the following Fourier properties

$$e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}_0} = \int d\vec{\mathbf{r}}\; \delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}_0)\, e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}} \tag{A.87a}$$

$$(2\pi)^3\, \delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}_0) = \int d\vec{\mathbf{k}}\; e^{i\vec{\mathbf{k}}\cdot(\vec{\mathbf{r}}-\vec{\mathbf{r}}_0)} \tag{A.87b}$$

It may we worth recalling that the Coulomb potentials satisfies the equation

$$\nabla^2 \left(\frac{1}{4\pi|\vec{\mathbf{r}}|}\right) = -\delta(\vec{\mathbf{r}}). \tag{A.88}$$

z1cpot

t:z1ft1 **Theorem A.10** *If the field $F(\vec{\mathbf{r}})$ is real, then its Fourier transform satisfies the requirement*

$$\tilde{F}^*(\vec{\mathbf{k}}) = \tilde{F}(-\vec{\mathbf{k}}) \tag{A.89}$$

z1tft1

It is straightforward to see that the transformations (z1ft1 A.85) and (z1ft2 A.86) are identical to the relation between wave functions in coordinate and momentum representation in quantum mechanics. In that context it is well–known that the overlap between two wave functions can be evaluated in either representation. This is the reflection of Parseval identity for Fourier transforms.

2t:z1ft2 **Theorem A.11** *If the fields $F(\vec{\mathbf{r}})$ and $G(\vec{\mathbf{r}})$ have Fourier transforms $\tilde{F}(\vec{\mathbf{k}})$ and $\tilde{G}(\vec{\mathbf{k}})$, then we have Parseval – Plancherel identity*

$$\int d\vec{\mathbf{r}}\; F^*(\vec{\mathbf{r}})\, G(\vec{\mathbf{r}}) = \int d\vec{\mathbf{k}}\; \tilde{F}^*(\vec{\mathbf{k}})\, \tilde{G}(\vec{\mathbf{k}}). \tag{A.90}$$

z1tft2

The fields F and/or G may be complex.

2t:z1ft3 **Theorem A.12** *The convolution of two fields $F(\vec{\mathbf{r}})$ and $G(\vec{\mathbf{r}})$ is defined as*

$$(F * G)(\vec{\mathbf{r}}) = \frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{x}}\ F(\vec{\mathbf{x}}) G(\vec{\mathbf{r}} - \vec{\mathbf{x}}). \tag{A.91}$$ z1ftcon

Fourier transform of the convolution is a product of the transforms, that is

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ (F * G)(\vec{\mathbf{r}}) = \tilde{F}(\vec{\mathbf{k}})\, \tilde{G}(\vec{\mathbf{k}}), \tag{A.92}$$ z1tft3a

while the Fourier transform of the product is the convolution of the transforms

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ F(\vec{\mathbf{r}}) G(\vec{\mathbf{r}}) = (\tilde{F} * \tilde{G})(\vec{\mathbf{k}}), \tag{A.93}$$ z1tft3b

Another result of the Fourier transform theory is also well–known in the context of quantum mechanics. It is the expression for the Fourier transform of the gradient of a function $F(\vec{\mathbf{r}})$.

2t:z1ft4 **Theorem A.13** *Fourier transform of the derivative $\partial_j F(\vec{\mathbf{r}})$ follows by partial integration, and is given as*

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ \partial_j F(\vec{\mathbf{r}}) = ik_j\, \tilde{F}(\vec{\mathbf{k}}), \tag{A.94}$$ z1tft4

This theorem is equivalent to the statement that the momentum operator in quantum mechanics (in properly chosen units) is $-i\boldsymbol{\nabla}$ in coordinate representation. This allows us to transform differential equations in coordinate space into algebraic equations in Fourier space.

2t:z1ft5 z1tft5 **Theorem A.14** *Simple generalization of the previous theorem (*2t:z1ft4 A.13*) yields*

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ [\,\boldsymbol{\nabla}\phi(\vec{\mathbf{r}})] = i\vec{\mathbf{k}}\,\tilde{\phi}(\vec{\mathbf{k}}), \tag{A.95a}$$

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ \Big[\,\mathrm{div}\ \vec{\mathbf{F}}(\vec{\mathbf{r}})\Big] = i\vec{\mathbf{k}}\cdot\tilde{\vec{\mathbf{F}}}(\tilde{\mathbf{k}}), \tag{A.95b}$$

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ \Big[\,\mathrm{rot}\ \vec{\mathbf{F}}(\vec{\mathbf{r}})\Big] = i\vec{\mathbf{k}}\times\tilde{\vec{\mathbf{F}}}(\tilde{\mathbf{k}}), \tag{A.95c}$$

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ [\,\boldsymbol{\nabla}^2\phi(\vec{\mathbf{r}})] = -k^2\,\tilde{\phi}(\vec{\mathbf{k}}), \tag{A.95d}$$

(A.95e)

2t:z1ft6 **Theorem A.15** *Fourier transform of the Coulomb potential is given as*

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ \left(\frac{1}{4\pi r}\right) = \frac{1}{(2\pi)^{3/2}}\ \left(\frac{1}{k^2}\right). \tag{A.96}$$ z1tft6

z1ft6a *As a consequence we get the following relations*

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{r}}\ e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ \left(\frac{\vec{\mathbf{r}}}{4\pi r^3}\right) = \frac{1}{(2\pi)^{3/2}}\ \left(\frac{-i\vec{\mathbf{k}}}{k^2}\right), \tag{A.97a}$$

$$\frac{1}{(2\pi)^{3/2}} \int d\vec{\mathbf{k}}\ e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}\ \left(\frac{-i\vec{\mathbf{k}}}{(2\pi)^{3/2}\,k^2}\right) = \frac{\vec{\mathbf{r}}}{4\pi r^3} \tag{A.97b}$$

* *

Appendix B

Useful operator identities

ap:oid

B.1 Similarity relations

Theorem B.1 *Let A and B be operators. Let ξ be a parameter which may be complex or real. Then, the following identity holds*

$$e^{\xi A} B e^{-\xi A} \;=\; B \;+\; \frac{\xi}{1!}\,[A,B] \;+\; \frac{\xi^2}{2!}\,[A,[A,B]] \;+\; \frac{\xi^3}{3!}\,[A,[A,[A,B]]] \;+\; \ldots \tag{B.1}$$

z2theo1

Before proving this theorem let us specify a superoperator $\hat{\mathcal{A}}$. For arbitrary operator B we define

$$\hat{\mathcal{A}} B = [A,B]\,. \tag{B.2}$$

z2supopa1

Formally we can also write

$$\hat{\mathcal{A}} = [A,\ \ ]\,, \tag{B.3}$$

z2supopa2

where an empty place at the second position within a commutator is understood as a place where the operator B, which is acted upon by the superoperator $\hat{\mathcal{A}}$, should be inserted. Having the definition of the superoperator $\hat{\mathcal{A}}$ we can rewrite the theorem (B.1) equivalently as

$$\exp(\xi A)\; B\; \exp(-\xi A) \;=\; \exp(\xi \hat{\mathcal{A}})\; B. \tag{B.4}$$

z2theo2

Proof. We introduce an operator-valued function

$$g(\xi) = e^{\xi A} B e^{-\xi A}, \qquad \text{with initial condition :} \qquad g(0) = B. \tag{B.5}$$

z2prth1a

Next, we expand $g(\xi)$ in Taylor series

$$g(\xi) = g(0) + \sum_{n=1}^{\infty} \frac{\xi^n}{n!}\; \frac{d^n g(\xi)}{d\xi^n}\bigg|_{\xi=0} \tag{B.6}$$

z2prth1b

It remains to compute explicitly the coefficients of the expansion, that is the derivatives evaluated at $\xi = 0$. The first derivative is as follows

$$\begin{aligned} \frac{d}{d\xi} g(\xi)\bigg|_{\xi=0} &= \frac{d}{d\xi}\left(e^{\xi A} B e^{-\xi A}\right)\bigg|_{\xi=0} = \left(A e^{\xi A} B e^{-\xi A} - e^{\xi A} B A e^{-\xi A}\right)\big|_{\xi=0} \\ &= (A g(\xi) - g(\xi) A)|_{\xi=0} = [A,\ g(\xi)]|_{\xi=0} = [A,\ B] \end{aligned} \tag{B.7}$$

where the first equality in the second line follows from the fact that operator A commutes with the exponential $e^{\xi A}$. The last equality follows from initial condition for the function $g(\xi)$. Substituting (B.7) into expansion (B.6) we obtain

$$g(\xi) = g(0) + \frac{\xi}{1!}\,[A,\,B] + \sum_{n=2}^{\infty} \frac{\xi^n}{n!}\,\left.\frac{d^n g(\xi)}{d\xi^n}\right|_{\xi=0} \tag{B.8}$$ z2prth1d

In the similar manner we calculate next terms of the expansion.

$$\begin{aligned} \left.\frac{d^2}{d\xi^2} g(\xi)\right|_{\xi=0} = \left.\frac{d}{d\xi}\,[A,\,g(\xi)]\right|_{\xi=0} &= \left.\left[A,\,\frac{dg(\xi)}{d\xi}\right]\right|_{\xi=0} \\ &= [A,\,[A,\,g(\xi)]]|_{\xi=0} = [A,\,[A,\,B]] \end{aligned} \tag{B.9}$$

where the last steps follow from Eq.(B.7). Thus, (B.8) transforms into the relation

$$g(\xi) = g(0) + \frac{\xi}{1!}\,[A,\,B] + \frac{\xi^2}{2!}\,[A,\,[A,\,B]] + \sum_{n=3}^{\infty} \frac{\xi^n}{n!}\,\left.\frac{d^n g(\xi)}{d\xi^n}\right|_{\xi=0} \tag{B.10}$$ z2prth1f

Further derivatives may be found in the same manner. It is also possible to employ the method of mathematical induction to show that the theorem (B.1) indeed holds.

Finally, we note that the relation (B.4) follows from (B.1) simply by expansion of the exponential in the right-hand-side of (B.4). Comparing the obtained expansion we easily see that right-hand-side of (B.1) is reproduced. This completes the proof of the theorem. ■

The previous theorem can easily be generalized. We shall now formulate a generalized similarity relation.

Theorem B.2 *Let $g(B_1, \ldots, B_k)$ be a function of k different operators. We assume that this function can be expanded into series*

$$g(B_1, B_2, \ldots, B_k) \;=\; \sum_{\{n_k\}} g_{n_1 n_2 \ldots n_k}\, B_1^{n_1} B_2^{n_2} \ldots B_k^{n_k}. \tag{B.11}$$ z2sr1

If it is necessary, commutation relations can be used to rearrange the operators $\{B_j\}$ in the power series. Then, the following similarity relation holds for operator A and a complex number ξ

$$e^{\xi A}\, g(B_1, B_2, \ldots, B_k)\, e^{-\xi A} \;=\; g\left(e^{\xi A} B_1 e^{-\xi A},\; e^{\xi A} B_2 e^{-\xi A},\; \ldots,\; e^{\xi A} B_k e^{-\xi A}\right), \tag{B.12}$$ z2sr2

that is, the function g is unchanged, only each of its arguments is transformed according to the given similarity.

Proof. Applying similarity operator $e^{\xi A}$ on the left of the expansion, and $e^{-\xi A}$ on the right, we can also introduce the $\hat{\mathbf{1}} = e^{-\xi A} e^{\xi A}$ between all factors in each term of the series. Then each of the operators undergoes the similarity transformation, and the series coefficients remain unchanged. Resummation yields rhs of the theorem. ■

B.2 Decomposition of the exponential

B.2.1 General idea of the decomposition

In many practical applications we need to express the operator $\exp[\xi(A+B)]$, where A and B are also operators, as a product of separate exponentials, that is

$$e^{\xi(A+B)} \;=\; e^{f_1(\xi)A}\, e^{f_2(\xi)B}\, e^{f_3(\xi)}. \tag{B.13}$$ z2de1

where $f_k(\xi)$ are ordinary (c-numbered, complex) functions of the parameter $\xi \in \mathbb{C}$. These functions must satisfy an obvious boundary condition $f_k(0) = 0$. The whole problem is to determine these functions. Before we start looking for the solution, let us note that we can easily write the relation inverse to (B.13), namely

$$e^{-\xi(A+B)} \;=\; e^{-f_3(\xi)}\, e^{-f_2(\xi)B}\, e^{-f_1(\xi)A}. \tag{B.14}$$ z2de2

Surely, $\exp[-f_3(\xi)]$ is a number so it commutes with all operators.

To find functions $f_k(\xi)$ let us differentiate both sides of)(B.13), thus obtaining

$$\begin{aligned}(A+B)\, e^{\xi(A+B)} \;=\; & f_1'(\xi) A\, e^{f_1(\xi)A}\, e^{f_2(\xi)B}\, e^{f_3(\xi)} \;+\; e^{f_1(\xi)A}\, f_2'(\xi) B\, e^{f_2(\xi)B}\, e^{f_3(\xi)} \\ & +\; e^{f_1(\xi)A}\, e^{f_2(\xi)B}\, e^{f_3(\xi)}\, f_3'(\xi),\end{aligned} \tag{B.15}$$

where the prime denotes the derivative with respect to ξ. Next, we multiply both sides of (B.15) on the right by both sides of the inverse relation (B.14). We get

$$A \;+\; B \;=\; f_1'(\xi)\, A \;+\; f_2'(\xi)\, e^{f_1(\xi)A}\, B\, e^{-f_1(\xi)A} \;+\; f_3'(\xi). \tag{B.16}$$ z2de4

Equating the coefficients multiplying operator A, we see that

$$f_1'(\xi) \;=\; 1, \qquad \Longrightarrow \qquad f_1(\xi) \;=\; \xi, \tag{B.17}$$ z2de5

which satisfies the boundary condition. Using (B.17) in (B.16) we reduce it to

$$B \;=\; f_2'(\xi)\, e^{\xi A}\, B\, e^{-\xi A} \;+\; f_3'(\xi). \tag{B.18}$$ z2de6

Now, we employ the similarity expansion (B.1) to write

$$B \;=\; f_2'(\xi) \left\{ B \;+\; \frac{\xi}{1!}\,[A,B] \;+\; \frac{\xi^2}{2!}\,[A,[A,B]] \;+\; \ldots \right\} \;+\; f_3'(\xi). \tag{B.19}$$ z2de7

Further steps obviously depend on the shape of the commutators which appear within the curly brackets. If we know the commutators, we can try to find the remaining functions of the parameter ξ.

B.2.2 The case of $[\,\mathbf{A},\ \mathbf{B}\,] = \mathbf{c}$

Let us now assume that the commutator $[\,A,\ B\,] = c$, where $c \in \mathbb{C}$. In such a case, all terms in (B.19), except the first two ones, vanish and we have

$$B \;=\; f_2'(\xi)\,(B \;+\; \xi\, c) \;+\; f_3'(\xi). \tag{B.20}$$ z2de8

Hence, we arrive at the equations

$$f_2^{'}(\xi) \;=\; 1, \qquad \text{and} \qquad f_2^{'}(\xi)\xi c \;+\; f_3^{'}(\xi) = 0. \tag{B.21}$$ z2de9

These equations are immediately integrated, and taking into account the boundary conditions we get

$$f_2(\xi) \;=\; \xi, \qquad \text{and} \qquad f_3(\xi) \;=\; -\,\frac{1}{2}\,\xi^2 c. \tag{B.22}$$ z2de10

Thus we can state the following

Theorem B.3 *If two operators A and B have the commutator $[\,A,\;B\,] = c \in \mathbb{C}$, then*

$$e^{\xi(A+B)} \;=\; e^{\xi A}\, e^{\xi B}\, e^{-c\xi^2/2}, \tag{B.23}$$ z2de11a

for any complex parameter ξ. Equivalently we can write

$$e^{\xi(A+B)} \;=\; e^{\xi B}\, e^{\xi A}\, e^{c\xi^2/2}, \tag{B.24}$$ z2de11b

B.2.3 Special case for annihilation and creation operators

We employ the theorem (B.23) taking $\xi = 1$ and specifying the operators as

$$A = \alpha\,\hat{a}, \qquad \text{and} \qquad B = \beta\hat{a}^\dagger, \tag{B.25}$$ z2de12

where $\hat{a}$ and $\hat{a}^\dagger$ are annihilation and creation operators. Since

$$\left[\,\alpha\hat{a},\;\beta\hat{a}^\dagger\,\right] = \alpha\,\beta, \tag{B.26}$$ z2de13

z2ac from Eqs.(B.23) and (B.24) we obtain

$$e^{\alpha\hat{a}+\beta\hat{a}^\dagger} \;=\; e^{\alpha\hat{a}}\, e^{\beta\hat{a}^\dagger}\, e^{-\alpha\,\beta/2} \tag{B.27a}$$

$$\;=\; e^{\beta\hat{a}^\dagger}\, e^{\alpha\hat{a}}\, e^{\alpha\,\beta/2}. \tag{B.27b}$$

These relations are very useful in many practical cases.

B.3 Similarity relation for annihilation operator

B.3.1 General relation

Let $\hat{a}$ and $\hat{a}^\dagger$ be the annihilation and creation operators, which satisfy the canonical commutation relation $\left[\,\hat{a},\;\hat{a}^\dagger\,\right] = 1$. Let us, moreover, define an operator

$$Z \;=\; \alpha\hat{a} \;+\; \beta\hat{a}^\dagger \;+\; \gamma\hat{a}^\dagger\hat{a}, \tag{B.28}$$ z2sra1

with α, β and γ being complex parameters (numbers). We consider the similarity relation

$$\hat{a}(\xi) \;=\; e^{-\xi Z}\,\hat{a}\,e^{\xi Z}, \tag{B.29}$$ z2sra2

with an obvious boundary condition $\hat{a}(0) = \hat{a}$. We can, in principle, use general expression (B.1). This is, however, inconvenient because due to the term $\gamma\hat{a}^\dagger\hat{a}$, the commutator series

do not truncate. Therefore, we employ a different approach. We differentiate Eq.(B.29) with respect to parameter ξ, obtaining

$$\frac{d}{d\xi}\,\hat{a}(\xi) \;=\; e^{-\xi Z}\left(-Z\hat{a}+\hat{a}^\dagger Z\right)e^{\xi Z} \;=\; e^{-\xi Z}\,[\,\hat{a},\;Z\,]\,e^{\xi Z}. \tag{B.30}$$

It is straightforward to compute the commutator

$$[\,\hat{a},\;Z\,] \;=\; \left[\,\hat{a},\;\alpha\hat{a}+\beta\hat{a}^\dagger+\gamma\hat{a}^\dagger\hat{a}\,\right] \;=\; \beta+\gamma\hat{a}. \tag{B.31}$$

Thus we have the differential equation

$$\frac{d}{d\xi}\,\hat{a}(\xi) \;=\; e^{-\xi Z}\,(\beta+\gamma\hat{a})\,e^{\xi Z} \;=\; \beta+\gamma\hat{a}(\xi). \tag{B.32}$$

This is an inhomogeneous differential equation. The homogeneous one: $\hat{a}'(\xi)=\gamma\hat{a}$ has an obvious solution $\hat{a}(\xi)=\hat{a}(0)e^{\gamma\xi}$. Hence, we look for the solution of (B.32) in the form

$$\hat{a}(\xi) \;=\; e^{\gamma\xi}\,b(\xi), \tag{B.33}$$

with boundary condition $b(0)=\hat{a}(0)$. Inserting (B.33) into (B.32) we obtain an equation for $b(\xi)$

$$b'(\xi) \;=\; e^{-\gamma\xi}\,\beta \qquad \text{which yields} \qquad b(\xi) \;=\; b_0-\frac{\beta}{\gamma}\,e^{-\gamma\xi}, \tag{B.34}$$

where the constant b_0 has to be fixed. From boundary condition we get $\hat{a}(0)=b(0)=b_0-\beta/\gamma$. Therefore, the sought solution to Eq.(B.32) follows as

$$\hat{a}(\xi) \;=\; e^{\gamma\xi}\left(\hat{a}(0)+\frac{\beta}{\gamma}-\frac{\beta}{\gamma}\,e^{-\gamma\xi}\right). \tag{B.35}$$

This completes our derivation and we can finally write

$$\hat{a}(\xi) \;=\; e^{-\xi(\alpha\hat{a}+\beta\hat{a}^\dagger+\gamma\hat{a}^\dagger\hat{a})}\,\hat{a}\,e^{\xi(\alpha\hat{a}+\beta\hat{a}^\dagger+\gamma\hat{a}^\dagger\hat{a})} \;=\; \hat{a}\,e^{\gamma\xi} \;+\; \frac{\beta}{\gamma}\left(e^{\gamma\xi}\;-\;1\right). \tag{B.36}$$

B.3.2 Some special cases

Let us take $\gamma=0,\ \xi=1$. Then, relation (B.36) reads

$$e^{-\alpha\hat{a}-\beta\hat{a}^\dagger}\,\hat{a}\,e^{\alpha\hat{a}+\beta\hat{a}^\dagger} \;=\; \hat{a}\;+\;\beta, \tag{B.37}$$

and it can be rewritten as

$$\hat{a}\,e^{\alpha\hat{a}+\beta\hat{a}^\dagger} \;=\; e^{\alpha\hat{a}+\beta\hat{a}^\dagger}\,\hat{a}\;+\;e^{\alpha\hat{a}+\beta\hat{a}^\dagger}\,\beta, \tag{B.38}$$

which yields the commutation relation

$$\left[\,\hat{a},\;e^{\alpha\hat{a}+\beta\hat{a}^\dagger}\,\right] \;=\; e^{\alpha\hat{a}+\beta\hat{a}^\dagger}\,\beta, \tag{B.39}$$

Let us note, that we can apply relations (B.27) to formula (B.37). This gives

$$e^{-\beta\hat{a}^\dagger}\,e^{-\alpha\hat{a}}\,e^{\alpha\beta/2}\,\hat{a}\,e^{\alpha\hat{a}}\,e^{\beta\hat{a}^\dagger}\,e^{-\alpha\beta/2} \;=\; e^{-\beta\hat{a}^\dagger}\,\hat{a}\,e^{\beta\hat{a}^\dagger} \;=\; \hat{a}+\beta, \tag{B.40}$$

because $e^{\pm\alpha\hat{a}}$ commutes with $\hat{a}$.

Another special case follows easily, when we put $\alpha=\beta=0$, and $\gamma=1$. Then (B.36) yields

$$\hat{a}(\xi) \;=\; e^{-\xi\hat{a}^\dagger\hat{a}}\,\hat{a}\,e^{\xi\hat{a}^\dagger\hat{a}} \;=\; \hat{a}\,e^{\xi}. \tag{B.41}$$

B.3.3 Applications of generalized similarity relation

The generalized similarity theorem (B.12) has several immediate applications. The first one is for arbitrary function $g(\hat{a},\, \hat{a}^\dagger)$ which can be expanded into power series of annihilation and creation operators, namely we have

$$\begin{aligned} e^{-\xi\hat{a}^\dagger\hat{a}}\, g(\hat{a},\, \hat{a}^\dagger)\, e^{\xi\hat{a}^\dagger\hat{a}} &= g\left(e^{-\xi\hat{a}^\dagger\hat{a}}\, \hat{a}\, e^{\xi\hat{a}^\dagger\hat{a}},\; e^{-\xi\hat{a}^\dagger\hat{a}}\, \hat{a}^\dagger\, e^{\xi\hat{a}^\dagger\hat{a}}\right) \\ &= g\left(\hat{a}\, e^{\xi},\; \hat{a}^\dagger\, e^{-\xi}\right) \end{aligned} \tag{B.42}$$

where we used relation (B.41).

Let us note, that (B.42 implies for $y \in \mathbb{R}$ that

$$\begin{aligned} e^{-iy\hat{a}^\dagger\hat{a}}\, D(z)\, e^{iy\hat{a}^\dagger\hat{a}} &= e^{-iy\hat{a}^\dagger\hat{a}}\, \exp\left(z\hat{a}^\dagger - z^*\hat{a}\right)\, e^{iy\hat{a}^\dagger\hat{a}} \\ &= \exp\left(ze^{-iy}\hat{a}^\dagger - z^*e^{iy}\hat{a}\right) \\ &= D(ze^{-iy}) \end{aligned} \tag{B.43}$$

B.4 Squeeze operator

We define squeezing operator, for a complex parameter $\xi \in \mathbb{C}$, as

$$S(\xi) \;=\; \exp\left[\frac{1}{2}\xi^*\,\hat{a}^2 \;-\; \frac{1}{2}\xi\,(\hat{a}^\dagger)^2\right]. \tag{B.44}$$ z2squ1

We easily see that

$$S^\dagger(\xi) \;=\; \exp\left[\frac{1}{2}\xi\,(\hat{a}^\dagger)^2 \;-\; \frac{1}{2}\xi^*\,\hat{a}^2\right], \;=\; S(-\xi) \;=\; S^{-1}(\xi), \tag{B.45}$$ z2squ2

which indicates that operator $S(\xi)$ is a unitary one.

In the spirit of previous sections, we intend to investigate the similarity transformation of the annihilation operator induced by the squeezing operator. That is, we are interested in the expression

$$a_S(\xi) = S^\dagger(\xi)\,\hat{a}\,S(\xi) = \exp\left[\frac{1}{2}\xi(\hat{a}^\dagger)^2 \;-\; \frac{1}{2}\xi^*\hat{a}^2\right]\,\hat{a}\,\exp\left[\frac{1}{2}\xi^*\hat{a}^2 \;-\; \frac{1}{2}\xi(\hat{a}^\dagger)^2\right]. \tag{B.46}$$ z2squ3

To consider this relation it is convenient to write the complex parameter in polar coordinates,

$$\xi \;=\; \rho\, e^{i\theta}. \tag{B.47}$$ z2squ4

Then, we can rewrite (B.46) in the form

$$a_S(\xi) = \exp\left[\,\rho\left(\frac{1}{2}(\hat{a}^\dagger)^2\,e^{i\theta} - \frac{1}{2}\hat{a}^2\,e^{-i\theta}\right)\right]\,\hat{a}\,\exp\left[-\,\rho\left(\frac{1}{2}(\hat{a}^\dagger)^2\,e^{i\theta} - \frac{1}{2}\hat{a}^2\,e^{-i\theta}\right)\right]. \tag{B.48}$$ z2squ5

We analyze this expression by means of formula (B.1), in which we make the identifications

$$\xi \to \rho, \qquad A \to \frac{1}{2}(\hat{a}^\dagger)^2\,e^{i\theta} \;-\; \frac{1}{2}\hat{a}^2\,e^{-i\theta}, \qquad B \to \hat{a}. \tag{B.49}$$ z2squ5a

We see that we have to consider the commutators of operator A with B which, due to the introduced identifications, reads

$$[A,\,B] \;=\; \left[\frac{1}{2}(\hat{a}^\dagger)^2\,e^{i\theta} \;-\; \frac{1}{2}\hat{a}^2\,e^{-i\theta},\;\hat{a}\right] \;=\; \frac{1}{2}\,e^{i\theta}\left[\hat{a}^\dagger\hat{a}^\dagger,\;\hat{a}\right] \;=\; -\,e^{i\theta}\hat{a}^\dagger. \tag{B.50}$$ z2squ6

Using the obtained commutator, we compute the next one, as it follows from the general expansion (B.1). We get

$$[A,[A,\,B]] \;=\; \left[\frac{1}{2}(\hat{a}^\dagger)^2\,e^{i\theta} \;-\; \frac{1}{2}\hat{a}^2\,e^{-i\theta},\;-\,e^{-i\theta}\,\hat{a}^\dagger\right] \;=\; \frac{1}{2}\left[\hat{a}\hat{a},\;\hat{a}^\dagger\right] \;=\; \hat{a}. \tag{B.51}$$ z2squ7

By careful inspection of the obtained commutators we conclude that:

- when operator A identified according to (B.49) occurs even number of times, the result of such a multiple commutator will always be equal to the annihilation operator $\hat{a}$;

- when operator A occurs odd number of times, the result of a corresponding multiple commutator will always be equal to the $-\,e^{i\theta}\hat{a}^\dagger$.

Therefore, the general similarity expansion (B.1) splits into two series: with odd and even terms, and we get

$$\begin{aligned} a_S(\xi) &= \hat{a}\left(1+\frac{\rho^2}{2!}+\frac{\rho^4}{4!}+\ldots\ldots\right) - \hat{a}^\dagger e^{i\theta}\left(\rho+\frac{\rho^3}{3!}+\frac{\rho^5}{5!}+\ldots\ldots\right) \\ &= \hat{a}\cosh(\rho) - \hat{a}^\dagger e^{i\theta}\sinh(\rho). \end{aligned} \tag{B.52}$$

Summarizing we write

$$a_S(\xi) = S^\dagger(\xi)\,\hat{a}\,S(\xi) = \hat{a}\cosh(\rho) - \hat{a}^\dagger e^{i\theta}\sinh(\rho), \tag{B.53}$$

z2squ9

The generalized similarity theorem (B.12) can be applied to find a transformation of the squeeze operator. Since the exponential function is expandable into the power series, we get for $y\in\mathbb{R}$:

$$\begin{aligned} e^{-iy\hat{a}^\dagger\hat{a}}\,S(\xi)\,e^{iy\hat{a}^\dagger\hat{a}} &= e^{-iy\hat{a}^\dagger\hat{a}}\,\exp\left(\frac{1}{2}\xi^*\,\hat{a}^2-\frac{1}{2}\xi(\hat{a}^\dagger)^2\right)\,e^{iy\hat{a}^\dagger\hat{a}} \\ &= \exp\left[\frac{1}{2}\xi^*\left(e^{-iy\hat{a}^\dagger\hat{a}}\,\hat{a}\,e^{iy\hat{a}^\dagger\hat{a}}\right)^2-\frac{1}{2}\xi\left(e^{-iy\hat{a}^\dagger\hat{a}}\,\hat{a}^\dagger\,e^{iy\hat{a}^\dagger\hat{a}}\right)^2\right] \\ &= \exp\left[\frac{1}{2}\xi^*\,\hat{a}^2\,e^{2iy}-\frac{1}{2}\xi(\hat{a}^\dagger)^2\,e^{-2iy}\right] \\ &= S\left(\xi\,e^{-2iy}\right) \end{aligned} \tag{B.54}$$

where in the third line we have used (B.41), while in the fourth we used the definition of the squeeze operator with shifted argument.

Next, we note that by means of the general similarity theorem (B.12) and using (B.52) and its hermitian conjugate, we can write

$$\begin{aligned} &S^\dagger(\xi)\,g(\hat{a},\,\hat{a}^\dagger)\,S(\xi) = \\ &\quad = g\left(\hat{a}\cosh(\rho) - \hat{a}^\dagger e^{i\theta}\sinh(\rho),\;\; \hat{a}^\dagger\cosh(\rho) - \hat{a}\,e^{-i\theta}\sinh(\rho)\right) \end{aligned} \tag{B.55}$$

where $g(.,.)$ is a function, which can be expanded into power series. In particular, taking function g as the displacement operator $g(\hat{a},\,\hat{a}^\dagger)=D(\alpha)=\exp(\alpha\hat{a}^\dagger-\alpha^*\hat{a})$ we obtain

$$\begin{aligned} S^\dagger(\xi)\,D(\alpha)\,S(\xi) &= \exp\big[\alpha\left(\hat{a}^\dagger\cosh(\rho)-\hat{a}\,e^{-i\theta}\sinh(\rho)\right) \\ &\qquad -\alpha^*\left(\hat{a}\cosh(\rho)-\hat{a}^\dagger e^{i\theta}\sinh(\rho)\right)\big] \\ &= \exp\big[\hat{a}^\dagger\left(\alpha\cosh(\rho)+\alpha^* e^{i\theta}\sinh(\rho)\right) \\ &\qquad -\hat{a}\left(\alpha^*\cosh(\rho)+\alpha e^{-i\theta}\sinh(\rho)\right)\big] \\ &= D\left(\alpha\cosh(\rho)+\alpha^* e^{i\theta}\sinh(\rho)\right) \\ &= D(z). \end{aligned} \tag{B.56}$$

which defines new argument $z=\alpha\cosh(\rho)+\alpha^* e^{i\theta}\sinh(\rho)$ of the transformed displacement operator. Relation (B.56) can be written as

$$D(\alpha)\,S(\xi) = S(\xi)\,D(z), \tag{B.57}$$

z2squ13

with z given via α and $\xi = \rho e^{i\theta}$ as above. Taking the expression for z and its complex conjugate, we multiply the first one by $\cosh(\rho)$ and the second one by $-\sinh(\rho)\, e^{i\theta}$. Then we add both equations, and using the hyperbolic unity we express α as

$$\alpha \;=\; z\cosh(\rho) - z^* e^{i\theta}\sinh(\rho) \tag{B.58}$$ z2squ14

which, together with

$$z \;=\; \alpha\cosh(\rho) + \alpha^* e^{i\theta}\sinh(\rho) \tag{B.59}$$ z2squ15

allows us to use Eq.(B.57) z2squ13 in an effective manner. From the last relation we see that

$$\begin{aligned} z\, e^{-i\theta/2} &= \alpha\, e^{-i\theta/2}\cosh(\rho) + \alpha^* e^{i\theta/2}\sinh(\rho) \\ &= \frac{1}{2}\, e^{\rho}\left(\alpha\, e^{-i\theta/2} + \alpha^* e^{i\theta/2}\right) + \frac{1}{2}\, e^{-\rho}\left(\alpha\, e^{-i\theta/2} - \alpha^* e^{i\theta/2}\right) \end{aligned} \tag{B.60}$$

This allows us to derive a useful relation between parameters α and z, namely

$$\begin{aligned} \mathrm{Re}\left(z\, e^{-i\theta/2}\right) &= e^{\rho}\,\mathrm{Re}\left(\alpha\, e^{-i\theta/2}\right) \\ \mathrm{Im}\left(z\, e^{-i\theta/2}\right) &= e^{-\rho}\,\mathrm{Im}\left(\alpha\, e^{-i\theta/2}\right) \end{aligned} \tag{B.61}$$

* *

Appendix C

Certain sum rule for Hermite polynomials

ap:suh

Here we will prove the following summation rule involving even Hermite polynomials

$$\sum_{k=0}^{\infty} \frac{t^k}{k!}\, H_{2k}(x) \;=\; \frac{1}{\sqrt{1+4t}}\, \exp\left(\frac{4tx^2}{1+4t}\right), \tag{C.1}$$ z3sh1

To prove this rule, we recall the generating function of Hermite polynomials

$$e^{-s^2+2sx} \;=\; \sum_{n=0}^{\infty} \frac{s^n}{n!}\, H_n(x). \tag{C.2}$$ z3sh2

We multiply both sides of (C.2) by e^{-as^2}, with a being a real positive parameter, and then we integrate both sides over $s \in \mathbb{R}^1$. Thus, we get

$$\int_{-\infty}^{\infty} ds\; e^{-(a+1)s^2+2sx} \;=\; \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} \int_{-\infty}^{\infty} ds\; s^n\, e^{-as^2}. \tag{C.3}$$ z3sh3

Both integrals appearing in (C.3) are simple. The one in the lhs we compute according to

$$\int_{-\infty}^{\infty} dy\; e^{-py^2-qy} \;=\; \sqrt{\frac{\pi}{p}}\, \exp\left(\frac{q^2}{4p}\right), \tag{C.4}$$ z3sh4

where in our case $p = a+1$ and $q = -2x$. The integral in the rhs of (C.3) vanishes for $n = 2k+1$, that is for odd n. Thus we have

$$\int_{-\infty}^{\infty} ds\; s^{2k}\, e^{-as^2} \;=\; \frac{\Gamma(k+1/2)}{a^{k+1/2}}, \qquad \text{for} \quad n = 2k. \tag{C.5}$$ z3sh5

Using (C.4) and (C.5) in (C.3) we get

$$\sqrt{\frac{a\pi}{a+1}}\, \exp\left(\frac{x^2}{a+1}\right) \;=\; \sum_{k=0}^{\infty} \frac{H_{2k}(x)}{a^k}\, \frac{\Gamma(k+1/2)}{(2k)!} \tag{C.6}$$ z3sh6

Next we consider the combinatorial term in the rhs. We know that

$$\Gamma(k+1/2) \;=\; \sqrt{\pi}\, \frac{(2k-1)!!}{2^k}. \tag{C.7}$$ z3sh7

Moreover, we have $(2k)! = (2k)!!(2k-1)!! = 2^k k!(2k-1)!!$, so by combining these relations

$$\frac{\Gamma(k+1/2)}{(2k)!} \;=\; \sqrt{\pi}\,\frac{1}{2^{2k}\,k!}. \tag{C.8}$$ z3sh8

Using (C.8) in the summation rule (C.6) we obtain

$$\sum_{k=0}^{\infty}\,\left(\frac{1}{4a}\right)^k\,\frac{H_{2k}(x)}{a^k} \;=\; \sqrt{\frac{a}{a+1}}\,\exp\left(\frac{x^2}{a+1}\right). \tag{C.9}$$ z3sh9

We see that substitution $a = 1/4t$ yields

$$\sum_{k=0}^{\infty}\,\frac{H_{2k}(x)}{k!}\,t^k \;=\; \sqrt{\frac{1}{1+4t}}\,\exp\left(\frac{4tx^2}{1+4t}\right), \tag{C.10}$$ z3sh10

which is the sum rule (C.1) which we intended to prove, so the proof is therefore completed. Finally we note that the obtained expression is well defined for $t > -1/4$.

* *

Appendix D

Pseudospin operators

ap:sop

D.1 Basic definitions

Identifications

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad |2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{D.1}$$

z4vecid

z4psdef

Construction of the pseudospin matrices

$$|1\rangle\langle 1| = \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0,\ 1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{D.2a}$$

$$|1\rangle\langle 2| = \begin{pmatrix} 0 \\ 1 \end{pmatrix}(1,\ 0) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{D.2b}$$

$$|2\rangle\langle 1| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(0,\ 1) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \tag{D.2c}$$

$$|2\rangle\langle 2| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1,\ 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{D.2d}$$

Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{D.3}$$

z4paul

z4spm

It is convenient to denote

$$S_- = |1\rangle\langle 2| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{D.4a}$$

$$S_+ = |2\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{D.4b}$$

We call these operators *lowering* and *raising*, respectively. We now define some more operators via their matrices.

z4sxyz

$$S_1 = \frac{1}{2}(S_+ + S_-) = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{D.5a}$$

$$S_2 = -\frac{i}{2}(S_+ - S_-) = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{D.5b}$$

$$S_3 = \frac{1}{2}(|2\rangle\langle 2| - |1\rangle\langle 1|) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{D.5c}$$

An obvious connection with Pauli matrices

$$S_j = \frac{1}{2}\,\sigma_j \tag{D.6}$$ z4spaul

explains why we call S_j operators the pseudospin. Before discussion of the properties of the pseudospin operators we make two additional comments. From Eqs.(D.5a) and (D.5b) it follows that

$$S_+ = S_1 + iS_2, \qquad S_- = S_1 - iS_2. \tag{D.7}$$ z4spm12

We also note the Hermiticity relations

$$S_j^\dagger = S_j \;\; - \text{Hermitian}, \qquad S_\pm^\dagger = S_\mp \;\; - \text{Hermitian conjugates}, \tag{D.8}$$ z4sherm

what follows by inspection of the matrix representation.

D.2 Various products of pseudospin operators

The products of pseudospin operators follow:

- from their ket-bra definitions;
- from their matrix representations;
- from the fundamental property of Pauli operators:

$$\sigma_j\,\sigma_k = i\epsilon_{jkm}\,\sigma_m \quad \text{for} \;\; j \neq k, \qquad \sigma_j^2 = 1 \quad \text{for} \;\; j = 1,2,3. \tag{D.9}$$ z4pamul

All this sources are in fact equivalent. The proofs of the given below relations are omitted since such proofs are very easy to do. Before we give many particular examples, we note that Eqs.(D.9) and (D.6) imply

$$S_j\,S_k = \frac{i}{2}\,\epsilon_{jkm}\,S_m \quad \text{for} \;\; j \neq k, \qquad S_j^2 = \frac{1}{4} \quad \text{for} \;\; j = 1,2,3. \tag{D.10}$$ z4smul

For raising and lowering operators we have

$$\begin{aligned} S_+\,S_+ &= 0 \qquad & S_+\,S_- &= 1/2 \;+\; S_3, \\ S_-\,S_- &= 0 \qquad & S_-\,S_+ &= 1/2 \;-\; S_3. \end{aligned} \tag{D.11}$$

D.3 Commutation relations

For Pauli operators we have

$$[\,\sigma_j,\;\sigma_k] \;=\; 2i\epsilon_{jkm}\,\sigma_m, \tag{D.12}$$ z4paulcom

which, together with Eq.(D.6), yields the commutation relation for the pseudospin operators

$$[\,S_j,\;S_k] \;=\; i\epsilon_{jkm}\,S_m, \tag{D.13}$$ z4pscom

For raising and lowering operators we have

$$[\,S_\pm,\ S_1] = \pm S_3, \qquad [\,S_\pm,\ S_2] = i\,S_3, \qquad [\,S_\pm,\ S_3] = \mp S_\pm, \tag{D.14}$$ z4rlcom1

and

$$[\,S_+,\ S_-] = 2S_3, \tag{D.15}$$ z4rlcom2

D.4 Useful identities and their consequences

z4th:sopid1 **Theorem D.1** *For numbers α and β real or complex, there holds an identity*

$$\exp[\,i\alpha\,S_+ + i\beta\,S_-\,] = \cos\sqrt{\alpha\beta}\ + \frac{i}{\sqrt{\alpha\beta}}\ (\,\alpha\,S_+ + \beta\,S_-\,)\sin\sqrt{\alpha\beta}\,. \tag{D.16}$$ z4sopid1

This identity has several interesting and useful consequences. Putting $\alpha = \beta$, we get

$$e^{i\alpha(S_+ + S_-)} = \cos\alpha + (S_+ + S_-)\sin\alpha. \tag{D.17}$$ z4sopid1a

Since $2S_1 = S_+ + S_-$, we also get

$$e^{2i\alpha S_1} = \cos\alpha + 2S_1\sin\alpha. \tag{D.18}$$ z4sopid1b

If we take a limit $\beta \to 0$ in (z4sopid1 D.16), we get

$$e^{i\alpha S_+} = 1 + i\alpha\,S_+. \tag{D.19}$$ z4sopid1c

Similar procedure, but with $\alpha \to 0$ yields

$$e^{i\beta S_-} = 1 + i\beta\,S_-. \tag{D.20}$$ z4sopid1d

Combining two last relations we have

$$e^{i\alpha S_\pm} = 1 + i\alpha\,S_\pm. \tag{D.21}$$ z4sopid1e

If we put $\alpha = -i\xi,\ \beta = i\xi$, then from (z4sopid1 D.16) we can derive

$$e^{i(\alpha S_+ + \beta S_-)} = e^{2i\xi S_2} = \cos\xi + 2iS_2\sin\xi, \tag{D.22}$$ z4sopid1f

which should be compared to (z4sopid1b D.18).

z4th:sopid2 **Theorem D.2** *For numbers α and β real or complex, there holds an identity*

$$\exp[\,i\alpha\,S_3 + i\beta\,S_1\,] = \\ = \cos\left(\frac{\sqrt{\alpha^2+\beta^2}}{2}\right) + \frac{2i}{\sqrt{\alpha^2+\beta^2}}\ (\,\alpha\,S_3 + \beta\,S_1\,)\sin\left(\frac{\sqrt{\alpha^2+\beta^2}}{2}\right) \tag{D.23}$$

This theorem also leads to many useful specific cases. Putting $\beta = 0$ we get

$$e^{i\alpha S_3} = \cos\left(\frac{\alpha}{2}\right) + 2iS_3 \sin\left(\frac{\alpha}{2}\right) \tag{D.24}$$ z4sopid2a

Combining (D.18), (D.22) and (D.24) we can write a useful relation

$$e^{i\alpha S_j} = \cos\left(\frac{\alpha}{2}\right) + 2iS_j \sin\left(\frac{\alpha}{2}\right), \qquad \text{for} \quad j = 1, 2, 3. \tag{D.25}$$ z4sopid2b1

As a conclusion from the above derived relations we get the third useful theorem.

Theorem D.3 *For any number α real or complex there holds an identity*

$$e^{i\alpha S_k}\, S_j\, e^{-i\alpha S_k} = \begin{cases} S_k & \text{for} \quad j = k, \\ S_j \cos\alpha + \epsilon_{jkm}\, S_m \sin\alpha & \text{for} \quad j \neq k. \end{cases} \tag{D.26}$$ z4sopid3

From this theorem it follows that

$$e^{i\alpha S_3}\, S_\pm\, e^{-i\alpha S_3} = S_\pm\, e^{\pm i\alpha} \tag{D.27}$$ z4sopid3a

* *