

Einführung in die Quantenoptik I

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The preliminary programme for this lecture:

I Interaction between light and atoms (light and matter)

- relevant observables
- the model of a two-level atom (a two-level medium)
- Bloch equations
- quantum states of one and two qubits, correlations, entanglement

II QED – field quantization

- elementary scheme with a mode expansion
- states of the radiation field: Fock, coherent, thermal, squeezed; distribution functions in phase space
- about vacuum energies

III Applications

- state transformation at a beamsplitter, homodyne detection
- cavity QED, Jaynes-Cummings-Paul model (collapse and revival)
basic elements of a quantum computer (quantum gates)
- spontaneous emission and vacuum fluctuations, photodetection
- laser theory
- squeezing in a cavity (nonlinear optics)

Outlook: quantum optics II

- master equations, open systems, system + bath paradigm
- quantum theory of the micromaser
- correlations and fluctuations, spectral characterization
- problems of current interest:
two-photon interference, intensity correlations
virtual vs real photons, strong coupling

These notes are a merger of previous years and contain more material than was actually delivered in WS 2013/14.

Chapter 1

Matter-light interaction

In this chapter, we review some basic physics about polarizable matter and its interaction with light. The focus is on developing simple approximations that describe the coupling to near-resonant light fields. The model of a two-level atom will play an important role.

To begin the lecture, we describe in this chapter the field classically. The arguments can be made, however, with the quantized field as well. We shall give here and there the corresponding formulas without going into the details (to be found in Chapter 2).

1.1 Relevant observables

matter responds with

- absorption of light
- electric dipole moments, i.e. a polarization field $\mathbf{P}(\omega, \mathbf{r})$

... two different processes. A minimal description that contains the two is a *two-level model*.

Reminder on polarization

Meaning of polarization used here¹: spatial density of electric dipole moments (a vector field). This is a ‘micro-macro relation’ typical for electrodynamics

$$\mathbf{P}(\omega, \mathbf{r}) = n_{\text{at}}(\mathbf{r})\mathbf{d}(\omega) \quad (1.1)$$

¹Other meaning for polarization: orientation of the electric field vector in an electromagnetic wave. Linear, circular, elliptic polarization. Unpolarized, partially polarized light.

where $n_{\text{at}}(\mathbf{r})$ is the spatial density of constituent ‘atoms’ (or molecules) and $\mathbf{d}(\omega)$ the dipole moment per atom. (Electrons are displaced relative to positive atomic cores, overall charge remains zero.)

Link to refractive index $n(\omega, \mathbf{r})$: polarization response to the electric field

$$\mathbf{P}(\omega, \mathbf{r}) = \varepsilon_0(n^2 - 1)\mathbf{E}(\omega, \mathbf{r}) \quad (1.2)$$

At the microscopic level: polarizability $\alpha(\omega)$ = response of dipole moment to an electric field

$$\mathbf{d}(\omega) = \alpha(\omega)\mathbf{E}(\omega, \mathbf{r}) \quad (1.3)$$

where \mathbf{r} is now the position of the atom in the field. In suitable units: $\alpha(\omega)/\varepsilon$ has the units of volume, typically comparable to the volume occupied by electrons in an atom.

1.1.1 Two level model

Occupation numbers

Two-level scheme to model absorption: from quantum mechanics. Suppose that constituent atoms (molecules, ...) are in either state $|g\rangle$ or $|e\rangle$. In a semiconductor, electronic bands (valence band, separated by an energy gap from the conduction band).

In a single atom, quantum mechanics provides probabilities p_g and p_e : if $|\psi\rangle$ is the state of the system, then

$$p_a = |\langle a|\psi\rangle|^2, \quad a = g, e \quad (1.4)$$

In a macroscopic piece of matter where $n(\mathbf{r})$ is the number density of atoms, we have level densities

$$n_a(\mathbf{r}, t) = n(\mathbf{r})p_a(t; \mathbf{r}) \quad (1.5)$$

where the probability p_a depends on \mathbf{r}) because it involves the local light fields, as we shall see in a moment.²

The total probability is conserved

$$p_g + p_e = 1 \quad (1.6)$$

and similarly the sum over the densities $n_a(\mathbf{r}, t)$. If this would not hold true, then the Hilbert space is ‘too small’ with only two states.

²Distinction between ‘local’ and ‘macroscopic’ field. Not a well-defined question, actually.

‘incoherent’: if a description with only populations p_a is sufficient. Is often the case in condensed matter. Also for atoms in the gas phase as long as the time scales are ‘long enough’.

Coming back to a single two-level atom, quantum mechanics also allows for coherent superpositions

$$|\psi(t)\rangle = \sum_a c_a(t)|a\rangle \quad (1.7)$$

which contains more information than just the probabilities $p_a = |c_a|^2$. The phases of the complex numbers are related to the polarization or the dipole moment of the atom.

1.1.2 Density operator

The concept of the density operator generalizes the state vector familiar from quantum mechanics. The main reason is that we also want to handle states (or ensembles) which have a nonzero entropy (like thermal states have) or which arise from processes that do not conserve entropy, like spontaneous decay.

See the *exercises* for a discussion of entropy.

In the field of quantum information, one adopts sometimes a quite mathematical language. We shall follow this route and define a density operator by the following properties

A density operator ρ is a hermitean operator on the Hilbert space \mathcal{H} of the system. (A $N \times N$ -matrix if $\dim \mathcal{H} = N$ is finite.)

ρ is normalized to unit trace, $\text{tr} \rho = 1$.

ρ is positive: for all $|\psi\rangle \in \mathcal{H}$, we have

$$0 \leq \langle \psi | \rho | \psi \rangle \leq \langle \psi | \psi \rangle \quad (1.8)$$

The expectation value of a system observable \hat{A} is given by the ‘trace rule’

$$\langle \hat{A} \rangle = \text{tr}(\hat{A}\rho) = \text{tr}(\rho\hat{A}) \quad (1.9)$$

where we have used a cyclic permutation under the trace.

These conditions imply that the eigenvalues of ρ are real numbers in the interval $0 \dots 1$ whose sum is unity. They can therefore be interpreted as probabilities. Indeed the diagonal matrix element $\langle \psi | \rho | \psi \rangle$ in Eq.(1.8) is physically interpreted as the probability to find the system in the state $|\psi\rangle$ when it has been prepared in the density operator ρ . (This does not tell anything how this measurement is implemented or what observable one has to measure.)

Projectors = pure states

One class of states is familiar from ordinary quantum mechanics:

If $|\psi\rangle$ is a normalized state vector in the Hilbert space, then the projector

$$\mathbb{P}_{|\psi\rangle} = |\psi\rangle\langle\psi| \quad (1.10)$$

is a density operator. It is *the* density operator for a system prepared in the state $|\psi\rangle$.

It is simple the check that $\mathbb{P}_{|\psi\rangle}$ satisfies all conditions for a density operator. As an example, let us work out its trace by using a set of basis vectors $|n\rangle$

$$\text{tr}(|\psi\rangle\langle\psi|) = \sum_n \langle n|\psi\rangle\langle\psi|n\rangle = \sum_n |\langle n|\psi\rangle|^2 = 1 \quad (1.11)$$

In the last sum, we recognize the sum over the squares of the coefficients $c_n = \langle n|\psi\rangle$ that represent the vector $|\psi\rangle$ in the chosen basis. This is just the norm of the state. Alternatively, we could have used the completeness relation $\sum_n |n\rangle\langle n| = \mathbb{1}$.

By a similar calculation, one also checks that the trace rule is equivalent to the standard expectation value of observables:

$$\text{tr}(\hat{A}\rho) = \sum_n \langle n|\hat{A}|\psi\rangle\langle\psi|n\rangle = \sum_n \langle\psi|n\rangle\langle n|\hat{A}|\psi\rangle = \langle\psi|\hat{A}|\psi\rangle \quad (1.12)$$

Density operators that are built from projectors are called *pure states*. A formal definition that requires only the knowledge of the density operator ρ is based on a well-known property of projectors:

A density operator ρ is called a pure state when $\rho^2 = \rho$.

It is easy to see that for a pure state, the eigenvalues p_n must satisfy the property $\sum_n p_n^2 = 1$. Since we have $0 \leq p_n \leq 1$, this can only be satisfied if exactly one term in the sum is nonzero, say $p_1 = 1$, while all others are zero. But this means, using the eigenvector $|\psi_1\rangle$, that the ‘spectral representation’ of the density operator reduces to a single term:

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n| = |\psi_1\rangle\langle\psi_1| \quad (1.13)$$

in other words: ρ is a projector.

Purity and entropy

The definition of a pure state above can be exploited to define a quantitative measure of how far a state is from the set of pure states:

The ‘mixedness’ $\text{Mx}(\rho)$ of a density operator is given by

$$\text{Mx}(\rho) = \frac{\text{tr}(\rho - \rho^2)}{\text{tr} \rho} = 1 - \text{tr} \rho^2 \quad (1.14)$$

where the last equation holds for trace-normalized density operators. Conversely, the *purity* is $\text{Pu}(\rho) = 1 - \text{Mx}(\rho)$.

For a pure state, we have $\text{Mx}(\rho) = 0$ and $\text{Pu}(\rho) = 1$. States with $\text{Mx}(\rho) > 0$ ($\text{Pu}(\rho) < 1$) are called non-pure or *mixed*.

An alternative measure of purity is provided by the entropy:

The *entropy* of a density operator is given formally and in terms of its eigenvalues p_n by

$$S(\rho) = -\text{tr} \rho \log \rho = -\sum_n p_n \log p_n \quad (1.15)$$

A pure state has entropy $S(\rho) = 0$ if we remember the limiting value $\lim_{x \rightarrow 0} x \log x = 0$. (Apply the De L'Hôpital rule to the ratio $x/(1/\log x)$ or to $\log x/(1/x)$.)

If we make the formal expansion $\log \rho \approx \log \mathbb{1} + \rho - \mathbb{1} + \dots$, define $\log \mathbb{1} = 0$, and stop after the linear term, we recover the purity defined above. The purity has the advantage that the logarithm of the matrix is never needed (and no diagonalization neither). In quantum information, one uses other types of entropy measures that share similar monotony properties: they are zero for pure states and increase as the state becomes mixed.

Mixed states and convexity

As an example of a mixed state, let us consider two pure states $|\psi\rangle, |\chi\rangle$ and form the following linear combination of projectors

$$\rho = p|\psi\rangle\langle\psi| + q|\chi\rangle\langle\chi|, \quad p, q > 0, \quad p + q = 1 \quad (1.16)$$

This is called a *statistical mixture* of the states $|\psi\rangle, |\chi\rangle$.

Let us interpret this as a state preparation procedure with incomplete knowledge: a machine prepares a state $|\psi\rangle$ with probability p and otherwise the state

$|\chi\rangle$. The only possible prediction of the average value of any observable \hat{A} that we can then make is the following

$$\langle \hat{A} \rangle = p \langle \psi | \hat{A} | \psi \rangle + q \langle \chi | \hat{A} | \chi \rangle = \text{tr}(\hat{A}\rho) \quad (1.17)$$

which is nothing but the definition of the average for a density operator. This equation combines in an elegant way ‘quantum’ and ‘classical’ probabilities: indeed, the expectation values $\langle \psi | \hat{A} | \psi \rangle$ are typical for quantum mechanics, with the distribution of possible values for \hat{A} given by the wave function of $|\psi\rangle$ (the expansion of the state over a basis of eigenstates of \hat{A}). On the other hand, the weighting factors p, q in Eq.(1.17) are simply what one would do in classical statistics, when events occur with some probabilities and an average outcome is asked for.

In a thermal state (statistical physics), a typical mixture occurs in thermal equilibrium: the states $|\psi\rangle$ and $|\chi\rangle$ are energy eigenstates (with energies E_e and E_g , say). The corresponding probabilities are proportional to the Boltzmann factor $p \sim e^{-E_e/kT}$ where T is the temperature of the system (and k the Boltzmann constant). The average value $\langle \hat{A} \rangle$ in thermal equilibrium is then the combination of quantum expectation values in the energy eigenstates, averaged over the classical probabilities of finding these states in the thermal ensemble. For a system with n energy levels (subscript T for thermal equilibrium):

$$\langle \hat{A} \rangle_T = \sum_n \frac{e^{-E_n/kT}}{Z} \langle n | \hat{A} | n \rangle \quad (1.18)$$

Here, $Z = \sum_n e^{-E_n/kT}$ is the partition function (*Zustandssumme*) that provides the normalization for the Boltzmann probabilities.

From a geometrical viewpoint, the ‘mixing rule’ (1.16) implies that for any two points in the set of density operators, also the straight line that joins them is included in the set. This straight line is just the linear combination with real coefficients between 0 and 1. In mathematics, this is called a *convex* linear combination. A set is called convex if it contains for any two points, also the line between the two.

We can of course generalize Eq.(1.16) to the mixing of any two density operators ρ_1, ρ_2

$$\rho = p\rho_1 + q\rho_2, \quad p, q > 0, \quad p + q = 1 \quad (1.19)$$

It is easy to check that ρ defined in this way is again a density operator. The physical interpretation can again be formulated in terms of an incomplete knowledge about state preparation.

In mathematics, convex sets are conveniently characterized when their ‘extreme points’ are known. Intuitively speaking, extreme points correspond to ‘corners’ of the convex set from which lines into its interior can be drawn. In quantum information, extreme points are closely related to pure states. We shall encounter below a very simple convex set: a sphere (the *Bloch sphere*). Its extreme points are all those on the surface of the sphere, while the points in the interior correspond to mixed states.

One even more formal way of introducing a density operator or a quantum state: in the axiomatic language of quantum information, a ‘state’ ρ is a mapping from a set of observables to their expectation values

$$\rho : A \mapsto \rho(A) = \langle A \rangle_\rho \quad (1.20)$$

Linear map with $\rho(\mathbb{1}) = 1$ (real or complex coefficients depending on choice of observable algebra) and $\rho(A)$ real for a hermitean A .

Consider the familiar linear combinations in Hilbert space, $|\phi\rangle = \alpha|e\rangle + \beta|g\rangle$, with basis vectors $|e\rangle$ and $|g\rangle$, say. These states play a special role and are called *pure states*. They also correspond to special observables: *projectors*

$$\mathbb{P}_\phi = |\phi\rangle\langle\phi| \quad (1.21)$$

This is also a hermitean operator with eigenvalues 0 or 1. A physical state has the property that it is *positive*:

$$\rho(\mathbb{P}_\phi) \geq 0 \quad \text{for all } |\phi\rangle \quad (1.22)$$

Physical interpretation: this is the probability of finding the system in the pure state $|\phi\rangle$, which clearly must be a positive number.

Definition of *density matrix* (or *density operator*): any linear map on the vector space of observables can be represented by a suitable linear form

$$\rho(A) = \text{tr}(\bar{\rho}A) \quad (1.23)$$

where $\bar{\rho}$ is a hermitean operator and $\text{tr}(\hat{A}\hat{B})$ is a natural scalar product on the space of (hermitean) observables. This rule corresponds to the usual calculation of expectation values for mixed states in quantum statistics. In a finite-dimensional system, it corresponds to the duality between linear forms and vectors: each linear form can be represented as a scalar product with a suitable vector. This becomes the Riesz representation theorem in an infinite-dimensional Hilbert space.

1.1.3 The Bloch sphere

Density matrix elements

Let us analyze the set of density operators for a two-level system using a simple parametrization. The operator ρ has a matrix representation in the basis $|e\rangle, |g\rangle$

$$\rho = \begin{pmatrix} p & \rho_{eg} \\ \rho_{eg}^* & q \end{pmatrix}, \quad p + q = 1 \quad (1.24)$$

We have $p, q > 0$ because these elements correspond to diagonal matrix elements $p = \langle e|\rho|e\rangle = (1, 0)\rho \begin{pmatrix} 1 \\ 0 \end{pmatrix} \geq 0$. Their sum is unity because of the trace-normalization. A single complex number ρ_{eg} gives both off-diagonal elements:

The off-diagonal elements of a density matrix are called *coherences*. They quantify to what extent (in this basis), the quantum state is rather a ‘coherent superposition’ as opposed to a ‘classical mixture’. In quantum optics, ‘states with large coherence’ are often very useful, but also fragile.

The coherences cannot be very large in order not to spoil the positivity of ρ . This can be worked out from $\langle \phi|\rho|\phi\rangle$ with an ‘optimized’ superposition state $|\phi\rangle$. We follow here a faster route and compute simply the mixedness of the density operator. It must be positive or zero:

$$\text{Mx}(\rho) = 1 - \text{tr} \rho^2 = 1 - (p^2 + |\rho_{eg}|^2 + |\rho_{eg}|^2 + q^2) = 1 - p^2 - q^2 - 2|\rho_{eg}|^2 \geq 0 \quad (1.25)$$

We thus have an upper bound for the modulus $|\rho_{eg}|$. For equal probabilities $p = q = \frac{1}{2}$ (which looks like a ‘mixed state’), we get the inequality $|\rho_{eg}| \leq 1/2$. At the upper limit $|\rho_{eg}| = 1/2$, we even get a pure state! On the other side, if $p = 1$, then necessarily $\rho_{eg} = 0$: in the vicinity of the basis states, there is little space for ‘coherence’. (We shall see in the next section how significant coherences can be achieved nevertheless.)

To summarize, we have found three independent real parameters (p , $\text{Re} \rho_{eg}$, and $\text{Im} \rho_{eg}$) whose range is some compact domain. What can be said about the geometry of this domain?

Bloch vector

Any hermitean 2×2 matrix with trace 1 can be written as a linear combination of hermitean matrices that are well known from quantum mechanics as the Pauli

matrices (check the signs in σ_2)

$$\rho = \frac{1}{2}(\mathbb{1} + s_3\sigma_3 + s_1\sigma_1 + s_2\sigma_2) = \frac{1}{2} \begin{pmatrix} 1 + s_3 & s_1 + is_2 \\ s_1 - is_2 & 1 - s_3 \end{pmatrix} \quad (1.26)$$

The three numbers s_i ($i = 1, 2, 3$) are called the components of the *Bloch vector*. If we remember our notation p, q for the diagonal elements, we have $s_3 = p - q$. Similarly, s_1 and s_2 are proportional to the real and imaginary parts of ρ_{eg} . The inequality (1.25) for the real parameters takes a very simple form for the Bloch vector

$$s_3^2 + s_1^2 + s_2^2 \leq 1 \quad (1.27)$$

This means that the vector $\mathbf{s} = (s_1, s_2, s_3)$ lies inside a sphere of radius 1 in three-dimensional space.

Exercises: the components of the Bloch vector are the expectation values of the Pauli matrices:

$$s_i = \langle \sigma_i \rangle = \text{tr}(\sigma_i \rho) \quad (1.28)$$

The mixedness is determined by the length of the Bloch vector only

$$\text{Mx}(\rho) = 1 - \text{tr}(\bar{\rho}^2) = \dots = \frac{1}{2}(1 - \mathbf{s}^2) \quad (1.29)$$

• picture!

1.2 Hamiltonian

An atom can be modelled as a collection of charged point particles. The simplest Hamiltonian one can write is therefore

$$H_A = \sum_{\alpha} \frac{\mathbf{p}_{\alpha}^2}{2M_{\alpha}} + \frac{1}{2} \sum_{\alpha \neq \beta} \frac{e_{\alpha} e_{\beta}}{4\pi\epsilon_0 |\mathbf{x}_{\alpha} - \mathbf{x}_{\beta}|} \quad (1.30)$$

where α labels the particles, M_{α}, e_{α} are their masses and charges. We try to use in this lecture SI units. (In cgs units, drop the $4\pi\epsilon_0$.) The interaction term corresponds to the electrostatic (or Coulomb) field created by the charges.

More advanced atomic models adopt a relativistic viewpoint, take into account the electron spin, the magnetic field created by the motion of the particles, the corresponding spin-orbit interaction, the spin-spin coupling, the hyperfine interaction etc. Theoretical atomic physics computes all these corrections to the energy levels and matrix elements ‘from first principles’ (see the textbook by

hydrogen		H	n	$l = 0$	$l = 1$	$l = 2$	\dots
lithium		Li	\dots	\dots	\dots	\dots	\dots
sodium	Natrium	Na	3	3s	3p	3d	
potassium	Kalium	K	2	2s	2p		
rubidium		Rb	1	1s			
cesium		Cs					
francium		Fr					

Table 1.1: Left: the series of alkaline atoms. Right: Spectroscopic notation for energy levels of hydrogen-like atoms.

Haken & Wolf (2000), for example). Typically, no simple analytical results can be found for atoms with more than two or three electrons, say.

For our purposes, we are not interested in so much detail. Instead, we use a simplified description of the atom states that captures their essential properties. Good examples are atoms with a single electron in the outer shell (the alkaline series), as listed in table 1.1. Their energy levels are to a good approximation given by a modified Balmer formula

$$E_{nl} = -\frac{e^2}{8\pi\epsilon_0 a_0 (n + \delta_l)^2} = -\frac{\text{Ryd}}{(n + \delta_l)^2}, \quad \begin{array}{l} n = 1, 2, \dots \\ l = 0, \dots, n - 1 \end{array} \quad (1.31)$$

The Bohr radius $a_0 = 4\pi\epsilon_0\hbar^2/me^2 \approx 0.5 \text{ \AA}$ gives the typical size of the electron cloud, and the ‘quantum defect’ δ_l lifts the degeneracy of the hydrogen levels. The energy scale is given by the Rydberg constant $\text{Ryd} \approx 13.6 \text{ eV}$.

The charge $Z|e|$ of the nucleus enters the Balmer formula via the quantum defects δ_l . In fact, the outer electron ‘sees’ the nucleus screened by the core electrons. This gives a Coulomb potential as for the hydrogen atom, with some modifications due to the core electrons. These are responsible for the lifted degeneracy between the l states.

The frequency of electromagnetic radiation emitted by atoms in a process $|i\rangle \rightarrow |f\rangle$ is given according to Bohr by

$$\omega_{if} = \frac{E_i - E_f}{\hbar} \quad (1.32)$$

For two typical energy levels $E_{i,f}$, $\hbar\omega_{if}$ is also of the order of 1 Ryd. If we compute the wavelength of the corresponding electromagnetic radiation, we find

$$\lambda_{if} \sim \frac{2\pi\hbar c}{\text{Ryd}} = \frac{4\pi}{\alpha_{\text{fs}}} a_0 \gg a_0 \quad (1.33)$$

$$\text{fine structure constant } \alpha_{\text{fs}} = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}, \quad (1.34)$$

which is much longer than the typical size of the atom (the Bohr radius gives the extension of the electronic orbitals). For typical light fields, the atom thus appears like a pointlike object. This property justifies the ‘long wavelength approximation’ that simplifies the Hamiltonian for the atom–light interaction.

Another way of looking at the result (1.33) is to interpret the inverse fine structure constant, $\alpha_{\text{fs}}^{-1} = c(4\pi\epsilon_0\hbar/e^2)$ as the ratio between the speed of light c and the typical velocity for an electron in the Hydrogen atom (the natural velocity scale in the so-called ‘atomic units’). We see that this velocity is only a few percent of c , hence we expect that the non-relativistic description we have used so far is a good approximation.

1.3 Atom-light interaction

1.3.1 Minimal coupling

According to the rules of electrodynamics, the interaction between a collection of charges with a given electromagnetic field is described by the ‘minimal coupling’ Hamiltonian. This corresponds to the replacement $\mathbf{p}_\alpha \mapsto \mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{x}_\alpha, t)$ where $\mathbf{A}(\mathbf{r}, t)$ is the vector potential. In this chapter, this is a given time-dependent function. It will become an operator when the field is quantized. In addition, there is the potential energy due to an ‘external’ scalar potential $\phi_{\text{ext}}(\mathbf{x}, t)$, so that we get

$$H_{AF} = \sum_{\alpha} \frac{(\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{x}_\alpha, t))^2}{2M_\alpha} + \frac{1}{2} \sum_{\alpha \neq \beta} \frac{e_\alpha e_\beta}{4\pi\epsilon_0 |\mathbf{x}_\alpha - \mathbf{x}_\beta|} + \sum_{\alpha} e_\alpha \phi_{\text{ext}}(\mathbf{x}_\alpha, t). \quad (1.35)$$

The minimal coupling prescription is related to the freedom of choosing the phase reference of the wave function, as is seen in more detail in the exercises.

Remark. This freedom is also called ‘local $U(1)$ gauge invariance’ because phase factors form the unitary group $U(1)$. Local changes in the phase of the wave function generate terms in the Schrödinger equation that can be combined with gauge transformations for the electromagnetic potentials. This connection to the electromagnetic gauge transformations is of great importance for quantum field theory. It allows to construct the coupling to the electromagnetic field from the symmetry properties of the quantum fields. For example, there are theories where electrons and neutrinos are combined into a two-component field, and the interactions are invariant under $SU(2)$ transformations that mix these two, plus $U(1)$ transformations of the phase common to the

two components. The group $SU(2) \times U(1)$ is four-dimensional and has four ‘generators’. Each of them corresponds to a vector potential that interacts with the two-component field. In addition to the standard electromagnetic potential (the ‘photon’), there are interactions associated to the ‘massive vector bosons’, called W^\pm and Z^0 . They convey the ‘weak interaction’ that is responsible for β decay. More details in any book on quantum field theory. I sometimes use the one by Itzykson & Zuber (2006).

When the minimal coupling Hamiltonian (1.35) is expanded to lowest order in the charges e_α , we obtain the so called ‘ $p \cdot A$ ’ interaction

$$H_{\text{int}} = - \sum_{\alpha} \frac{e_{\alpha}}{2M_{\alpha}} \{ \mathbf{p}_{\alpha} \cdot \mathbf{A}(\mathbf{x}_{\alpha}, t) + \mathbf{A}(\mathbf{x}_{\alpha}, t) \cdot \mathbf{p}_{\alpha} \} + \sum_{\alpha} e_{\alpha} \phi_{\text{ext}}(\mathbf{x}_{\alpha}, t). \quad (1.36)$$

In the Coulomb gauge where $\nabla \cdot \mathbf{A} = 0$, the ordering of the operators is irrelevant. This interaction is linear in the vector potential, but there is also a second-order (or ‘diamagnetic’) term

$$H_{\text{dia}} = \sum_{\alpha} \frac{e_{\alpha}^2 \mathbf{A}^2(\mathbf{x}_{\alpha}, t)}{2M_{\alpha}} \quad (1.37)$$

When calculations are pushed to second order in the $p \cdot A$ -coupling, the diamagnetic interaction must be included as well, for consistency. This makes the ‘book-keeping’ in perturbation theory complicated.

Gauge transformation. There are essentially two schools that treat the scalar potential in very different ways.

(1) Either one is interested in electromagnetic fields on short scales compared to the wavelength (called “non-retarded limit”). Then one can ignore the vector potential and use only the scalar potential ϕ_{ext} to describe the matter-field interaction. This applies, for example, to the interaction of atoms or matter with electrons (scattering experiments).

(2) Or the wavelength is an important scale. Then one can even choose a gauge where $\phi_{\text{ext}} = 0$, and only the vector potential is nonzero.

Sometimes a mixture of the two schemes is needed, for example when light creates charge carriers, like in semiconductors or in the photoelectric effect.

1.3.2 Electric dipole coupling

A simpler approach is possible, however. We first make the approximation that the field varies slowly on the scale of the displacements \mathbf{x}_{α} of the charges in the atom. Then we can replace, to lowest order, $\mathbf{A}(\mathbf{x}_{\alpha}, t) \approx \mathbf{A}(\mathbf{R}, t)$ where \mathbf{R} is the atomic center of charge. This is called the ‘long-wavelength approximation’ that is well justified for fields near-resonant with typical atomic transitions. Within this approximation, we can find a simpler interaction Hamiltonian that is linear

in the electromagnetic field. It is called the ‘ $d \cdot E$ ’ coupling and is strictly linear in the electric field:

$$\begin{aligned} H_{\text{int}} &= -\mathbf{d} \cdot \mathbf{E}(\mathbf{R}, t), \\ \mathbf{d} &= \sum_{\alpha} e_{\alpha}(\mathbf{x}_{\alpha} - \mathbf{R}), \end{aligned} \quad (1.38)$$

where \mathbf{d} is the electric dipole moment of the atom relative to \mathbf{R} . This version of the $d \cdot E$ interaction can be derived from the minimal coupling Hamiltonian with a gauge transformation (see the exercises) from the minimal coupling Hamiltonian in the long-wavelength approximation, without invoking an additional approximation.

Gauge transformation. Change from the vector potential $\mathbf{A}(\mathbf{x}, t)$ to

$$\mathbf{A}'(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t) - \nabla\chi(\mathbf{x}, t), \quad \chi(\mathbf{x}, t) = (\mathbf{x} - \mathbf{R}) \cdot \mathbf{A}(\mathbf{R}, t) \quad (1.39)$$

where $\chi(\mathbf{x}, t)$ is called the ‘gauge function’. It ensures that $\mathbf{A}'(\mathbf{R}, t) = 0$ at all times. Since the gauge function is time-dependent, the scalar potential also changes:

$$\phi'(\mathbf{x}, t) = \phi(\mathbf{x}, t) + \partial_t\chi(\mathbf{x}, t) = \phi(\mathbf{x}, t) + (\mathbf{x} - \mathbf{R}) \cdot \partial_t\mathbf{A}(\mathbf{R}, t) \quad (1.40)$$

If we simply insert these ‘new potentials’ into the minimal coupling Hamiltonian, we get

$$H'_{\text{dia}} = 0, \quad H'_{\text{int}} = + \sum_{\alpha} e_{\alpha} \{ \phi_{\text{ext}}(\mathbf{x}_{\alpha}, t) + (\mathbf{x}_{\alpha} - \mathbf{R}) \cdot \partial_t\mathbf{A}(\mathbf{R}, t) \} \quad (1.41)$$

Note that the diamagnetic term cancels without further approximation. We expand the scalar potential for small $\mathbf{x}_{\alpha} - \mathbf{R}$ and get

$$H'_{\text{int}} = +\phi_{\text{ext}}(\mathbf{R}, t) \sum_{\alpha} e_{\alpha} + \sum_{\alpha} e_{\alpha}(\mathbf{x}_{\alpha} - \mathbf{R}) \cdot \{ \nabla\phi_{\text{ext}}(\mathbf{R}, t) + \partial_t\mathbf{A}(\mathbf{R}, t) \} \quad (1.42)$$

The first term cancels if the system of charges is globally neutral. In the second term, we recognize the expression of the electric field $\mathbf{E}(\mathbf{R}, t)$ in terms of the potentials. Hence we find the electric dipole Hamiltonian (1.38).

The advantages of the electric dipole coupling are: the atom couples directly to the field; there is no quadratic interaction term. One must not forget that between the two interactions, the wave function (the atomic state) differs by a unitary transformation. Otherwise, some matrix elements or transition rates may come out differently. This issue is discussed in great detail in the book ‘Molecular Quantum Electrodynamics’ by Craig & Thirunamachandran (1984) and in Chap. IV of ‘Photons and Atoms – Introduction to Quantum Electrodynamics’ by Cohen-Tannoudji & al. (1987).

1.3.3 Selection rules

Since the electric dipole moment determines the interaction with the light field, a few remarks on its matrix elements are in order. We take as a starting point the basis of the stationary states of an atom, described by the Hamiltonian (1.30). These states are typically described by quantum numbers like parity, angular momentum etc. The ‘selection rules’ specify for which states we know by symmetry that the matrix elements of the electric dipole moment vanish. In that case, the corresponding states are not connected by an ‘electric dipole transition’, or the transition is ‘dipole-forbidden’.

Parity. We say that a state $|a\rangle$ has a defined parity $P_a = \pm 1$ when the electronic wave function $\psi(\{\mathbf{x}_\alpha\})$ “transforms like” $P_a \psi(\{\mathbf{x}_\alpha\})$ when all coordinates are transformed as $\mathbf{x}_\alpha \mapsto -\mathbf{x}_\alpha$. This means that

$$(\hat{P}\psi)(\{-\mathbf{x}_\alpha\}) = \psi(\{-\mathbf{x}_\alpha\}) = P_a \psi(\{\mathbf{x}_\alpha\}) \quad (1.43)$$

where $(\hat{P}\psi)$ denotes the action of the parity operator on the wave function.³ If now $|a\rangle$ has a well-defined parity, then it is easy to show that $\langle a|\mathbf{d}|a\rangle = 0$ (see lecture). In addition, the matrix element $\langle a|\mathbf{d}|b\rangle$ is only nonzero when $|a\rangle$ and $|b\rangle$ have different parity. This is an example of a “selection rule”. It provides a simple argument to exclude certain transitions from happening under the electric-dipole coupling. We shall see below that an off-diagonal matrix element like $\langle a|\mathbf{d}|b\rangle$ is essential when one wants to induce a “quantum jump” from one level to another with light.

Energy. Selection rules often arise when the system has certain symmetries. See a few examples below. The simplest symmetry is “translation in time”, i.e., the system Hamiltonian does not depend on time. We then know from classical mechanics that energy is a conserved quantity. This is also true in quantum mechanics and quantum optics. The corresponding selection rule for atom-light interaction is the Bohr-Sommerfeld rule for the photon (angular) frequency ω that can induce a transition between two levels $|a\rangle$ and $|b\rangle$:

$$\hbar\omega = |E_b - E_a|. \quad (1.44)$$

³In the simple one-dimensional problems you remember from Quantum Mechanics I, wave functions that are ‘even’ or ‘odd’ have a well-defined parity. But there are also wave functions that are neither even nor odd. One says that these do not have a well-defined parity.

This formula is in fact one of the birth certificates of quantum theory – remember that quantum mechanics was developed to explain the discrete frequencies observed in the radiation spectra of atoms.

Angular momentum. If there is no electron spin, this is given by l , and by $j = l \pm \frac{1}{2}$ for hydrogen-like atoms where one spin of a non-paired electron is present. The vector operator \mathbf{d} transforms under rotation like a spin 1 (there are three different basis vectors). One can introduce a basis \mathbf{e}_q ($q = -1, 0, 1$) that are eigenvectors of L_3 as well and write $\mathbf{d} = \sum_q d_q \mathbf{e}_q$. The product $\mathbf{e}_q |l, m\rangle$ then is an eigenstate of L_3 with eigenvalue $q + m$. Therefore, the matrix element with $|l', m'\rangle$ is only nonzero when $m' = q + m$. We find the selection rule

$$|m - m'| \leq 1.$$

In addition, the product states $\mathbf{e}_q |l, m\rangle$ can be expanded onto eigenstates of \mathbf{L}^2 . The rules for the ‘addition of angular momentum’ imply that only angular momenta $l' = l - 1, l, l + 1$ occur in this expansion. This gives the selection rule

$$|l - l'| \leq 1.$$

Total momentum. An atom that is in a plane wave state regarding its centre-of-mass motion, with momentum \mathbf{P} receives an additional momentum $\hbar\mathbf{k}$ when a photon from a plane electromagnetic wave with wave vector \mathbf{k} is absorbed. The corresponding ‘recoil velocity’ $\hbar\mathbf{k}/M$ is of the order of a few mm/s to a few cm/s for typical atoms. The atomic recoil plays an important role for atom deceleration and cooling with laser light.

1.4 Two-level atoms

For the rest of this lecture, it will be sufficient to write the atomic Hamiltonian in the form

$$H_A = \sum_n E_n |n\rangle\langle n|, \quad (1.45)$$

where the states $|n\rangle$ are the stationary states corresponding to the energy eigenvalue E_n . But even this form is too complicated: it contains too many terms when dealing with near-resonant laser light. This is the setting we shall focus on here. One can then retain only a few states to describe the atom.

1.4.1 Two-level language

Two-level observables

Atomic Hamiltonian. The standard notation for the two states is $|g\rangle$ for the ground state and $|e\rangle$ for the excited state. The Bohr frequency is often written

$\omega_A = \omega_e - \omega_g > 0$. The atomic energy levels are often referenced to a zero energy lying between both states, this gives:

$$H_A = \frac{\hbar\omega_A}{2}|e\rangle\langle e| - \frac{\hbar\omega_A}{2}|g\rangle\langle g| \quad (1.46)$$

It is also useful to identify the two-dimensional Hilbert space of the two-level atom with the \mathbb{C}^2 , using the basis vectors $(1, 0)^T \leftrightarrow |e\rangle$ and $(0, 1)^T \leftrightarrow |g\rangle$. The Hamiltonian then becomes the diagonal matrix

$$H_A = \frac{\hbar\omega_A}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar\omega_A}{2}\sigma_3 \quad (1.47)$$

where σ_3 is the third Pauli matrix. Indeed, it is obvious that a two-dimensional Hilbert space can be identified with the Hilbert space of a spin 1/2.

Observables energy, inversion, dipole.

$$\mathbf{d} = \mathbf{d}_{ge}\sigma + \mathbf{d}_{ge}^*\sigma^\dagger = \mathbf{d}_{ge}|g\rangle\langle e| + \mathbf{d}_{ge}^*|e\rangle\langle g| \quad (1.48)$$

where the vector of matrix elements of the dipole operator is $\mathbf{d}_{ge} = \langle g|\mathbf{d}|e\rangle$. Only off-diagonal matrix elements because of the parity selection rule.

State of a two-level system

This section contains details on a somewhat more axiomatic approach than what we did in the lecture in WS 11/12. You may jump directly to Eqs.(3.40, 1.59) that have been discussed in the Problem sessions.

The expectation values $\langle\sigma_3\rangle$ and $\langle\sigma\rangle$ completely specify the state of the two-level system.

Why is this so? A general observable is a hermitean 2×2 matrix. All these matrices are linear combinations of Pauli matrices

$$\begin{aligned} A &= \begin{pmatrix} a_{ee} & a_{eg} \\ a_{ge} & a_{gg} \end{pmatrix} = \frac{a_{ee} + a_{gg}}{2} \mathbb{1} + \frac{a_{ee} - a_{gg}}{2} \sigma_3 + a_{ge}\sigma + a_{eg}\sigma^\dagger \\ &= \frac{a_{ee} + a_{gg}}{2} \mathbb{1} + \sum_j a_j \sigma_j, \end{aligned} \quad (1.49)$$

$$\sigma_1 = \sigma + \sigma^\dagger \quad (1.50)$$

$$\sigma_2 = i(\sigma - \sigma^\dagger) \quad (1.51)$$

with real coefficients a_j .

The above statement is true even for a more general definition of a *state* than you may be used to. In the axiomatic language of quantum information, a state is a mapping from a set of observables to their expectation values

$$\rho : A \mapsto \rho(A) = \langle A \rangle_\rho \quad (1.52)$$

Linear map with $\rho(\mathbb{1}) = 1$ (real or complex coefficients depending on choice of observable algebra) and $\rho(A)$ real for a hermitean A .

Now, the action of this map is determined by evaluation on basis vectors = Pauli matrices for a two-level system:

$$\rho(A) = \frac{a_{ee} + a_{gg}}{2} \rho(\mathbb{1}) + \sum_j a_j \rho(\sigma_j) = \frac{a_{ee} + a_{gg}}{2} \rho(\mathbb{1}) + \sum_j a_j s_j \quad (1.53)$$

with components of *Bloch vector* $\mathbf{s} = (s_1, s_2, s_3)$.

This definition is more general than complex linear combinations of $|e\rangle$ and $|g\rangle$. These states play a special role and are called *pure states*. They also correspond to special observables: *projectors*

$$\mathbb{P}_\phi = |\phi\rangle\langle\phi| \quad (1.54)$$

This is also a hermitean operator with eigenvalues 0 or 1. A physical state has the property

$$\rho(\mathbb{P}_\phi) \geq 0 \quad \text{for all } |\phi\rangle \quad (1.55)$$

Physical interpretation: this is the probability of finding the system in the pure state $|\phi\rangle$, which clearly must be a positive number.

Definition of *density matrix* (or *density operator*): any linear map on the vector space of observables can be represented by a suitable linear form

$$\rho(A) = \text{tr}(\bar{\rho}A) \quad (1.56)$$

where $\bar{\rho}$ is a hermitean operator. This rule corresponds to the usual calculation of expectation values for mixed states in quantum statistics. In a finite-dimensional system, it corresponds to the duality between linear forms and vectors: each linear form can be represented as a scalar product with a suitable vector. This becomes the Riesz representation theorem in an infinite-dimensional Hilbert space.

Using this for projector observables, we find from Eq.(1.55):

$$0 \leq \rho(\mathbb{P}_\phi) = \text{tr}(\bar{\rho}|\phi\rangle\langle\phi|) = \langle\phi|\bar{\rho}|\phi\rangle \quad (1.57)$$

Hence the diagonal elements of the density matrix are positive, in any basis. This connects again to the interpretation of the probability of finding the system in the state $|\phi\rangle$.

Density operator as observable itself. Expectation value is called purity

$$\text{Pu}(\rho) = \langle \bar{\rho} \rangle_\rho = \text{tr}(\bar{\rho}^2) = \dots = \frac{1}{2}(1 + \mathbf{s}^2) \quad (1.58)$$

Calculation uses representation in terms of Bloch vector and Pauli matrices

$$\bar{\rho} = \frac{1}{2} \left(\mathbb{1} + \sum_j s_j \sigma_j \right) = \frac{\mathbb{1} + \mathbf{s} \cdot \boldsymbol{\sigma}}{2} \quad (1.59)$$

Bloch sphere

The language of a spin 1/2 is often used to visualize the dynamics of a two-level atom. Let us compute the components of the average spin vector $(s_1, s_2, s_3)^T \equiv \langle \boldsymbol{\sigma} \rangle$ (the ‘Bloch vector’) in the pure state $|\psi(t)\rangle = (c_e(t), c_g(t))^T$:

$$s_3 = |c_e|^2 - |c_g|^2 \quad (1.60)$$

$$s_1 - is_2 = 2c_g^* c_e \quad (1.61)$$

Observe that $\mathbf{s}^2 = s_1^2 + s_2^2 + s_3^2 = 1$ for a pure state. The component s_3 is related to the occupation probabilities $|c_e(t)|^2$, $|c_g(t)|^2$ (the ‘populations’): it gives the *inversion*, i.e., the difference of the ground and excited state populations. In the ground state, one has $\langle \sigma_3 \rangle = -1$. The other two components (1.61) are only nonzero when the atom is in a superposition of the ground and excited states.

In the exercises, you show that the Bloch vector is in general constrained by $\mathbf{s}^2 \leq 1$, due to the positivity condition (1.57) of the density matrix. It can thus be represented by a point in a sphere, the ‘Bloch sphere’ (see Fig.1.1). On the sphere surface are located the pure states: the ‘south pole’ corresponds to an atom in the ground state, while an excited atom is at the ‘north pole’. In between these two, the atom is in a superposition of ground and excited states. In particular, around the equator, both ground and excited state are occupied with probability 1/2 (the inversion is zero). The longitude along the equator is fixed by the phase difference between ground and excited state.

If no external laser field is applied, the Bloch vector rotates at the frequency ω_A clockwise around the vertical axis. In particular, the occupation probabilities do not change with time: the inversion, being the projection onto the vertical axis, is constant. With the laser on, we shall see that the rotation axis gets tilted so that an atom initially in the ground state develops an excited component.

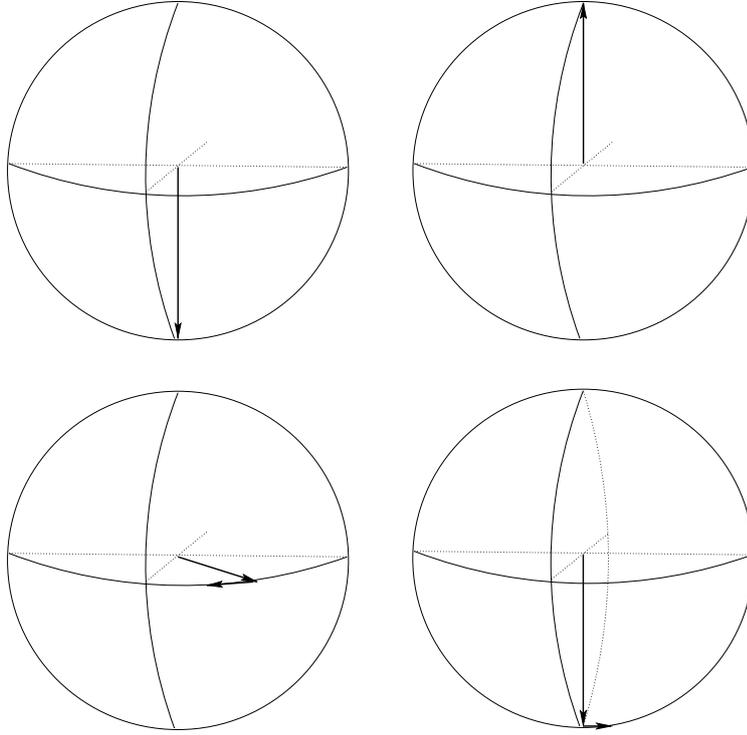


Figure 1.1: Upper left: Bloch vector for an atom in the ground state. Upper right: excited state. Lower left: superposition of ground and excited states with equal weight. The arrow along the ‘equator’ indicates the direction of free rotation of the Bloch vector without a laser field. Lower right: an initial ground state starts to undergo resonant Rabi oscillations, as indicated by the arrow tangent to the ‘south pole’. The x_1 -axis points to the right, the x_3 -axis upwards.

1.4.2 Resonance approximation

Interaction Hamiltonian

The interaction with a monochromatic laser field can be described by the Hamiltonian

$$\begin{aligned}
 H &= H_A - \mathbf{d} \cdot \mathbf{E}(t) \\
 \mathbf{E}(t) &= \mathbf{E} e^{-i\omega_L t} + \text{c.c.} \\
 \mathbf{d} &= \mathbf{d}_{ge} |g\rangle\langle e| + \text{h.c.}
 \end{aligned} \tag{1.62}$$

where the complex vector \mathbf{E} gives the amplitude of the electric field. It is evaluated at the position of the atom, we drop this dependence here. The laser (an-

gular) frequency is ω_L . The term $\mathbf{E} e^{-i\omega_L t}$ is called the ‘positive frequency part’ of the field: its time evolution is the same as for a solution of the time-dependent Schrödinger equation (with positive energy $\hbar\omega_L$).

We re-write Eq.(1.62) in terms of two separately hermitean operators

$$\begin{aligned} -\mathbf{d} \cdot \mathbf{E}(t) &= \frac{\hbar}{2} \left(\Omega e^{-i\omega_L t} |e\rangle\langle g| + \text{h.c.} \right) \\ &\quad + \frac{\hbar}{2} \left(\Omega' e^{i\omega_L t} |e\rangle\langle g| + \text{h.c.} \right) \end{aligned} \quad (1.63)$$

$$\frac{\hbar\Omega}{2} = -\mathbf{d}_{ge}^* \cdot \mathbf{E}, \quad (\text{Rabi frequency}) \quad (1.64)$$

where Ω is a complex-valued frequency, and Ω' has a similar expression as Eq.(1.64). (We follow the Paris convention and notation for Ω .)

If the field is quantized, Eq.(1.62) applies in similar form in the interaction picture and involves photon annihilation operators a_L in place of the complex amplitude \mathbf{E} (and creation operators a_L^\dagger in place of \mathbf{E}^*). The fully quantized interaction Hamiltonian is derived from the quantized field operator and takes the form:

$$\begin{aligned} -\mathbf{d}(t) \cdot \mathbf{E}(t) &\mapsto \\ -\sum_k \mathcal{E}_k \left(a_k(t) \mathbf{f}_k \cdot \mathbf{d}(t) + a_k^\dagger(t) \mathbf{f}_k^* \cdot \mathbf{d}(t) \right) \end{aligned} \quad (1.65)$$

where $\mathcal{E}_k = \sqrt{\hbar\omega_k/(2\varepsilon_0 V)}$ is the electric field amplitude at the one-photon level and $\mathbf{f}_k = \mathbf{f}_k(\mathbf{R})$ is the normalized mode function, evaluated at the position \mathbf{R} of the atom. We have written Eq.(1.65) in the “interaction picture” where all operators carry their “free” time dependence. For the photon annihilation operator $a_k(t) = a_k e^{-i\omega_k t}$, which is the operator in the Heisenberg picture under the free field Hamiltonian. The time dependence of the (freely evolving) dipole operator is given by $\mathbf{d}(t) = \exp(iH_A t) \mathbf{d} \exp(-iH_A t)$.

In order to examine what happens to an atom illuminated by a laser field, we make the *Ansatz*

$$|\psi(t)\rangle = \tilde{c}_e(t) e^{-i\omega t/2} |e\rangle + \tilde{c}_g(t) e^{+i\omega t/2} |g\rangle \quad (1.66)$$

where the frequency ω is chosen later. The amplitudes describe the two-level system in a *picture* that differs from the usual choice $c_e(t)$, $c_g(t)$. The Schrödinger equation for \tilde{c}_e contains a correction term because of the time-dependent exponential. One gets

$$\begin{aligned} i\hbar\partial_t \tilde{c}_e &= \left(E_e - \frac{\hbar\omega}{2} \right) \tilde{c}_e + \frac{\hbar}{2} \Omega e^{-i(\omega_L - \omega)t} \tilde{c}_g \\ &\quad + \frac{\hbar}{2} \Omega' e^{i(\omega_L + \omega)t} \tilde{c}_g \end{aligned} \quad (1.67)$$

Now, we can take the choice $E_e = \frac{1}{2}\hbar\omega_A$ for the excited state energy. There are now two “natural choices” for ω :

- (1) **interaction picture:** $\omega = \omega_A$, and the first term disappears. The time dependence of \tilde{c}_e is then only due to the atom-laser interaction. This picture is suitable for perturbation theory.
- (2) **rotating frame:** $\omega = \omega_L$, and the second term becomes time-independent. This picture is suitable for concrete calculations in quantum optics, once we have convinced ourselves what is the meaning of the third term.

Time-dependent perturbation theory

We now make the choice (1) of the interaction picture and solve the equation for \tilde{c}_e with the help of time-dependent perturbation theory. This proceeds by identifying the interaction Hamiltonian as a “small term” and by counting ascending powers.

At the order zero, H_A is the only Hamiltonian. Keeping in mind the choice $\omega = \omega_A$, Eq.(1.67) reduces to

$$\partial_t \tilde{c}_e^{(0)} = 0, \quad \partial_t \tilde{c}_g^{(0)} = 0 \quad (1.68)$$

where the equation for \tilde{c}_g is similar to Eq.(1.67). As expected from the analogy to the time-dependent Schrödinger equation (for the “free” atom), the amplitudes are constants at order zero. The natural initial condition “atom is in state $|g\rangle$ ” translates into

$$\tilde{c}_e^{(0)}(t) = 0, \quad \tilde{c}_g^{(0)}(t) = 1. \quad (1.69)$$

To the first order, we get from Eq.(1.67)

$$i\hbar\partial_t \tilde{c}_e^{(1)} = \frac{\hbar}{2}\Omega e^{-i(\omega_L - \omega_A)t} \tilde{c}_g^{(0)} + \frac{\hbar}{2}\Omega' e^{i(\omega_L + \omega_A)t} \tilde{c}_g^{(0)} \quad (1.70)$$

Now, since we know $\tilde{c}_g^{(0)}(t)$ as a (constant) function of time, this can be integrated immediately to give

$$c_e(t) = c_e(0) + \frac{\Omega}{2} \frac{e^{-i(\omega_L - \omega_A)t} - 1}{\omega_L - \omega_A} - \frac{\Omega'}{2} \frac{e^{i(\omega_A + \omega_L)t} - 1}{\omega_A + \omega_L} \quad (1.71)$$

The two terms in this result have distinct physical interpretations, related to the denominators.

Absorption. The first denominator leads to a ‘large’ result when $\omega_A = \omega_L$. One says that the atom went from the state $|g\rangle$ to the higher-lying state $|e\rangle$ by absorbing one ‘energy quantum’ (‘photon’). (Recall that the amplitude c_e for the state $|e\rangle$ is increased in Eq.(1.71).) This process is governed by the ‘positive frequency’ component $\Omega e^{-i\omega_L t}$ of the interaction Hamiltonian (corresponding to the positive frequency component of the electromagnetic field). In the quantized description of the light field, this component corresponds to an ‘annihilation operator’ that removes one photon from the field. If we fix the states $|g\rangle$ and $|e\rangle$ such that the condition for absorption is satisfied, then the second term in Eq.(1.71) has a ‘large’ denominator, $\omega_A + \omega_L \approx 2\omega_A$. This term is therefore much smaller than the first one, by a factor of the order $\mathcal{O}(10^{-6})$ for laser fields of reasonable intensity (see exercise). This suggests that we can neglect this term. This approximation is called the ‘resonance approximation’ (or the ‘rotating wave approximation’, an admittedly strange name). If we keep the non-resonant term, we deal in the quantum theory with a ‘virtual’ process where the atom passes into a state with a higher energy and at the same time, a photon is created.

Emission. If we had started with the atom in the excited state $|e\rangle$, one would get a resonant contribution again for $\omega_L = \omega_A$, with a large amplitude being created in $|g\rangle$. This corresponds to a transition with the energy balance $E_e = E_g + \hbar\omega_L$: the atom makes a transition to a lower-lying state, and in the quantized field description, a ‘photon’ is created (by the creation operator a_k^\dagger in the expansion of the field operator). The non-resonant term in this setting would correspond to the atom decaying to the ground state and absorbing a photon, clearly a virtual process.

To summarize, in the resonance approximation, we only retain those parts of the interaction Hamiltonian where the excitation of the atom (the operator $\sigma^\dagger = |e\rangle\langle g|$) is accompanied by a positive frequency laser field $\mathbf{E}e^{-i\omega_L t}$. This approximation is consistent with the two-level approximation where right from start, we only considered atomic levels whose Bohr frequencies are near-resonant with the laser.

This approximation is possible for a ‘detuning’ $\Delta = \omega_L - \omega_A$ small compared to the typical differences between atomic transition frequencies. This condition is easily achieved since transition frequencies (spectral lines) differ easily by energies of the order of 1 eV, and this is a ‘huge’ detuning to drive an atomic transition.

Remark. The description of absorption and emission, as we encounter it here, does not explicitly require the quantization of the light field. These processes also occur in a ‘classical’ time-dependent potential because energy is not conserved there, as is well known in classical mechanics. One can push the analogy even further: a weak monochromatic excitation of a mechanical system reveals the system’s ‘resonance frequencies’. For an atom, these are apparently given by the Bohr frequencies. The only difference to a mechanical system is that we are inclined to use different names for the excitations with positive and negative frequencies, since in the atomic energy spectrum, there is a definite difference between ‘going up’ and ‘going down’ (there exists a ground state).

Atomic polarizability

The perturbative calculation can be used to determine the dipole moment that the laser field induces in the atom. This dipole is, within the lowest order in the perturbation, linear in the amplitude \mathbf{E} of the laser, or equivalently, in the Rabi frequency Ω . As is discussed in more detail in the exercises (Problem 3.2), the polarizability is defined by equating the average (induced) dipole moment with a function linear in the laser amplitude,

$$\langle \psi(t) | (\mathbf{d}_{ge}\sigma + \text{h.c.}) | \psi(t) \rangle = \alpha(\omega_L) \mathbf{E} e^{-i\omega_L t} + \text{h.c.} \quad (1.72)$$

Note that the asymptotic regime $t \rightarrow \infty$ is taken here where the atomic dipole oscillates at the frequency of the external field. Now, for the initial condition that the atom starts in its ground state, the polarizability is

$$\alpha_g(\omega) = \frac{(2\omega_{eg}/\hbar) \mathbf{d}_{ge} \otimes \mathbf{d}_{ge}^*}{\omega_{eg}^2 - \omega^2} \quad (1.73)$$

where two peaks at $\omega = \pm\omega_{eg}$ appear. These peaks are not damped – which is an artefact because we ignored any damping processes to far. In practice, processes called spontaneous emission, thermal absorption, and dephasing remove the divergence of the polarizability $\omega = \pm\omega_{eg}$ and lead to a Lorentzian profile with a nonzero linewidth. To calculate this, we need the quantum theory of the light field.

RWA Hamiltonian in the rotating frame

We come back to the (near-)resonant interaction: it can be described by the (effective) Hamiltonian

$$H_{AL} = -\mathbf{d}_{ge}^* \mathbf{E} e^{-i\omega_L t} \sigma^\dagger - \mathbf{d}_{ge} \mathbf{E}^* e^{i\omega_L t} \sigma \quad (1.74)$$

This is called the “rotating wave approximation”, a physically more transparent name would be “resonance approximation”. The change into the picture (2) (rotating frame) mentioned on p.22 above ($\omega = \omega_L$) corresponds to the unitary transformation

$$|\psi(t)\rangle = e^{-i\frac{\omega_L t}{2}\sigma_3}|\tilde{\psi}(t)\rangle \quad (1.75)$$

This gives for the state $|\tilde{\psi}(t)\rangle$ the following Hamiltonian

$$H = -\frac{\hbar\Delta}{2}\sigma_3 + \frac{\hbar}{2}(\Omega^*\sigma + \Omega\sigma) \quad \Delta = \omega_L - \omega_A \quad (1.76)$$

where the time-dependence of Eq.(1.74) has disappeared (exactly) and where only the *detuning* Δ instead of the laser frequency appears (Paris convention for the sign of Δ).

With a quantized field, add the Hamiltonian H_F for the field and make the replacement

$$\frac{\hbar}{2}(\Omega^*\sigma + \sigma^\dagger\Omega) \mapsto -\sum_k \mathcal{E}_k \left\{ a_k^\dagger \mathbf{f}_k^* \cdot \mathbf{d}_{\text{eg}}^* \sigma + \sigma^\dagger a_k \mathbf{f}_k \cdot \mathbf{d}_{\text{eg}} \right\} \quad (1.77)$$

One could also read this as an operator-valued Rabi frequency per mode, $\hat{\Omega}_k$.

1.4.3 Overview

The Hamiltonian (1.76), combined with its quantized field formulation, is the basis for most of the phenomena that have been studied in the quantum optics of two-level system. One can discuss the following topics (we give a selection in this lecture):

- Rabi oscillations in a classical monochromatic field;
- spontaneous decay of an excited atom into the continuum of vacuum field modes (initially in the ground state);
- interaction of light with a medium of two-level atoms. One has to re-interpret the density matrix as giving the state of a macroscopic number of atoms. The occupations p_e, p_g , for example, then are proportional to the number of atoms (or molecules) in the excited and ground state. The atomic dipole becomes, after multiplication with the atom density, the polarization field (electric dipole moment per volume). Coupled to the Maxwell equations where this polarization field enters as a source term, one then has a simple “semiclassical” description for a laser, for a solar cell, for a semi-conductor. The Bloch equations in this case may contain more complicated terms.

- collapse and revival of Rabi oscillations when the atom couples to a single quantized field mode. The collapse and the revival occurs because the Rabi frequency depends on the photon number, and the oscillations for the different Fock state components of a field state (a coherent state, for example) get out of phase;
- resonance fluorescence is the radiation emitted by an atom driven by a near-resonant laser field. This combines Rabi oscillations in a classical field with the emission of photons into the empty mode continuum. Of particular interest is the spectrum of this emission: it contains, for sufficiently strong driving, two sidebands, split by the Rabi frequency from the central line (centered at the laser frequency). The central line contains a monochromatic component ('elastic scattering', related to the laser-induced dipole moment as in classical electrodynamics) and a broadened component of Lorentzian shape, related to spontaneous emission. This spectrum is a cornerstone of quantum optics and one of the few examples of a non-perturbative calculation in quantum electrodynamics.

Spin 1/2 analogy. We now come back to the spin 1/2 analogy. The Hamiltonian (1.74) with the atomic energies and the atom–laser interaction has the same form as the Hamiltonian for a spin 1/2 in a time-dependent magnetic field,

$$H_{\text{spin}} = \boldsymbol{\sigma} \cdot \mathbf{B}(t) \quad (1.78)$$

where $\boldsymbol{\sigma}$ is the vector of Pauli matrices and the 'magnetic field' $\mathbf{B}(t)$ actually has the dimensions of an energy (we took a unity magnetic moment). The magnetic field rotates at the laser frequency around the x_3 -axis:

$$\mathbf{B}(t) = \frac{\hbar}{2} \begin{pmatrix} \Omega \cos \omega_L t \\ \Omega \sin \omega_L t \\ \omega_A \end{pmatrix} \quad (1.79)$$

It is useful to change the coordinate frame such that it co-rotates with this field (this is the 'rotating frame'). In this frame, the 'effective magnetic field' is static⁴,

$$\mathbf{B}_{\text{eff}} = \frac{\hbar}{2} \begin{pmatrix} \Omega \\ 0 \\ \omega_A \end{pmatrix}. \quad (1.80)$$

The transformation into the rotating frame also changes the wave function of our two-state particle by a unitary transformation (this is the way a two-component spinor transforms under a rotation of the coordinate axes)

$$U(t) = \exp\{-i\omega_L t \sigma_3 / 2\} = \begin{pmatrix} e^{-i\omega_L t / 2} & 0 \\ 0 & e^{i\omega_L t / 2} \end{pmatrix} \quad (1.81)$$

⁴If we had kept the nonresonant terms in the Hamiltonian, the magnetic field would also show a time-dependent component rotating at the frequency $2\omega_L$.

We observe that this is the transformation we used in Eq.(1.66) to go into the interaction picture (on resonance where $\omega_L = \omega_A$). This unitary transformation being time-dependent, we get also a modification of the Hamiltonian proportional to $-i\hbar U^\dagger \partial_t U = -\hbar\omega_L \sigma_3$. All told, we find the Hamiltonian *in the rotating frame*

$$H = -\frac{\hbar\Delta}{2}\sigma_3 + \frac{\hbar\Omega}{2}\sigma_1 \quad (1.82)$$

where the *detuning* is given by the difference between the laser frequency and the atomic transition frequency

$$\Delta = \omega_L - \omega_A. \quad (1.83)$$

Note that the laser and atomic frequencies have disappeared from the Hamiltonian and only their difference (the detuning) occurs. As a consequence, the relevant time scales (given by $1/\Delta$ and $1/\Omega$) are typically much longer than the optical period $2\pi/\omega_L$. On these long time scales, nonresonant processes remain ‘virtual’ and cannot be directly observed. This is consistent with the neglect of nonresonant levels (two-state approximation) and of the nonresonant two-state coupling (rotating wave approximation).

1.5 Two-level dynamics

1.5.1 Rabi oscillations

The most simple case of atom-laser dynamics is a laser ‘on resonance’, i.e., $\omega_L = \omega_A$. The Schrödinger equation for the Hamiltonian (1.76) yields (we drop the tildes)

$$i\hbar\dot{c}_e = \frac{\hbar\Omega}{2}c_g \quad (1.84)$$

$$i\hbar\dot{c}_g = \frac{\hbar\Omega}{2}c_e. \quad (1.85)$$

where the Rabi frequency is chosen real for simplicity. With the initial conditions $c_g(0) = 1$, $c_e(0) = 0$, the solution is

$$\dot{c}_e = -i \sin(\Omega t/2) \quad (1.86)$$

$$c_g = \cos(\Omega t/2). \quad (1.87)$$

The excited state probability thus oscillates between 0 and 1 at a frequency $\Omega/2$. This phenomenon is called ‘Rabi flopping’. It differs from what one would guess from ordinary time-dependent perturbation theory where one typically gets linearly increasing probabilities. That framework, however, applies only if the final

state of the transition lies in a continuum which is not the case here. Rabi flopping also generalizes the perturbative result (1.70) which would give a quadratic increase $|c_e|^2 \propto t^2$ that cannot continue for long times. But instead of saturating, the atomic population returns to the ground state.

Every experimentalist is very happy when s/he observes Rabi oscillations. It means that any dissipative processes have been controlled so that they happen at a slower rate. In a realistic setting, one gets a damping of the oscillation amplitude towards equilibrium populations.

Rabi pulses. Rabi oscillations with a fixed interaction time are often used to implement coherent operations on an atom or spin. The corresponding evolution operator is given by (we focus on the resonant case)

$$U_\theta = \exp\{-i\theta\sigma_1/2\} = \cos(\theta/2) - i\sigma_1 \sin(\theta/2) \quad (1.88)$$

with $\theta = \Omega t$. After one cycle of Rabi oscillations, $\Omega t = 2\pi$ (a ‘ 2π -pulse’), the atom returns to its ground state — but its wave function has changed sign. This sign change is well-known from spin 1/2 particles: the corresponding unitary transformation reads

$$U_{2\pi} = \cos(\pi) - i\sigma_1 \sin(\pi) = -1 \quad (1.89)$$

A more interesting manipulation is a ‘ π -pulse’, $\Omega t = \pi$, that flips the ground and excited state:

$$U_\pi = \cos(\pi/2) - i\sigma_1 \sin(\pi/2) = -i\sigma_1 \quad (1.90)$$

Finally, a ‘ $\pi/2$ -pulse’ takes the atom into a superposition of ground and excited states with equal weight (a Bloch vector on the equator of the Bloch sphere)

$$U_{\pi/2} = \cos(\pi/4) - i\sigma_1 \sin(\pi/4) = \frac{1 - i\sigma_1}{\sqrt{2}}$$

$$U_{\pi/2}|g\rangle = \frac{1}{\sqrt{2}}|g\rangle - \frac{i}{\sqrt{2}}|e\rangle$$

If the laser is shut off after such a pulse, the Bloch vector will continue to rotate along the equator at the frequency Δ .

1.5.2 Dissipation and Bloch equations

We now describe how the dynamics of the atomic Bloch vector is modified when so-called dissipative processes are taken into account. These processes occur

because the two-level system is not closed: it is in contact with the electromagnetic field that carries away energy and information (entropy). In addition, it is subject to vacuum fluctuations (see Chapter ??). The challenge of including dissipation into quantum optics is that the equations of motion must be compatible some basic principles of quantum mechanics: states cannot evolve in an arbitrary way because probabilities remain positive, for example.

Spontaneous emission

As a consequence of the coupling to the quantized electromagnetic field, the excited state of the two-level atom decays by emitting a photon into an ‘empty’ mode of the electromagnetic field. This phenomenon can conveniently be described by the equations of ‘radioactive decay’ (a pair of ‘rate equations’)

$$\frac{dp_e}{dt} = -\gamma p_e, \quad \frac{dp_g}{dt} = +\gamma p_g \quad (1.91)$$

The rate γ gives the probability per unit time of emitting a photon and putting the atomic population from the excited state down to the ground state. The total population is conserved, as it should be for a process where the atom just changes its internal state. (In radioactive decay, ‘e’ would be a plutonium and ‘g’ an uranium atom, and the ‘photon’ an α -particle.) In terms of the third component of the Bloch vector (the inversion), we have the following equation

$$\left. \frac{d}{dt} \langle \sigma_3 \rangle \right|_{\text{decay}} = -\gamma (\langle \sigma_3 \rangle + 1) \quad (1.92)$$

We also need a prescription how to take into account such a process in the dynamics of off-diagonal elements of the density matrix like ρ_{eg} . These equations cannot be chosen arbitrarily because we require that the density operator ρ remains positive under time evolution. We discuss this in more detail later in the lecture. The result is that also the dipole components of the Bloch vector decay exponentially

$$\left. \frac{d}{dt} \langle \sigma \rangle \right|_{\text{decay}} = -\Gamma \langle \sigma \rangle \quad (1.93)$$

The rate must satisfy the inequality $\Gamma \geq \gamma/2$, otherwise one can find initial conditions that evolve into state outside the Bloch sphere (i.e., a density matrix with negative probabilities). The process (1.93) is sometimes called “dephasing” or “decoherence” because it happens when the relative phase of a superposition

state, $\alpha|g\rangle + \beta e^{i\theta}|e\rangle$ is “diffusing” in time (with a variance that increases linearly with t like in Brownian motion). The off-diagonal elements of the density matrix are sometimes called “coherences”, they determine to what extent one has a genuine quantum superposition, distinct from a “classical” (or thermodynamical) mixture.

To compute the spontaneous decay rate γ , we need Fermi’s Golden Rule, a standard result from time-dependent perturbation theory. We derive this after we have learned about the quantization of the electromagnetic field, but the result is

$$\gamma = \frac{|\mathbf{d}_{ge}|^2 \omega_{eg}^3}{3\pi\epsilon_0 \hbar c^3} \quad (1.94)$$

with a typical value $1/\gamma \sim 10$ ns for transitions in the visible range and dipole moments of the order of the Bohr magneton. We just note the scaling with the fine structure constant

$$\frac{\gamma}{\omega_{eg}} \sim \frac{e^2}{3\pi\epsilon_0 \hbar c} \frac{a_0^2}{\lambda_{eg}^2} \sim \alpha_{fs}^3 \quad (1.95)$$

On the scale of the Bohr frequencies in the atom, the decay is thus very slow.

Bloch equations

One finds by applying the model for spontaneous decay that the average spin vector evolves according to the following set of equations, now including dissipation,

$$\frac{d}{dt}\langle\sigma\rangle = -(\mathrm{i}\omega_A + \Gamma)\langle\sigma\rangle + \mathrm{i}(\Omega/2) e^{-\mathrm{i}\omega_L t} \langle\sigma_3\rangle \quad (1.96)$$

$$\frac{d}{dt}\langle\sigma_3\rangle = -\gamma(\langle\sigma_3\rangle + 1) + \mathrm{i}\left(\Omega^* e^{\mathrm{i}\omega_L t} \langle\sigma\rangle - \Omega e^{-\mathrm{i}\omega_L t} \langle\sigma^\dagger\rangle\right) \quad (1.97)$$

This is written within the rotating wave approximation (the Hamiltonian (1.74)) but not yet in the frame rotating at the laser frequency ω_L (choice (2) on p.22). Using the transformation (1.75), one finds $\sigma(t) = \tilde{\sigma}(t) e^{-\mathrm{i}\omega_L t}$ with

$$\frac{d}{dt}\langle\tilde{\sigma}\rangle = (\mathrm{i}\Delta - \Gamma)\langle\tilde{\sigma}\rangle + \mathrm{i}(\Omega/2) \langle\sigma_3\rangle \quad (1.98)$$

$$\frac{d}{dt}\langle\sigma_3\rangle = -\gamma(\langle\sigma_3\rangle + 1) + \mathrm{i}\left(\Omega^* \langle\tilde{\sigma}\rangle - \Omega \langle\sigma^\dagger\rangle\right) \quad (1.99)$$

Here, the frequencies enter via the detuning $\Delta = \omega_L - \omega_A$ (Paris convention, some authors use the other sign).

Rate equation limit

Assume that dephasing rate Γ is “faster” than all other time scales. “Adiabatic elimination of coherences” leads to

$$\langle \tilde{\sigma} \rangle_{\text{ad}} \approx \frac{i(\Omega/2) \langle \sigma_3 \rangle}{\Gamma - i\Delta} \quad (1.100)$$

found by solving Eq.(1.98) in the steady state. *Idea:* find stationary state after an initial transient. Time scale for transient is $1/\Gamma$, hence short by assumption. Assume that $\langle \sigma_3 \rangle$ evolves slowly on this scale (“adiabatic following” of $\langle \tilde{\sigma} \rangle$).

Insert into Eq.(1.99) for the inversion gives the *rate equation*

$$\begin{aligned} \frac{d}{dt} \langle \sigma_3 \rangle &= -\gamma(\langle \sigma_3 \rangle + 1) - 2 \text{Im} (\Omega^* \langle \tilde{\sigma} \rangle_{\text{ad}}) \\ &= -\gamma(\langle \sigma_3 \rangle + 1) - \underbrace{\frac{\Gamma |\Omega|^2}{\Gamma^2 + \Delta^2}}_{\text{absorption}} \langle \sigma_3 \rangle \end{aligned} \quad (1.101)$$

The last term is the rate by which the two-level system absorbs energy from the laser (and gets excited). Indeed, for initial conditions in the ground state $\langle \sigma_3 \rangle = -1$, one gets a positive derivative from Eq.(1.101).

Exercise. Calculate the time-averaged power absorbed by the two-level atom using the formula from mechanics, $P_{\text{abs}} = \langle \dot{\mathbf{d}}(t) \cdot \mathbf{E}(t) \rangle$ by taking the time average and the quantum expectation value in the stationary state. Compare $P_{\text{abs}}/\hbar\omega_L$ to the absorption rate in Eq.(1.101).

Rate equations are often used in condensed matter when fluorescent systems like molecules or quantum dots are embedded in a solid environment. In that case, the contact with the surrounding atoms and molecules leads to a large value for Γ . In this limit, the induced dipole moment is quite small (see Eq.(1.100)), and the relevant dynamics is well approximated by considering only probabilities (occupation numbers, the inversion).

1.5.3 Collapse and revival

If the light field is described as a single quantized mode, an additional feature occurs in the Rabi oscillations. The key point is that the coupling Hamiltonian, $g(a^\dagger \sigma + \sigma^\dagger a)$, now couples the states $|g, n\rangle$ and $|e, n-1\rangle$ where n is the photon number. These states are split (on resonance) in energy by the ‘Rabi splitting’

$g\sqrt{n}$. Recall that this splitting was $|\Omega|$ for a classical laser field, proportional to the field amplitude. This is mimicked by the scaling with \sqrt{n} since the photon number n is proportional to the field intensity.

In each sub-space spanned by $|g, n\rangle$ and $|e, n-1\rangle$, the system thus performs Rabi oscillations with a slightly different frequency. If one starts with a coherent state $|\alpha\rangle$ for the field mode, the Rabi oscillations will thus evolve at a mean frequency $\approx g|\alpha|$, but at large times, the oscillations will ‘get out of phase’. This leads to a ‘collapse’ of the Rabi oscillation amplitude, as illustrated in Figure 1.2. It happens on the time scale $1/g$ which is a factor $|\alpha|$ times longer than the period

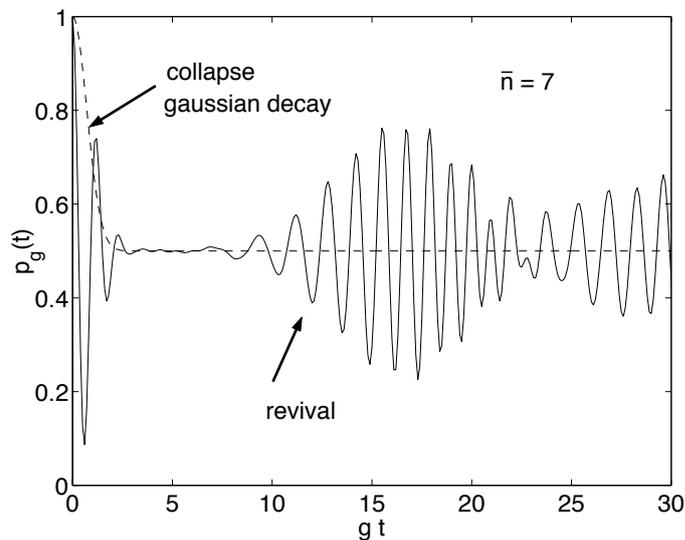


Figure 1.2: Ground state occupation $p_g(t)$ for a two-level atom coupled to a single mode, initially in the coherent state $|\alpha\rangle$ with $|\alpha|^2 = 7$. Time is in units of the ‘single-photon Rabi frequency’ g .

of the initial Rabi oscillations. At still larger times, of order $|\alpha|/g$, the amplitude of the oscillations ‘revives’ again. This is due to the fact that the Rabi frequencies form a discrete, incommensurable set (the frequencies are proportional to the irrational numbers \sqrt{n} , on resonance). A more detailed analysis is presented in Sec. ??.

1.6 A few notes on quantum dissipation

Material not covered in WS 11/12.

1.6.1 How to generate mixed states

If a quantum system is closed and can be prepared in a pure state, then the time evolution is simply Hamiltonian, $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, and we don't have to talk about quantum dissipation. This is not so in many settings, however.

There are a few examples how mixed (or non-pure) states arise.

(i) Initial mixed state. If the initial state is prepared within some probabilistic scheme, we have to work with an initial density matrix $\rho(0) \neq |\psi(0)\rangle\langle\psi(0)|$. This translates our incomplete knowledge about the initial conditions. Recall that density matrices can be “mixed” by forming so-called convex linear combinations

$$\rho = p\rho_1 + q\rho_2, \quad p + q = 1, \quad p, q \geq 0, \quad \text{tr } \rho_{1,2} = 1 \quad (1.102)$$

where the two density matrices $\rho_{1,2}$ are both normalized and p, q can be interpreted as probabilities for preparing the two.

The time evolution is still simple if the system is closed (Hamiltonian evolution):

$$\rho(t) = U(t)\rho(0)U^\dagger(t) \quad (1.103)$$

or in differential form (the von Neumann equation)

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H, \rho] \quad (1.104)$$

A typical example is an initial state prepared with a given temperature, $\rho(0) \propto \exp(-H_I/T)$. Interesting dynamics then happens only if $H_I \neq H$.

Exercise. We actually don't need to solve the von Neumann equation (1.104): by expanding $\rho(0)$ in terms of its eigenvectors, we can just evolve these eigenvectors under Schrödinger's equation and mix the final states. By linearity, the result is the same.

(ii) Reduced density matrix. The second example is that of a “system” S coupled to another one, let's call it “bath” or “environment” B . In this setting, we restrict ourselves (*by construction*) to observables that do not give any information about the state of the environment. These observables can be written in the form $\hat{A} \otimes \mathbb{1}_B$ where $\mathbb{1}_B$ is the unit operator in the environment's Hilbert space. The key observation is that the expectation values for all system observables of this type can be calculated with the help of a density operator ρ for the system,

$$\langle \hat{A} \otimes \mathbb{1}_B \rangle_{S+B} = \text{tr}(\hat{A}\rho_S) \quad (1.105)$$

Note that there are many authors who do not make the distinction between $\hat{A} \otimes \mathbb{1}_B$ and \hat{A} . The object ρ_S is called a *reduced density operator* (or matrix). It is sometimes written

$$\rho_S = \text{tr}_B \rho_{S+B} = \text{tr}_B |\psi_{S+B}\rangle\langle\psi_{S+B}| \quad (1.106)$$

where the last writing assumes that system+environment are in a pure state $|\psi_{S+B}\rangle$. This procedure is called “taking the partial trace” over the environment (symbolic: tr_B), *tracing out the environment*, or “projecting into the system Hilbert space”. More precisely, the partial trace and the reduced density operator can be written in terms of the matrix elements ($|a\rangle, |b\rangle$ are arbitrary system states)

$$\langle a|\rho_S|b\rangle = \sum_n \langle a, n|\rho_{S+B}|b, n\rangle \quad (1.107)$$

where the $\{|n\rangle\}$ form a complete basis for the environment. You will encounter sometimes the writing

$$\text{tr}_B \rho_{S+B} = \sum_n \langle n|\rho_{S+B}|n\rangle \quad (\text{symbolic}) \quad (1.108)$$

where the object on the rhs has to be understood as having still the character of an operator in the Hilbert space of the system.

The time evolution of a system coupled to an environment produces mixed states in a dynamical way:

$$\rho_S(t) = \text{tr}_B \left[U_{S+B}(t) \rho_{S+B}(0) U_{S+B}^\dagger(t) \right] \quad (1.109)$$

even if $\rho_{S+B}(0)$ starts off in a pure state. This is called the “Nakajima-Zwanziger” projection. This construction is, of course, only relevant if (i) the initial state is not factorized (it is entangled) or (ii) there is some interaction between S and B . Otherwise $U_{S+B}(t)$ factorizes, and the partial trace simply reduces to

$$\begin{aligned} & \text{tr}_B (U_S \otimes U_B) (\rho_S \otimes \rho_B) (U_S \otimes U_B)^\dagger \\ &= \text{tr}_B (U_S \rho_S U_S^\dagger) \otimes (U_B \rho_B U_B^\dagger) \\ &= U_S \rho_S U_S^\dagger \text{tr}_B (U_B \rho_B U_B^\dagger) \\ &= U_S \rho_S U_S^\dagger \end{aligned} \quad (1.110)$$

The Nakajima-Zwanziger projection (1.109) shares many physically interesting features and is at the basis of many generalizations of the Schrödinger equation to “open quantum systems”. The system+environment setting thus provides a conceptual framework to introduce dissipation into quantum mechanics. We shall use it in the later parts of the quantum optics course.

(iii) Measure and forget. This procedure of mixing states is related to the system+environment setting, but it arises from the basic postulates and can be formulated without introducing explicitly an environment. We recall the standard rule (von Neumann and Lüders) of what happens to a quantum state when an observable \hat{A} has been measured (with eigenvalue a):

$$|\psi\rangle \mapsto |a\rangle \quad (1.111)$$

The system has “collapsed” to an eigenstate $|a\rangle$ of the observable. This is still a pure state and corresponds to a “perfect” or projective measurement.

Now introduce probabilities and forgetting. The probability that we get the eigenvalue a is, of course, given by $p(a) = |\langle a|\psi\rangle|^2 = \text{tr}(|a\rangle\langle a|\rho)$ where $\rho = |\psi\rangle\langle\psi|$ for an initially pure state. Hence if we start off with a non-pure state, the von-Neumann-Lüders rule reads

$$\rho \mapsto |a\rangle\langle a| \quad (1.112)$$

In this way, we can even “purify” a mixed state! After all, the states in quantum mechanics just reflect the knowledge we have about the system.

The perfect measurement is often quite difficult to perform, however, and many states can be found that are still compatible with the measured eigenvalue a . In other words, our measurement cannot distinguish precisely among the different eigenstates $|a\rangle$. This is the typical scenario if the eigenvalues are continuously distributed.

Now let us imagine that we only know that we have performed the measurement “Is the system in state $|a\rangle$?”, but have forgotten the result. We know that with probability $p(a)$, the state has collapsed (projective measurement). But with probability $1 - p(a)$, something else has happened. Let us assume that the state remained unchanged. By forgetting the result of the measurement, we are forced to assign to the system a mixed state:

$$\rho \mapsto (1 - p(a))\rho + p(a)|a\rangle\langle a| \quad (\text{simplest approximation}) \quad (1.113)$$

This scenario is called an “imperfect” or weak measurement. If the probability $p(a)$ is small, the state change is also small. This is the scenario we shall use to motivate the dissipative evolution of a two-level system. An alternative notation for the probabilistic mixture of the two states can be given

$$\rho \mapsto \begin{cases} \rho & \text{with prob } 1 - p(a) \\ |a\rangle\langle a| & \text{with prob } p(a) \end{cases} \quad (1.114)$$

Remark. We can re-phrase this procedure within a system+environment setting. Suppose that we couple the system to an environment that can “measure” whether the system is in state $|a\rangle$. After some evolution time, we get an entangled state ($|\psi\rangle$ is the initial system density state, assumed pure and $|0\rangle$ the initial environment state)

$$|\psi, 0\rangle \mapsto \langle a|\psi\rangle|a, 1_a\rangle + U_{S+B}|\psi_\perp, 0\rangle$$

where $|1_a\rangle$ is the (“conditional”) environment state and $|\psi_\perp\rangle$ is the (non-normalized) system state orthogonal to $|a\rangle$. We construct the reduced density operator and get a mapping (between system operators)

$$|\psi\rangle\langle\psi| \mapsto \text{tr}_B(\langle a|\psi\rangle|a, 1_a\rangle + U_{S+B}|\psi_\perp, 0\rangle)(\langle a|\psi\rangle|a, 1_a\rangle + U_{S+B}|\psi_\perp, 0\rangle)^\dagger$$

Now comes the key assumption: the coupling to the environment has been sufficiently strong so that one can distinguish the environment states $|1_a\rangle, |0\rangle$, and the environment states contained in $U_{S+B}|\psi_\perp, 0\rangle$. The best we can do is that these states are orthogonal

$$\langle 1_a|0\rangle \approx 0, \quad \text{tr}_B U_{S+B}|\psi_\perp, 0\rangle\langle a, 1_a| \approx 0 \quad (1.115)$$

This removes the mixed (crossed) terms in the partial trace, and we get a mixture (with $p(a) = |\langle a|\psi\rangle|^2$ as in QM I)

$$|\psi\rangle\langle\psi| \mapsto |a\rangle\langle a|p(a) + \text{tr}_B U_{S+B}|\psi_\perp, 0\rangle\langle\psi_\perp, 0|U_{S+B}^\dagger$$

where the first term contains the projection onto the eigenstate. The simplest assumption for the second term is that the environment does not evolve at all, provided the system is in the orthogonal state $|\psi_\perp\rangle$. Then $U_{S+B}|\psi_\perp, 0\rangle \approx |\psi_\perp, 0\rangle$, and the partial trace gives

$$|\psi\rangle\langle\psi| \mapsto |a\rangle\langle a|p(a) + \mathbb{P}_\perp|\psi\rangle\langle\psi|\mathbb{P}_\perp$$

where \mathbb{P}_\perp projects into the subspace orthogonal to $|a\rangle$. The last term has a trace $1 - p(a)$, as in Eq.(1.113), but differs slightly because of the projection. We come back to this when discussing spontaneous emission.

See the introductory article “Decoherence and the transition from quantum to classical” by Zurek (1991) for more details on this discussion. The main message is that the coupling to an environment can provide the same physics as measuring a quantum system.

1.6.2 Quantum dissipation in a two-level system

Evolution over time step Δt . “Sufficiently small” in some sense to put together Hamiltonian evolution and measurement (“monitoring”) by an environment.

Pure Hamiltonian (for simplicity, time-independent, applies in rotating frame) ($\hbar = 1$)

$$\rho(t + \Delta t) \approx (\mathbb{1} - iH\Delta t)\rho(t)(\mathbb{1} + iH\Delta t) = \rho(t) - i[H\Delta t, \rho(t)] + \mathcal{O}(\Delta t^2) \quad (1.116)$$

Now observing and forgetting about the results. We consider two scenarios.

Dephasing: measuring energy states. We assume that with a probability Δp , we have been able to determine in which energy eigenstate the two-level system is. This can be achieved, for example, by performing measurements on the environment. The rule for “measure and forget” then gives (we have three outcomes)

$$\rho(t + \Delta t) = \begin{cases} \rho(t) & \text{with prob } 1 - \Delta p \\ |g\rangle\langle g| & \text{with prob } \Delta p \rho_{gg}(t) \\ |e\rangle\langle e| & \text{with prob } \Delta p \rho_{ee}(t) \end{cases} \quad (1.117)$$

This gives the mixed state, as a simple calculation shows

$$\begin{aligned}\rho(t + \Delta t) &= (1 - \Delta p)\rho(t) + \Delta p \sum_{a=g,e} \langle a|\rho(t)|a\rangle |a\rangle\langle a| \\ &= (1 - \frac{1}{2}\Delta p)\rho(t) + \frac{1}{2}\Delta p \sigma_3 \rho(t) \sigma_3\end{aligned}\quad (1.118)$$

Concatenate the two elementary processes (1.116, 1.118) and construct an approximate time derivative

$$\frac{\Delta\rho}{\Delta t} \approx -i[H, \rho(t)] + \frac{\Delta p}{2\Delta t} \{\sigma_3 \rho(t) \sigma_3 - \rho(t)\} \quad (1.119)$$

This is the dynamical equation for a system subject to dephasing. The equation is in the so-called Lindblad form (see Eq.(1.127)), a general form for the time evolution of an open system that we shall derive later in the lecture. The rate $\Delta p/2\Delta t$ is called the “dephasing rate”.

Exercise. Switch to the Heisenberg picture and calculate from Eq.(1.119) the rate of change $\langle \Delta\sigma/\Delta t \rangle$ of the Bloch vector. Show that the non-Hamiltonian terms give

$$\left. \frac{\langle \Delta\sigma \rangle}{\Delta t} \right|_{\text{non-H}} \approx -\frac{\Delta p}{2\Delta t} \langle \sigma \rangle \quad (1.120)$$

while $\langle \Delta\sigma_3/\Delta t \rangle = 0$. The monitoring of the energy levels thus does not change the inversion which is not surprising, since we made the assumption that the measured eigenstate is not changed. The dipole, that captures the relative phase of superposition states in the energy basis, however, decays with a rate $\Delta p/2\Delta t$. We can thus interpret the dipole relaxation rate as the rate at which the environment acquires information about the system’s energy. Note also that the decay of the dipole is the price to pay for the measurement in the energy basis – the quantum-mechanical rule that “any measurement perturbs the system” still holds.

Spontaneous emission: quantum jumps. The second scenario is based on the observation of the photons that a two-level atom can emit. We assume that over the evolution time Δt , the probability to detect an emitted photon is $\Delta p \rho_{ee}(t)$. We have clearly $\Delta p = \gamma\Delta t$ according to the law of radioactive decay. In addition, once this photon has been detected, we know that the atom must be in the ground state $|g\rangle$. This feature is different from the previous scenario where the measurement perturbed the system in a weaker way.

Now imagine that we throw away the information that a photon has been emitted. The state then mixes into

$$\rho(t + \Delta t) = \begin{cases} \rho' & \text{with prob } 1 - \Delta p \\ |g\rangle\langle g| & \text{with prob } \Delta p \rho_{ee}(t) \end{cases} \quad (1.121)$$

where the state ρ' is normalized and corresponds to the event “no photon detected”. This can be translated into

$$\rho(t + \Delta t) = \rho'' + \Delta p \rho_{ee}(t) |g\rangle\langle g| = \rho'' + \Delta p \sigma \rho(t) \sigma^\dagger \quad (1.122)$$

where ρ'' is a non-normalized state with trace $1 - \Delta p \rho_{ee}(t)$. The second term appearing here is called a “quantum jump”: the photon emission happens when the atom jumps from the excited to the ground state $|e\rangle \rightarrow |g\rangle$. The ladder (or annihilation) operator σ plays here a very intuitive role. If $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ is a pure state, the system jumps to the state $\sigma|\psi(t)\rangle$ at the photon emission.

The first term ρ'' in Eq.(1.122) now takes care of the conservation of probabilities. In our first guess (1.113) we simply took $\rho'' = (1 - \Delta p \rho_{ee})\rho$. This recipe must be refined here, for two reasons.

One reason is more formal: we want that $\rho(t + \Delta t)$ to be expressed as a linear map of the state $\rho(t)$, but $\Delta p \rho_{ee} \rho$ is quadratic in ρ . This reason is deeply rooted in the linearity of quantum mechanics. The Nakajima-Zwanziger scheme (1.109) which provides a very general framework for quantum dissipation, is also a linear map between density matrices.

The second reason is that the event “no photon has been detected” actually *changes our knowledge* about the system. Qualitatively speaking, it increases our confidence that the system might be in the ground state. We are having less the tendency to think it is in the excited state. After all, if the system is in the excited state, we would expect at some point a photon to appear! In the opposite limit, if over a very long time we do not detect any photons, the system must be (with a very high probability) in the ground state, and we have gained this knowledge from the sequence of “no-photon” events.

We are thus led to the following refined approximation

$$\begin{aligned} \rho'' &\approx \left(\mathbb{1} - \frac{1}{2} \Delta p |e\rangle\langle e| \right) \rho(t) \left(\mathbb{1} - \frac{1}{2} \Delta p |e\rangle\langle e| \right) \\ &\approx \rho(t) - \frac{1}{2} \Delta p \left\{ \sigma^\dagger \sigma \rho(t) + \rho(t) \sigma^\dagger \sigma \right\} \end{aligned} \quad (1.123)$$

Putting Eqs.(1.122, 1.123), together, we find the so-called “master equation” for a two-level system with spontaneous decay

$$\frac{\Delta \rho}{\Delta t} \approx -i [H, \rho(t)] + \frac{\Delta p}{\Delta t} \left\{ \sigma \rho(t) \sigma^\dagger - \frac{1}{2} \sigma^\dagger \sigma \rho(t) - \frac{1}{2} \rho(t) \sigma^\dagger \sigma \right\} \quad (1.124)$$

More details on this derivation can be found in the paper by Dalibard & al. (1992) on a “Wave-Function Approach to Dissipative Processes in Quantum Optics”.

Exercise. By working out matrix elements of this equation, identify $\gamma = \Delta p / \Delta t$ with the spontaneous decay rate. The important message of this equation is that spontaneous

emission changes *both* the inversion and the dipole:

$$\left. \frac{\langle \Delta \sigma \rangle}{\Delta t} \right|_{\text{non-H}} \approx -\frac{1}{2} \gamma \langle \sigma \rangle \quad (1.125)$$

$$\left. \frac{\langle \Delta \sigma_3 \rangle}{\Delta t} \right|_{\text{non-H}} \approx -\gamma (\langle \sigma_3 \rangle + 1) \quad (1.126)$$

1.6.3 Lindblad master equation

Without going into the details of the derivation, we just state here that the generalized von-Neumann equations (1.119, 1.124) are special cases of a general theorem about the time evolution of a quantum system, the

Lindblad theorem. If a time evolution $T_t : \rho(0) \mapsto \rho(t)$ satisfies the following conditions:

- the map T_t is linear and maps density matrices onto density matrices;
- the map T_t is completely positive⁵;
- expectation values evolve continuous in time;
- repeating the map corresponds to adding time lapses, $T_t T_{t'} = T_{t+t'}$,

then there exists a hermitean operator H and a countable set of system operators L_k ($k = 1 \dots K$) such that the state $\rho(t) = T_t \rho(0)$ solves the differential equation

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_{k=1}^K \left\{ L_k \rho L_k^\dagger - \frac{1}{2} L_k^\dagger L_k \rho - \frac{1}{2} \rho L_k^\dagger L_k \right\} \quad (1.127)$$

The operators L_k are called Lindblad or jump operators.

For spontaneous emission and dephasing, only a single Lindblad operator appears, as shown in this Table:

	spont. decay	dephasing
Lindblad operator	$\sqrt{\gamma} \sigma$	$\sqrt{\kappa/2} \sigma_3$

where κ is the dephasing rate. Keeping both Lindblad operators in the time evolution, gives the Bloch equations (1.98, 1.99) with a dephasing rate $\Gamma = \kappa + \gamma/2$. The Lindblad theorem is proven later on in the quantum optics lecture. A simple proof can be found in Nielsen & Chuang (2000) and Henkel (2007).

⁵Qualitatively speaking: density matrices are mapped onto density matrices even if the system is augmented by some environment and the map T_t augmented by “nothing happens with the environment”.

Chapter 2

The quantized field

We give here an elementary introduction to the quantization of the electromagnetic field. We adopt the Coulomb gauge and a canonical framework. We then discuss examples for the quantum states of the field and the properties of vacuum fluctuations.

A few general remarks. The procedure followed here is also called “second quantization”. This refers, taken literally, to the quantum mechanics of a many-body system where “first quantization” corresponds to introducing operators \hat{x} , \hat{p} for a single particle (or equivalently: introducing a wave function $\psi(\mathbf{x})$). The second-quantized theory then promotes the wave function to an operator $\hat{\psi}(\mathbf{x})$. We see this procedure at work in electrodynamics where the starting point is a “classical field theory”. The result is the same: the fields $\mathbf{E}(\mathbf{x}, t)$, $\mathbf{B}(\mathbf{x}, t)$ will be replaced by operators (denoted with carets = “hats”).

In the modern language of quantum field theory, any physical object is described by a suitable field operator. Photons appear in the quantized Maxwell fields. For electrons, the Schrödinger equation is quantized (either in its relativistic form, the Dirac equation, to describe high-energy electrons, or in the non-relativistic form, to describe a many-electron system like in a solid).

There is an analogue of “first quantization” (or its “reverse” = going to the classical limit) in electrodynamics: the passage to geometrical optics.

Statements from Cohen-Tannoudji, Dupont-Roc and Grynberg. The electromagnetic field is not the wave function for the photon because the equation of motion contains a source term = photons can be created and annihilated.

You can postulate that the electromagnetic energy is the Hamiltonian of the quantum theory, with the conventional commutation relations. The Heisenberg

equations of motion then give the Maxwell–Lorentz equations. *But* this short-circuits the identification of canonically conjugate coordinates in the classical Maxwell theory (incl the freedom of gauge).

The positive-frequency part of the electromagnetic field operator is well-defined only for the free field. Sources potentially mix positive and negative frequencies.

2.1 Canonical quantization

2.1.1 Fields

Maxwell equations. We want to quantize the vacuum Maxwell equations for the electromagnetic field. With a given charge and current density, these read

$$\begin{aligned} \nabla \cdot \mathbf{B} &= 0 & \varepsilon_0 \nabla \cdot \mathbf{E} &= \rho \\ \nabla \times \mathbf{E} + \partial_t \mathbf{B} &= 0 & \nabla \times \mathbf{B} - \mu_0 \varepsilon_0 \partial_t \mathbf{E} &= \mu_0 \mathbf{j} \end{aligned} \quad (2.1)$$

Introducing the scalar and vector potentials via

$$\mathbf{B} = \nabla \times \mathbf{A} \quad (2.2)$$

$$\mathbf{E} = -\nabla\phi - \partial_t \mathbf{A}, \quad (2.3)$$

the left column of (2.1) is identically fulfilled. The Coulomb law then becomes

$$-\varepsilon_0 \nabla^2 \phi - \varepsilon_0 \nabla \partial_t \mathbf{A} = \rho \quad (2.4)$$

If we impose the Coulomb gauge, $\nabla \cdot \mathbf{A} = 0$, the vector potential drops out and the scalar potential is determined by the charge density alone:

$$-\varepsilon_0 \nabla^2 \phi = \rho \quad (2.5)$$

In this gauge, the scalar potential is thus not a dynamical degree of freedom of the field: its dynamics is ‘enslaved’ by that of the charges. This holds with suitable boundary conditions such that the homogeneous equation $\nabla^2 \phi = 0$ has no nontrivial solutions. In free space, with $\phi(\mathbf{x} \rightarrow \infty) \rightarrow 0$, we get

$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int d^3x' \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \quad (2.6)$$

which is a superposition of well-known Coulomb potentials.

Wave equation. We are left with the wave equation for the vector potential

$$\nabla \times (\nabla \times \mathbf{A}) + \frac{1}{c^2} \partial_t^2 \mathbf{A} = \mu_0 (\mathbf{j} - \varepsilon_0 \partial_t \nabla \phi) \equiv \mu_0 \mathbf{j}_\perp. \quad (2.7)$$

On the right hand side, we have introduced the ‘transverse current’. Its divergence is zero because of Eq.(2.5) and charge conservation:

$$\nabla \cdot \mathbf{j}_\perp = \nabla \cdot \mathbf{j} + \partial_t \rho = 0. \quad (2.8)$$

The name ‘transverse’ comes from the fact that in spatial Fourier components, the current $\mathbf{j}_\perp(\mathbf{k})$ must be perpendicular to \mathbf{k} . One also says that the vector potential in the Coulomb gauge is transverse because $\nabla \cdot \mathbf{A} = 0$. The transversality of the source term in (2.7) ensures that if \mathbf{A} is transverse at one time, it is also transverse at all later times.

Conservation laws. Charge: $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$.

Energy (Poynting theorem):

$$\partial_t u + \nabla \cdot \mathbf{S} = -\mathbf{j} \cdot \mathbf{E} \quad (2.9)$$

$$u = \frac{\varepsilon_0}{2} \mathbf{E}^2 + \frac{1}{2\mu_0} \mathbf{B}^2 \quad \text{energy density} \quad (2.10)$$

$$\mathbf{S} = \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B} \quad \text{Poynting vector} \quad (2.11)$$

Momentum and angular momentum.

2.1.2 Plane wave expansion

The canonical quantization scheme starts from the classical theory in its Hamilton formulation. We first identify the field and its canonically conjugate momentum. For a classical single particle, position \mathbf{x} and $\mathbf{p} = \partial L / \partial \dot{\mathbf{x}}$ from the Lagrangian do the job. The Lagrangian of electrodynamics is discussed in the exercises and contains the vector potential \mathbf{A} as coordinate and gives as canonical momentum the electric field (\mathcal{L} is the Lagrangian density)

$$\mathbf{\Pi} = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{A}}} = -\varepsilon_0 \mathbf{E} \quad (2.12)$$

We next have to check (see exercises) that the following expression generates the Maxwell equations by the canonical equations

$$H = \int dV \left(\frac{1}{2\varepsilon_0} \mathbf{\Pi}^2 + \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 \right) \quad (2.13)$$

This is not surprising since we are dealing with the volume integral over the electromagnetic energy density. Note that we quantize only the free field here (no charges or currents).

In classical Hamiltonian electrodynamics, the fact that \mathbf{A} and $\mathbf{\Pi}$ are canonically conjugate is expressed by the following Poisson bracket

$$\{A_i(\mathbf{x}), \Pi_j(\mathbf{x}')\} = -\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') \quad (2.14)$$

where $\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}')$ is the so-called transverse δ -function. It acts like the unit operator on the space of transverse vector fields \mathbf{F} :

$$F_i(\mathbf{x}) = \sum_j \int d^3x' \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') F_j(\mathbf{x}') \quad (2.15)$$

while vector fields that are not transverse are projected into the subspace of transverse fields. The Poisson bracket in Eq.(2.14) is an integral over (functional derivatives) with respect to the vector potential and the conjugate momentum field. More details follow in Section 2.4.

Diagonalize the field energy. In the field Hamiltonian (2.13), the field value $\mathbf{A}(\mathbf{x})$ is coupled to its neighboring values by the derivative. The Hamiltonian is therefore not in “diagonal form”. But it can be brought into one by expanding the field in suitable mode functions, with plane waves being a natural choice. We note that this expansion has nothing to do with quantum field theory: it is done already at the classical level (when “eigenmodes” of a laser cavity are calculated, for example). The names “quantization volume” and “quantized wave vector” are therefore ill chosen. Don’t confuse this with the next step where really quantization happens (see Section ??).

The complex character of plane waves, combined with the polarization of the field, leads to some technical difficulties as we see in a moment. We take plane waves in a box of volume V with periodic boundary conditions, and expand (the same expansion applies to the momentum field $\mathbf{\Pi}$)

$$\mathbf{A}(\mathbf{x}) = \sum_{\mathbf{k}} \mathbf{A}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \quad (2.16)$$

where the wave vectors \mathbf{k} are discrete and have a spacing of the order $V^{-1/3}$. Some simple manipulations then bring the Hamiltonian in the form

$$H = V \sum_{\mathbf{k}} \left(\frac{1}{2\varepsilon_0} \mathbf{\Pi}_{\mathbf{k}} \cdot \mathbf{\Pi}_{-\mathbf{k}} + \frac{\varepsilon_0 c^2 k^2}{2} \mathbf{A}_{\mathbf{k}} \cdot \mathbf{A}_{-\mathbf{k}} \right). \quad (2.17)$$

We have used that for the Fourier amplitudes of transverse fields, $\mathbf{k} \cdot \mathbf{A}_{\mathbf{k}} = 0$ and the expression for the speed of light. We recognize here the dispersion relation in free space $\omega_{\mathbf{k}}^2 = k^2/\varepsilon_0\mu_0 = c^2k^2$.

This already decomposes into a sum over the wave vectors \mathbf{k} . Only waves with \mathbf{k} and $-\mathbf{k}$ are coupled. The complex number $A_{\mathbf{k}\mu}$ therefore encodes two degrees of freedom that are related to the plane waves with wave vectors \mathbf{k} and $-\mathbf{k}$.

The main task of quantization is to replace the fields by operators such that the Poisson bracket becomes the commutator. Referring to Eq.(2.14), we introduce the plane wave expansion of the transverse δ -function:

$$\delta_{ij}^{\perp}(\mathbf{x} - \mathbf{x}') = \sum_{\mathbf{k}\mu} \frac{e_{\mathbf{k}\mu i} e_{\mathbf{k}\mu j}^*}{V} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \quad (2.18)$$

where the polarization vectors $\mathbf{e}_{\mathbf{k}\mu}$ are normalized (there are two basis vectors with $\mathbf{k} \perp \mathbf{e}_{\mathbf{k}\mu}$). We have taken complex polarization vectors here, this is useful for circular polarization and to discuss the spin of the electromagnetic field.

2.1.3 Field operators

Now, quantization. The Poisson bracket $\{\cdot, \cdot\}$ is replaced by a commutator $(i/\hbar)[\cdot, \cdot]$. For the field and its conjugate momentum, we therefore get

$$i \left[\hat{A}_i(\mathbf{x}), \hat{\Pi}_j(\mathbf{x}') \right] = -\hbar \delta_{ij}^{\perp}(\mathbf{x} - \mathbf{x}') \quad (2.19)$$

You know from quantum mechanics I that this commutator provides uncertainty relations. Recalling that $\mathbf{\Pi}$ is the electric field, we therefore find that it cannot be measured simultaneously with the vector potential at the same position. The situation is actually worse because the transverse δ -function is not local in space (see the exercises).

When we insert the mode expansions for \mathbf{A} and $\mathbf{\Pi}$ in the commutator (2.19), we get a (double) sum over \mathbf{k}, μ . Comparing each term in the sum to the plane-wave expansion of the transverse δ -function [Eq.(2.18)], we get

$$i \left[\hat{A}_{\mathbf{k}i}, \hat{\Pi}_{\mathbf{k}'j} \right] = -\frac{\hbar}{V} \delta_{\mathbf{k}+\mathbf{k}',0} \sum_{\mu} e_{\mathbf{k}\mu i} e_{\mathbf{k}\mu j}^* \quad (2.20)$$

We implement this commutator by introducing annihilation and creation operators $a_{\mathbf{k}\mu}, a_{\mathbf{k}\mu}^{\dagger}$, see Eqs.(2.28, 2.29) below. Before we look at this expression, let us step back and simplify the problem.

Reminder: harmonic oscillator. Let us consider canonical coordinates x and p with the Hamiltonian (a simplified version of (2.17))

$$\hat{H} = \frac{V}{2\varepsilon_0} \hat{p}^2 + \frac{V\varepsilon_0\omega_k^2}{2} \hat{x}^2 \quad (2.21)$$

We also simplify the commutation relation (2.19) into

$$i[\hat{x}, \hat{p}] = -\frac{\hbar}{V} \quad (2.22)$$

To implement this, we try the definitions

$$\hat{x} = \sqrt{\frac{\hbar}{2V}} \lambda (a + a^\dagger) \quad (2.23)$$

$$\hat{p} = \sqrt{\frac{\hbar}{2V}} \frac{1}{i\lambda} (a - a^\dagger) \quad (2.24)$$

This choice is motivated by the fact that both \hat{x} and \hat{p} are hermitean operators. Note that the scale factor λ is not specified by the commutation relation. That one is implemented if we take

$$-\frac{\hbar}{V} \stackrel{!}{=} i[\hat{x}, \hat{p}] = \frac{\hbar}{2V} [\hat{a} + \hat{a}^\dagger, \hat{a} - \hat{a}^\dagger] = -\frac{\hbar}{V} [\hat{a}, \hat{a}^\dagger] \implies [\hat{a}, \hat{a}^\dagger] = 1 \quad (2.25)$$

The operators \hat{a} and \hat{a}^\dagger are known as ladder operators from the quantum mechanics I lecture. They are clearly dimensionless, the factor λ can hence be used to give \hat{x} and \hat{p} the correct physical dimension. More fundamentally, it provides a way to simplify (in fact: minimize) the Hamiltonian (2.21). Inserting Eqs.(2.23, 2.24), we get

$$\hat{H} = \frac{\hbar}{4} \left(-\frac{1}{\varepsilon_0\lambda^2} (\hat{a} - \hat{a}^\dagger)^2 + \varepsilon_0\omega_k^2\lambda^2 (\hat{a} + \hat{a}^\dagger)^2 \right) \quad (2.26)$$

The terms with a^2 and $a^{\dagger 2}$ drop out from this difference if we choose $\varepsilon_0\lambda^2 = 1/\omega_k$. This gives (here, the anticommutator is denoted by $\{\cdot, \cdot\}_+$)

$$\hat{H} = \frac{\hbar\omega_k}{2} \{\hat{a}, \hat{a}^\dagger\}_+ = \frac{\hbar\omega_k}{2} (2\hat{a}^\dagger\hat{a} + 1) \quad (2.27)$$

We are going to see that the full electromagnetic Hamiltonian has a similar structure, with just a sum over wave vectors and polarizations to be added.

Interpretation: photons and particles. The physical interpretation of this Hamiltonian in ordinary quantum mechanics is well known: the operator $\hat{a}^\dagger \hat{a}$ has integer eigenvalues $n = 0, 1, 2, \dots$. One has a ground state $|0\rangle$ with energy $\frac{1}{2}\hbar\omega_k$ and excited states with an equidistant spacing $\hbar\omega_k$ in energy.

This interpretation is essentially changed in the quantum field theory: the energy levels are interpreted as the presence of particles (“photons”) in a given mode of the field, each particle carrying an energy $\hbar\omega_k$. The classical mode frequency is thus translated into an energy: note how the scale factor \hbar postulated by de Broglie arises from the commutator between the quantum operators. The equidistant energy levels are a consequence of our assumption that the particles (photons) are not interacting with each other. The ladder operators of QM I can now be interpreted literally as “creation” and “annihilation” operators and implement mathematically the non-conservation of particles. Example: the decay process of particle “b” into a pair of particles “a” ($b \rightarrow a+a$) is implemented by an operator product $a^\dagger b$ in the Hamiltonian. This kind of products of more than two operators are called interaction Hamiltonians: they will be treated systematically in perturbation theory (and graphically represented by Feynman diagrams).

Creation and annihilation operators

For the full quantum field, we modify the rules (2.23, 2.24) for the canonical operators to include the polarization label

$$\hat{\mathbf{A}}_{\mathbf{k}} = \sqrt{\frac{\hbar}{2\varepsilon_0\omega_k V}} \sum_{\mu} \left(\hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} + \hat{a}_{-\mathbf{k}\mu}^\dagger \mathbf{e}_{-\mathbf{k}\mu}^* \right) \quad (2.28)$$

$$\hat{\mathbf{\Pi}}_{\mathbf{k}} = \sqrt{\frac{\hbar\varepsilon_0\omega_k}{2V}} (-i) \sum_{\mu} \left(\hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} - \hat{a}_{-\mathbf{k}\mu}^\dagger \mathbf{e}_{-\mathbf{k}\mu}^* \right) \quad (2.29)$$

These expressions are constructed to satisfy the “hermiticity condition” $(\hat{\mathbf{A}}_{\mathbf{k}})^\dagger = \hat{\mathbf{A}}_{-\mathbf{k}}$ that replaces conventional hermiticity in the simpler example before. The annihilation and creation operators are postulated to satisfy the following commutation relations (the generalization of (2.25)):

$$\left[\hat{a}_{\mathbf{k}\mu}, \hat{a}_{\mathbf{k}'\mu'} \right] = 0, \quad \left[\hat{a}_{\mathbf{k}\mu}, \hat{a}_{\mathbf{k}'\mu'}^\dagger \right] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\mu\mu'} \quad (2.30)$$

The commutator $[\hat{A}_{\mathbf{k}i}, \hat{\Pi}_{\mathbf{k}'j}]$ now gets contributions only from the ‘mixed term’ $[\hat{a}_{\mathbf{k}\mu}, \hat{a}_{-\mathbf{k}\mu}^\dagger]$ that appears twice. Putting the prefactors together, we find

$$i \left[\hat{A}_{\mathbf{k}i}, \hat{\Pi}_{\mathbf{k}'j} \right] = -\frac{\hbar}{2V} \delta_{\mathbf{k},-\mathbf{k}'} \sum_{\mu} \left\{ e_{\mathbf{k}\mu i} e_{\mathbf{k}\mu j}^* + e_{-\mathbf{k}\mu i}^* e_{-\mathbf{k}\mu j} \right\} \quad (2.31)$$

The polarization vectors can be constructed in such a way that $\mathbf{e}_{-\mathbf{k}\mu}^* = \mathbf{e}_{\mathbf{k}\mu}$ (this works with real vectors or with circular polarization vectors, see the exercises). Then the two terms in curly brackets combine, and we get exactly what we asked for in Eq.(2.20).

2.1.4 The observables of quantum electrodynamics

Field Hamiltonian

We have now all elements together that we need for field quantization. In the following, the results are illustrated by working out the basic observables of the theory: the field Hamiltonian and the field operators, written as mode expansions.

To get the Hamiltonian, we have to add one physical consideration, however. In which order do we take the operator products that replace the classical products $\mathbf{A}^2(\mathbf{x})$ or $\mathbf{A}_{\mathbf{k}} \cdot \mathbf{A}_{-\mathbf{k}}$? After all, the Fourier operators need not commute. (And indeed, they don't, as Eq.(2.28) shows.) The operator ordering has fundamental consequences for the vacuum energy, as we shall see. There are two conventional choices

— *symmetric order* $|\mathbf{A}_{\mathbf{k}}|^2 \mapsto \frac{1}{2} \sum_i \{ \hat{A}_{\mathbf{k}i}, \hat{A}_{-\mathbf{k}i} \}_+$

This has the advantage that the Hamilton operator is hermitean by construction.

— *normal order* $|\mathbf{A}_{\mathbf{k}}|^2 \mapsto \sum_i : \hat{A}_{\mathbf{k}i} \hat{A}_{-\mathbf{k}i} :$

Here, the notation $: \cdots :$ denotes a re-arrangement of annihilation and creation operators in such a way that the annihilation operators act first:

$$: a_{\mathbf{k}\mu} a_{\mathbf{k}'\mu'}^\dagger : = a_{\mathbf{k}'\mu'}^\dagger a_{\mathbf{k}\mu}. \quad (2.32)$$

This has the advantage that in the ground state of the quantum field (all modes have zero excitations), $\langle 0 | : \hat{H} : | 0 \rangle = 0$. The ground state therefore has zero energy, and we get rid of potentially divergent zero-point fluctuations. Note that for the normal ordering scheme, we have to know already what is the ground state.

Let us start with the symmetrically ordered Hamiltonian. Inserting the field operators into the mode expansion (2.17), one gets

$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar\omega_{\mathbf{k}}}{8} (-) \sum_{\mu\mu'} \left\{ \hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} - \hat{a}_{-\mathbf{k}\mu}^\dagger \mathbf{e}_{-\mathbf{k}\mu}^*, \hat{a}_{-\mathbf{k}\mu'} \mathbf{e}_{-\mathbf{k}\mu'} - \hat{a}_{\mathbf{k}\mu'}^\dagger \mathbf{e}_{\mathbf{k}\mu'}^* \right\}_+$$

$$+ \sum_{\mathbf{k}} \frac{\hbar\omega_{\mathbf{k}}}{8} \sum_{\mu\mu'} \left\{ \hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} + \hat{a}_{-\mathbf{k}\mu}^\dagger \mathbf{e}_{-\mathbf{k}\mu}^*, \hat{a}_{-\mathbf{k}\mu'} \mathbf{e}_{-\mathbf{k}\mu'} + \hat{a}_{\mathbf{k}\mu'}^\dagger \mathbf{e}_{\mathbf{k}\mu'}^* \right\}_+ \quad (2.33)$$

As in our simple example before, the products of “like” operators $\hat{a}_{\mathbf{k}\mu} \hat{a}_{-\mathbf{k}\mu'}$ drop out of this difference. For the “mixed” products, we observe the orthogonality of the polarization vectors,

$$\mathbf{e}_{\mathbf{k}\mu} \cdot \mathbf{e}_{\mathbf{k}\mu'}^* = \mathbf{e}_{-\mathbf{k}\mu}^* \cdot \mathbf{e}_{-\mathbf{k}\mu'} = \delta_{\mu\mu'} \quad (2.34)$$

which brings us to a single sum over polarizations:

$$\hat{H} = \sum_{\mathbf{k}\mu} \frac{\hbar\omega_{\mathbf{k}}}{4} \left(\left\{ \hat{a}_{\mathbf{k}\mu}, \hat{a}_{\mathbf{k}\mu}^\dagger \right\}_+ + \left\{ \hat{a}_{-\mathbf{k}\mu}^\dagger, \hat{a}_{-\mathbf{k}\mu} \right\}_+ \right) \quad (2.35)$$

The second term gives, after the summation, the same result as the first term because the mode frequency $\omega_{\mathbf{k}}$ does not depend on the sign of \mathbf{k} . Hence, we get a sum over modes as a simple generalization of Eq.(2.27):

$$\hat{H} = \sum_{\mathbf{k}\mu} \frac{\hbar\omega_{\mathbf{k}}}{2} (2\hat{a}_{\mathbf{k}\mu}^\dagger \hat{a}_{\mathbf{k}\mu} + 1) \quad (2.36)$$

We discuss the structure of the Hilbert space (the eigenstates of \hat{H}) in Sec.2.3.2. But the ground state is a transparent concept already at this stage. It is denoted $|0\rangle$ or $|\text{vac}\rangle$ and is defined by the state annihilated by *all* annihilation operators,

$$\hat{a}_{\mathbf{k}\mu} |\text{vac}\rangle = 0, \quad \text{for all } \mathbf{k}, \mu \quad (2.37)$$

This state is called the “vacuum” because obviously, all excitation numbers are zero: there are no particles. Obviously, the vacuum state is an eigenstate of the field Hamiltonian (2.36) with an energy

$$\hat{H} |\text{vac}\rangle = E_{\text{vac}} |\text{vac}\rangle, \quad E_{\text{vac}} = \sum_{\mathbf{k}\mu} \frac{\hbar\omega_{\mathbf{k}}}{2} \quad (2.38)$$

This (divergent) vacuum energy is discussed in the exercises. We touch here one of the big open problems in fundamental physics: there are several reasonable cutoffs that can be taken to make this sum convergent, none of them gives physically reasonable results. Observable consequences of the vacuum energy (despite it being divergent, one can extract finite and measurable quantities) are discussed in Secs.2.3.3, ??.

Exercise. Show that the Heisenberg equation of motion for the mode operators $a_{\mathbf{k}\mu}$ has the solution

$$a_{\mathbf{k}\mu}(t) = a_{\mathbf{k}\mu} e^{-i\omega_k t} \quad (2.39)$$

Since this looks like the solution to the time-dependent Schrödinger equation, this is called a “positive frequency” operator. The creation operator $a_{\mathbf{k}\mu}^\dagger(t)$ is a “negative frequency” operator.

Mode expansion of field operators

We now come back to the operator for the vector potential. We combine the Fourier operators Eq.(2.28) with the mode expansion to get

$$\hat{\mathbf{A}}(\mathbf{x}, t) = \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar}{2\varepsilon_0\omega_k V}} \left(\hat{a}_{\mathbf{k}\mu}(t) \mathbf{e}_{\mathbf{k}\mu} + \hat{a}_{-\mathbf{k}\mu}^\dagger(t) \mathbf{e}_{-\mathbf{k}\mu}^* \right) e^{i\mathbf{k}\cdot\mathbf{x}} \quad (2.40)$$

In the second term, we can use $-\mathbf{k}$ as wave vector index. It is then easy to see that this produces the hermitean conjugate of the first term, bringing the field operator into a manifestly hermitean form:

$$\hat{\mathbf{A}}(\mathbf{x}, t) = \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar}{2\varepsilon_0\omega_k V}} \left(\hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_k t} + \text{h.c.} \right) \quad (2.41)$$

This is called the mode expansion of the quantized electromagnetic field. The rotation of the vector potential gives us the mode expansion of the magnetic field operator. It involves the polarization vectors $\mathbf{k} \times \mathbf{e}_{\mathbf{k}\mu} = (\omega_k/c) \mathbf{b}_{\mathbf{k}\mu}$ where for circular polarizations $\mathbf{b}_{\mathbf{k}\mu}$ is actually proportional to $\mathbf{e}_{\mathbf{k}\mu}$. With linear polarizations, one gets a vector orthogonal to the electric field, of course.

The electric field operator is found from the conjugate momentum field $\hat{\mathbf{E}} = -\hat{\mathbf{\Pi}}/\varepsilon_0$ and its mode expansion is

$$\hat{\mathbf{E}}(\mathbf{x}, t) = \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}} i \left(\hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_k t} - \text{h.c.} \right) \quad (2.42)$$

$$\hat{\mathbf{B}}(\mathbf{x}, t) = \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar\omega_k \mu_0}{2V}} i \left(\hat{a}_{\mathbf{k}\mu} \mathbf{b}_{\mathbf{k}\mu} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_k t} - \text{h.c.} \right) \quad (2.43)$$

It is a useful check that the relation $\mathbf{E} = -\partial_t \mathbf{A}$ also holds for the quantum fields.

These mode expansions are the basic “work horse” for quantum optics. To memorize the formulas, a simple shortcut: the quantum theory works with the same “mode functions” (here: plane waves) as in classical electrodynamics. The electric field energy density for each mode, $\frac{1}{2}\epsilon_0|\mathbf{E}|^2$, is equal to $\frac{1}{2}\hbar\omega_k/V$ (sum the squares of the two terms in the brackets), times the photon number $\hat{a}_{\mathbf{k}\mu}^\dagger\hat{a}_{\mathbf{k}\mu}$. The magnetic energy density gives the same contribution so that one photon carries an energy density $\hbar\omega_k/V$. (This is for a plane wave mode delocalized over the volume V , of course.)

Field commutators, second turn

It is an instructive exercise to work out that the mode expansions (2.41, 2.42, 2.43) yield the following commutation relations between the field operators (all of them follow from the basic commutator (2.19)):

$$i \left[\hat{A}_i(\mathbf{x}), \hat{E}_j(\mathbf{x}') \right] = \frac{\hbar}{\epsilon_0} \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') \quad (2.44)$$

$$i \left[\hat{B}_i(\mathbf{x}), \hat{E}_j(\mathbf{x}') \right] = -\frac{\hbar}{\epsilon_0} \epsilon_{ijk} \partial_k \delta(\mathbf{x} - \mathbf{x}') \quad (2.45)$$

where the in the second equation, we have made use of the fact that under the rotation $\nabla \times$, there is no difference between the normal and the transverse δ -function.

Interaction with matter

If we keep the interaction with matter in the description, there is one additional term in the Hamiltonian (density), $-\mathbf{j} \cdot \mathbf{A}$. To be precise, we need in the Coulomb gauge the transverse current \mathbf{j}^\perp – in this way the theory becomes gauge invariant with respect to gauge transformation allowed under the Coulomb gauge ($\mathbf{A}' = \mathbf{A} + \nabla\chi$ with $\nabla^2\chi = 0$).

The interaction Hamiltonian with the transverse current takes the following form in the quantized theory:

$$H_{\text{int}} = - \int d^3x \mathbf{j}^\perp(\mathbf{x}) \cdot \mathbf{A}(\mathbf{x}) \quad (2.46)$$

$$= - \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar}{2\epsilon_0\omega_k V}} \left\{ a_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} \cdot \mathbf{j}_{\mathbf{k}}^{\perp*} + \text{h.c.} \right\}, \quad (2.47)$$

where $\mathbf{j}_{\perp,\mathbf{k}}$ is the spatial Fourier transform. It is, of course, also possible to work with the electric dipole interaction. The gauge transformation that leads to this

formulation can be read as a unitary transformation in the quantized field theory (see the book by Cohen-Tannoudji & al. (1987) for a discussion).

2.2 Alternative formulations

- with continuous momentum (Fourier integrals).
- with general mode functions (Sec.2.4.4)
- a bit more of functional analysis (functional derivatives etc)
- the full matter+field quantum theory, incl relativistic matter

Continuous wave vectors. Mode expansion of electric field operator

$$\mathbf{E}(\mathbf{x}, t) = \int d^3k \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0(2\pi)^3}} \sum_{\mu} \left(\mathbf{e}_{\mathbf{k}\mu} a_{\mathbf{k}\mu} e^{i\mathbf{k}\cdot\mathbf{x}} + \text{h.c.} \right) \quad (2.48)$$

We read off the replacement rule by comparison to (2.42): substitute $V \mapsto (2\pi)^3$ and replace the summation over \mathbf{k} by an integral. This changes, of course, the dimensions of the annihilation operators. The commutation relation (2.30) becomes

$$[\hat{a}_{\mathbf{k}\mu}, \hat{a}_{\mathbf{k}'\mu'}^{\dagger}] = \delta(\mathbf{k} - \mathbf{k}') \delta_{\mu\mu'} \quad (2.49)$$

The interpretation is now that the operator

$$d\hat{N} = \hat{a}_{\mathbf{k}\mu}^{\dagger} \hat{a}_{\mathbf{k}\mu} d^3k \quad (2.50)$$

gives the photon number in an element d^3k of the wavevector space. The total photon number and the field energy are, for instance, given by

$$\hat{N} = \int d^3k \sum_{\mu} \hat{a}_{\mathbf{k}\mu}^{\dagger} \hat{a}_{\mathbf{k}\mu}, \quad \hat{H} = \int d^3k \sum_{\mu} \hbar\omega_k \hat{a}_{\mathbf{k}\mu}^{\dagger} \hat{a}_{\mathbf{k}\mu} \quad (2.51)$$

while they are sums in a finite quantization volume.

Quantization of wave packets. We can also associate a bosonic operator to a ‘wavepacket’. Consider two orthogonal, transverse vector fields $\mathbf{f}(\mathbf{k})$ and $\mathbf{g}(\mathbf{k})$ and construct

$$\begin{aligned} \hat{a} &= \int d^3k \sum_{\mu} \mathbf{f}(\mathbf{k}) \cdot \mathbf{e}_{\mathbf{k}\mu} a_{\mathbf{k}\mu} \\ \hat{b} &= \int d^3k \sum_{\mu} \mathbf{g}(\mathbf{k}) \cdot \mathbf{e}_{\mathbf{k}\mu} a_{\mathbf{k}\mu} \end{aligned} \quad (2.52)$$

Then the commutator is

$$\begin{aligned}
[\hat{a}, \hat{b}^\dagger] &= \int d^3k d^3k' \sum_{\mu\mu'} \mathbf{f}(\mathbf{k}) \cdot \mathbf{e}_{\mathbf{k}\mu} \mathbf{g}^*(\mathbf{k}') \cdot \mathbf{e}_{\mathbf{k}'\mu'}^* [a_{\mathbf{k}\mu}, a_{\mathbf{k}'\mu'}] \\
&= \int d^3k \sum_{\mu} \mathbf{f}(\mathbf{k}) \cdot \mathbf{g}^*(\mathbf{k}) = 0
\end{aligned} \tag{2.53}$$

where we get the L^2 scalar product in the space of transverse vector fields. If the vector field \mathbf{f} is normalized in the corresponding L^2 -norm, we get $[\hat{a}, \hat{a}^\dagger] = 1$. The operator $\hat{a}^\dagger \hat{a}$ thus counts the photon number in the “wave packet” described by \mathbf{f} . These kinds of wave packets play the role of the normalizable mode functions of the simple formulation with a finite quantization volume. They are useful to describe few-photon pulses that are localized spatially and spread over some frequency range.

2.3 Photons and the quantum vacuum

2.3.1 ‘Photons’

The present quantized description of the electromagnetic field allows us to give a more precise meaning to the word ‘photon’. *A photon is an excitation of a mode of the field.* We have seen that the quantized field reduces to a collection of harmonic oscillators, one for each mode. As we know from the harmonic oscillator, its stationary states are labelled by non-negative numbers $n = 0, 1, \dots$. One says that in these states, the mode contains ‘ n photons’. The creation operator a^\dagger whose action on these states is $a^\dagger |n\rangle \propto |n+1\rangle$, thus ‘creates one photon’. This picture is consistent with the assumption (dating back to Einstein (1905)) that photons correspond to ‘energy packets’ of $\hbar\omega_k$ of the electromagnetic field. If a plane wave mode expansion is used, we can also say that the momentum of a photon is $\hbar\mathbf{k}$, as we know from de Broglie (1926) or from the Compton effect.

It is however possible to use different mode expansions for the same field. For example, we could have used an expansion in terms of spherical vector harmonics which differs from the plane wave expansion by a (infinite-dimensional) unitary transformation. A single-photon state in the plane wave basis thus becomes a superposition of single-photon states in infinitely many spherical modes. Conversely, a ‘photon’ in this description would not correspond to a plane wave (its momentum would not be $\hbar\mathbf{k}$), but it would have a definite angular momentum with respect to the origin. It is even possible to define photons that are wavepackets localized in time, by superposing plane waves with neighboring frequencies. This picture allows to describe experiments with ‘single-photon

pulses'. We refer to the exercises to look at these properties in more detail.

Finally, we precall that the computation of a suitable set of mode functions is a 'classical' problem: no quantum theory is needed to state it. Using a cubic 'quantization' box, one can show that the plane waves with wave vectors $\mathbf{k} = (2\pi/L)(n_x, n_y, n_z)^T$ ($n_i \in \mathbb{Z}$) are orthogonal with respect to the scalar product

$$\int_{L^3} d^3x \mathbf{f}^*(\mathbf{x}) \cdot \mathbf{g}(\mathbf{x}). \quad (2.54)$$

This is clear for different wave vectors, $\mathbf{k} \neq \mathbf{k}'$. But for a given \mathbf{k} , one can also find two orthogonal polarization vectors $\boldsymbol{\varepsilon}_{1,2}$ that give orthogonal modes (the scalar product $\boldsymbol{\varepsilon}_1^* \cdot \boldsymbol{\varepsilon}_2$ is zero). The corresponding magnetic field mode functions are also orthogonal. The electrodynamics becomes a 'quantum' theory only when the amplitudes of the mode functions become suitably normalized operators.

2.3.2 The Fock-Hilbert space

The Hilbert space of the quantized field is constructed from the mode operators a_κ and a_κ^\dagger . The state of lowest energy is called the 'vacuum state', $|\text{vac}\rangle$ or $|0\rangle$:

$$a_\kappa |\text{vac}\rangle = 0 \quad (2.55)$$

No confusion between the normalizable state $|0\rangle$ and the zero vector 0 in the Hilbert space. This is why we often prefer to write $|\text{vac}\rangle$.

The 'one-photon sector' is spanned by the infinitely many states with one photon per mode

$$|1_\kappa\rangle = a_\kappa^\dagger |\text{vac}\rangle \quad (2.56)$$

...and so on. A typical state can be labelled by its 'occupation numbers' $|n_1, \dots, n_\kappa, \dots\rangle = |\{n_\kappa\}\rangle$, it contains n_κ photons in the mode κ . The so-called Fock-Hilbert space is generated by taking linear combinations of these basis vectors with complex coefficients. From linear combinations with a finite number of terms, one completes the space by limiting procedures with respect to a suitable topology (related to the usual scalar product). Since the field theory ultimately contains a infinitely many modes and even a continuum, the topological structure can be quite intricate.

The field operators (vector potential, electric and magnetic fields) act between the N - and $N \pm 1$ -photon sectors via the ladder operators a_κ and a_κ^\dagger they contain. Their expectation values in the state $|\{n_\kappa\}\rangle$ are thus zero. To get a nonzero expectation value, one must construct superpositions of number states

with different particle numbers. These states are not stationary in general. In quantum optics, an example of such states are the coherent states, useful to describe classical fields or to approximate a laser field. In high-energy physics, one usually discards such superpositions by a ‘super-selection rule’: one argues that for massive particles, the rest mass is so large that the relative phase between the components that differ in particle number varies so rapidly that one cannot distinguish, in practice, between a superposition state and a mixed state (to be described by a density matrix, see below).

2.3.3 Vacuum fluctuations

In the vacuum state, the expectation value $\langle \mathbf{E}(\mathbf{x}, t) \rangle = \langle \text{vac} | \mathbf{E}(\mathbf{x}, t) | \text{vac} \rangle = 0$ because a_κ annihilates the vacuum state and a_κ^\dagger can be made to act to the left on the vacuum state which is annihilated. **Note.** The same is true for any stationary (or number) state, see Sec. 3.3.2.

The vacuum fluctuations become visible in the next moment of the field: for a given mode κ ,

$$\frac{\hbar\omega_\kappa}{2\varepsilon_0} \langle (\mathbf{f}_\kappa(\mathbf{x})a(t) + \text{h.c.})^2 \rangle = \frac{\hbar\omega_\kappa}{2\varepsilon_0} |\mathbf{f}_\kappa(\mathbf{x})|^2 \langle a_\kappa(t)a_\kappa^\dagger(t) \rangle = \frac{\hbar\omega_\kappa}{2\varepsilon_0} |\mathbf{f}_\kappa(\mathbf{x})|^2 \quad (2.57)$$

in the last step, we have used that $a_\kappa(t) = a_\kappa(0) e^{-i\omega_\kappa t}$. In the case of plane wave modes, we have $|\mathbf{f}_\kappa(\mathbf{x})|^2 = 1/V$. The sum over wave vectors \mathbf{k} and polarization indices λ can be written in the form

$$\langle \mathbf{E}^2(\mathbf{x}, t) \rangle = \int_0^\infty \frac{d\omega}{2\pi} \frac{\hbar\omega}{2\varepsilon_0} \rho(\omega) \quad (2.58)$$

where $\rho(\omega)$ is the so-called ‘local density of modes’ (per unit frequency and unit volume):

$$\rho(\mathbf{x}; \omega) = 2\pi \sum_\kappa |\mathbf{f}_\kappa(\mathbf{x})|^2 \delta(\omega - \omega_\kappa) = \frac{2\pi}{V} \sum_\kappa \delta(\omega - \omega_\kappa) \quad (2.59)$$

For the plane wave modes, ω_κ only depends on the magnitude of \mathbf{k} , and in the continuum limit,

$$\sum_{\mathbf{k}} = V \int \frac{d^3k}{(2\pi)^3} \quad (2.60)$$

we get after a simple integration

$$\rho(\omega) = \frac{2}{\pi} \frac{\omega^2}{c^3} \quad (2.61)$$

The full vacuum fluctuation of the electric field is then infinite

$$\langle \mathbf{E}^2(\mathbf{x}, t) \rangle = \frac{\hbar}{\pi \varepsilon_0 c^3} \int_0^\infty \frac{d\omega}{2\pi} \omega^3 \quad (2.62)$$

because the integral diverges at the upper limit. This correlates with an infinite electromagnetic energy density in vacuum (multiply with $\varepsilon_0/2$ and add the magnetic component, which doubles the result). This “infinite vacuum energy” is one of the unresolved problems in physics. “Intuitive cutoffs” at short wavelengths, for example, at the Planck scale (10^{-35} m) give a finite energy density, but with a value that differs by something like 120 orders of magnitude from the energy density associated with cosmological observations (including “dark energy”, “cosmological constants” and so on). A simple discussion of the vacuum energy problem has been given by Adler & al. (1995).

Exercise. Find a cutoff such that the vacuum energy density equals the ‘critical density of the Universe’ (the critical mass density is roughly 10^{-29} g/cm³, given the current expansion rate of the Universe.)

A finite value can be found, if we compute an autocorrelation function of the electric field. A similar calculation gives

$$\langle \mathbf{E}(\mathbf{x}, t) \cdot \mathbf{E}(\mathbf{x}, t') \rangle = \int_0^\infty \frac{d\omega}{2\pi} \frac{\hbar \omega}{2\varepsilon_0 c^3} \rho(\omega) e^{-i\omega(t-t')} \quad (2.63)$$

This leads to the integral representation of the Γ -function in the complex plane and finally to

$$\langle \mathbf{E}(\mathbf{x}, t) \cdot \mathbf{E}(\mathbf{x}, t') \rangle = \frac{3\hbar}{\pi^2 \varepsilon_0 c^3 \tau^4} \quad (2.64)$$

which is finite for all $\tau = t - t' \neq 0$. For any finite value of τ , the electric vacuum energy density is thus of the order of $\hbar \omega_\tau / \lambda_\tau^3$ with the characteristic frequency $\omega_\tau = 1/\tau$ and wavelength $\lambda_\tau = c\tau$.

2.4 Second turn

We give in this section a few more technical details on field quantization. The information contained here is not part of the ordinary curriculum of this year.

2.4.1 Transverse δ -function

We have encountered the ‘transverse δ -function’ $\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}')$ in the commutator (2.19) between the vector potential and its canonically conjugate momentum. This is a distribution that acts

like a δ -function on fields with zero divergence, and projects an arbitrary vector field \mathbf{F} on its transverse part \mathbf{F}^\perp

$$F_l^\perp(\mathbf{x}) = \int d^3x' \delta_{lm}^\perp(\mathbf{x} - \mathbf{x}') F_m(\mathbf{x}') \quad (2.65)$$

By definition, the transverse part has zero divergence, $\nabla \cdot \mathbf{F}^\perp = 0$. The projection is most easily constructed in Fourier space

$$F_j^\perp(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \frac{k^2 \delta_{jl} - k_j k_l}{k^2} \tilde{F}_l(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} \quad (2.66)$$

where $\tilde{\mathbf{F}}(\mathbf{k})$ is the spatial Fourier transform of $\mathbf{F}(\mathbf{x})$. This relation allows to deduce explicit expressions for the transverse δ -function.

Note that in the wave equation (2.7) for the vector potential, we have an alternative relation between the current density \mathbf{j} and its transverse part:

$$\mathbf{j}_\perp = \mathbf{j} - \varepsilon_0 \partial_t \nabla \phi,$$

The ‘longitudinal part’ that is subtracted here is thus related to the electrostatic field created by the corresponding charge density. More details are discussed in the exercises.

2.4.2 Matter

Let us consider that all matter is made from charged point particles with charges e_α and positions \mathbf{r}_α . The electric charge and current densities are then given by

$$\rho(\mathbf{x}, t) = \sum_\alpha e_\alpha \delta(\mathbf{x} - \mathbf{r}_\alpha(t)), \quad \mathbf{j}(\mathbf{x}, t) = \sum_\alpha e_\alpha \mathbf{v}_\alpha(t) \delta(\mathbf{x} - \mathbf{r}_\alpha(t)) \quad (2.67)$$

The sum runs over all the particles. Charge conservation is ensured provided that $\dot{\mathbf{r}}_\alpha = \mathbf{v}_\alpha$.

The point charges are thus the ‘sources’ for the electromagnetic field. But their motion is also influenced by the fields via the Newton-Lorentz equations:

$$\frac{d}{dt} \frac{m_\alpha \mathbf{v}_\alpha}{\sqrt{1 - v_\alpha^2/c^2}} = e_\alpha (\mathbf{E}(\mathbf{r}_\alpha) + \mathbf{v}_\alpha \times \mathbf{B}(\mathbf{r}_\alpha)) \quad (2.68)$$

We use a relativistic framework here, and with the Lorentz factor, the time derivative is actually the one for the relativistic particle momentum. Note that in these equations, the coordinate \mathbf{r}_α enters generally in a nonlinear way. This differs from the Maxwell equations that are linear in the fields and potentials and whose solutions are linear in the charge and current distributions. (The superposition principle can be applied, see Eq.(2.6).) All nonlinear effects in optics can ultimately be traced back to the nonlinear response of matter to an applied electromagnetic field.

Quantization. The theory outlined so far describes physics at the end of the 19th century. It is unable to describe a stable state of matter because of the ‘radiation catastrophe’: positive and negative charges circle around each other, radiate electromagnetic waves and lose energy. Stable bound states exist only when the particle dynamics is quantized—recall the hydrogen atom.

Let us recall the typical energy and length scales for the hydrogen atom. The energy levels in Hydrogen are given by

$$E_n = -\frac{\text{Ryd}}{n^2} = -\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2} \frac{1}{n^2} \quad (2.69)$$

where the Rydberg constant is $1 \text{ Ryd} \approx 13.6 \text{ eV}$. (In cgs units, drop the factor $(4\pi\epsilon_0)^2$.) The size of the Hydrogen atom is of the order of the Bohr radius

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \quad (2.70)$$

The typical wavelength of an electromagnetic wave resonant with a transition in Hydrogen is therefore of the order of

$$\lambda = \frac{\hbar c}{\text{Ryd}} = \frac{2}{\alpha_{\text{fs}}} a_0 \quad (2.71)$$

$$\frac{1}{\alpha_{\text{fs}}} = \frac{4\pi\epsilon_0 \hbar c}{e^2} \approx 137 \quad (2.72)$$

Here, α_{fs} is the fine structure constant. Its inverse can be understood as a measure of the speed of light in ‘atomic units’ (the natural units for the Hydrogen problem). The value $1/\alpha_{\text{fs}} \approx 137$ is fairly large. This means two things:

- the size of the hydrogen atom is small compared to the wavelength of resonant radiation: the Lorentz force (2.68) has therefore only a weak dependence on \mathbf{r}_α ;
- the typical velocity of an electron in the Hydrogen atom is in the non-relativistic regime: we can therefore use non-relativistic mechanics to describe the matter response.

This will justify several approximations for the atom-light interaction that we are going to make in the rest of the lecture.

2.4.3 Lagrange-Hamilton formulation

Lagrangian. We now proceed to quantize the wave equation (2.7) in the ‘canonical way’. The first step is to guess the corresponding Lagrangian. A good guess is the Lagrangian

$$L = -\sum_{\alpha} m_{\alpha} c^2 \sqrt{1 - \dot{\mathbf{r}}_{\alpha}^2/c^2} + \int d^3x \mathcal{L}_{F+I} \quad (2.73)$$

where the Lagrangian density for the field and its interaction with the electric charges is given by

$$\mathcal{L}_{F+I} = \frac{\epsilon_0}{2} (\dot{\mathbf{A}} + \nabla\phi)^2 - \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 - \phi\rho + \mathbf{A} \cdot \mathbf{j}. \quad (2.74)$$

Via the Euler-Lagrange equations, one gets the Maxwell equations (2.5,2.7) for the fields and the Newton-Lorentz equation (2.68) for the particles. Note that the Lagrangian (2.73,2.74) is invariant under gauge transformations

$$\phi \mapsto \phi - \partial_t \chi, \quad \mathbf{A} \mapsto \mathbf{A} + \nabla \chi \quad (2.75)$$

where $\chi(\mathbf{x}, t)$ is an arbitrary smooth function. This gauge invariance is connected to charge conservation.

Coulomb gauge. We now proceed to specialize to the Coulomb gauge, simplify the Lagrangian and derive the Hamiltonian. We start with the terms involving the scalar potential in the Lagrangian (2.74). The mixed term is

$$\dot{\mathbf{A}} \cdot \nabla \phi = \nabla \cdot (\dot{\mathbf{A}} \phi) - \phi \nabla \cdot \dot{\mathbf{A}} \quad (2.76)$$

The first term is a divergence, and leads to a surface integral when integrated over the volume. We adopt the usual boundary condition that at the (infinitely remote) surface, the fields vanish: then this term is zero. The second term is zero in the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$.

The term quadratic in the scalar potential is

$$(\nabla \phi)^2 = \nabla \cdot (\phi \nabla \phi) - \phi \nabla^2 \phi = \nabla \cdot (\phi \nabla \phi) + \phi \rho / \varepsilon_0 \quad (2.77)$$

using the Laplace equation (2.5). The second term thus combines with the interaction part $-\phi \rho$ in the Lagrangian that becomes $-\frac{1}{2} \phi \rho$. This energy can be interpreted as the Coulomb interaction energy between the charges:

$$V_{\text{Coul}} = \frac{1}{2} \int d^3x \phi \rho = \frac{1}{2} \int d^3x d^3x' \frac{\rho(\mathbf{x}) \rho(\mathbf{x}')}{4\pi \varepsilon_0 |\mathbf{x} - \mathbf{x}'|} \quad (2.78)$$

$$= \frac{1}{2} \sum_{\alpha\beta} \frac{e_\alpha e_\beta}{4\pi \varepsilon_0 |\mathbf{r}_\alpha - \mathbf{r}_\beta|} \quad (2.79)$$

where the factor $\frac{1}{2}$ ensures that all pairs of charges are only counted once. The divergent self-interaction for $\mathbf{r}_\alpha = \mathbf{r}_\beta$ also appears here. It is usually discarded. *The key point to note is that in the Coulomb gauge, the contribution of the scalar potential depends only on the particle coordinates. It is not a proper degree of freedom of the fields.*

To summarize, in the Coulomb gauge, the Lagrangian can be split into the following form:

$$L = - \sum_{\alpha} m_{\alpha} c^2 \sqrt{1 - v_{\alpha}^2 / c^2} - V_{\text{Coul}}(\{\mathbf{r}_{\alpha}\}) + \int d^3x \mathcal{L}_{\text{F+I}}^{\perp} \quad (2.80)$$

with

$$\mathcal{L}_{\text{F+I}}^{\perp} = \frac{\varepsilon_0}{2} \dot{\mathbf{A}}^2 - \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 + \mathbf{A} \cdot \mathbf{j}. \quad (2.81)$$

We have added the subscript \perp to remind ourselves that this is only valid if the vector potential is transverse.

Hamiltonian. For the Hamiltonian, we need the canonical momenta conjugate to \mathbf{r}_{α} and \mathbf{A} :

$$\mathbf{p}_{\alpha} = \frac{\partial L}{\partial \dot{\mathbf{r}}_{\alpha}} = \frac{m \dot{\mathbf{r}}_{\alpha}}{\sqrt{1 - \dot{\mathbf{r}}_{\alpha}^2 / c^2}} + e_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha}) \quad (2.82)$$

$$\mathbf{\Pi}(\mathbf{x}) = \frac{\delta L}{\delta \dot{\mathbf{A}}(\mathbf{x})} = \varepsilon_0 \dot{\mathbf{A}}(\mathbf{x}) \quad (2.83)$$

The particle momentum contains the relativistic kinetic momentum and an electromagnetic contribution. For the field momentum, it looks as if ε_0 were the ‘mass’ and $\dot{\mathbf{A}}$ the velocity. But the derivative looks strange, it is a ...

Functional derivative. In the field case, we have a continuous collection of degrees of freedom, labelled by the space-points \mathbf{x} . This requires a generalization of the notion of a derivative to the infinite-dimensional case: the ‘functional derivative’ $\delta L/\delta \dot{\mathbf{A}}(\mathbf{x})$. It is the generalization of a gradient.

In mathematical terms, if we have a ‘functional’ $L[\mathbf{A}(\mathbf{x})]$, i.e. a mapping from the space of vector fields into the real numbers, its functional derivative is defined by the following approximation:

$$L[\mathbf{A}(\mathbf{x}) + \delta \mathbf{A}(\mathbf{x})] \approx L[\mathbf{A}(\mathbf{x})] + \int d^3x \left. \frac{\delta L}{\delta \mathbf{A}(\mathbf{x})} \right|_{\mathbf{A}(\mathbf{x})} \delta \mathbf{A}(\mathbf{x}) + \mathcal{O}(\delta \mathbf{A}^2) \quad (2.84)$$

Here, the second line is an example of a linear functional because the integral is linear in $\delta \mathbf{A}(\mathbf{x})$. The function with which the small deviation $\delta \mathbf{A}(\mathbf{x})$ is weighted under the integral *defines* the functional derivative. A mathematical theorem ensures that in a suitable space of functions, all linear functionals take this integral form.

It is a simple exercise to derive with (2.84) expression (2.83) for the field momentum $\mathbf{\Pi}$. We shall return to a less trivial example below.

The Hamiltonian is given by

$$H = \sum_{\alpha} \mathbf{p}_{\alpha} \cdot \dot{\mathbf{r}}_{\alpha} + \int d^3x \mathbf{\Pi} \cdot \dot{\mathbf{A}} - L \quad (2.85)$$

where the field part is the obvious generalization to a continuous set of degrees of freedom. Putting everything together, we get

$$H = \sqrt{[\mathbf{p}_{\alpha} - e_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha})]^2 c^2 + m^2 c^4} + V_{\text{Coul}}(\{\mathbf{r}_{\alpha}\}) + \int d^3x \left[\frac{\mathbf{\Pi}^2}{2\epsilon_0} + \frac{(\nabla \times \mathbf{A})^2}{2\mu_0} \right] \quad (2.86)$$

where the interaction between matter and (transverse) field arises due to the ‘minimal coupling’ prescription only. (The term linear in \mathbf{j} in the Lagrangian cancels with the term linear in $\dot{\mathbf{r}}_{\alpha}$ in (2.85).)

Canonical equations. The motion of particles and fields in the Hamiltonian formalism can be described in a compact way in terms of Poisson brackets. We discuss this in some detail because they provide another example of functional derivatives and because they bear strong similarities to the commutators of the quantum theory. In addition, it turns out to be tricky to get the transverse wave equation (2.7).

The Poisson bracket provides the time evolution of any function Q (or functional) of the coordinates and momenta by

$$\dot{Q} = \{H, Q\} \quad (2.87)$$

where we define

$$\{A, B\} = \sum_{\alpha} \frac{\partial A}{\partial \mathbf{p}_{\alpha}} \cdot \frac{\partial B}{\partial \mathbf{r}_{\alpha}} - \frac{\partial A}{\partial \mathbf{r}_{\alpha}} \cdot \frac{\partial B}{\partial \mathbf{p}_{\alpha}} + \int d^3x \left[\frac{\delta A}{\delta \mathbf{\Pi}(\mathbf{x})} \cdot \frac{\delta B}{\delta \mathbf{A}(\mathbf{x})} - \frac{\delta A}{\delta \mathbf{A}(\mathbf{x})} \cdot \frac{\delta B}{\delta \mathbf{\Pi}(\mathbf{x})} \right] \quad (2.88)$$

Here, functional derivatives with respect to \mathbf{A} and $\mathbf{\Pi}$ appear for the fields. The Poisson bracket is antisymmetric in A and B and satisfies a ‘Jacobi identity’ (as does the commutator).

By working out $\{H, \mathbf{r}_\alpha\}$, only the second term of the first line in (2.88) contributes, and we get (after some calculations) the relativistic relation between velocity and momentum, Eq.(2.82). This is left as an exercise. Similarly, one gets $\dot{\mathbf{A}} = \mathbf{\Pi}/\varepsilon_0$.

A more complicated calculation is needed for $\dot{\mathbf{\Pi}}$ where we have to evaluate

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})} \sqrt{[\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha)]^2 c^2 + m^2 c^4} \quad (2.89)$$

We note first that

$$\frac{\delta \mathbf{A}(\mathbf{r}_\alpha)}{\delta \mathbf{A}(\mathbf{x})} = \delta(\mathbf{r}_\alpha - \mathbf{x}) \quad (2.90)$$

because the ‘evaluation functional’ $\mathbf{A} \mapsto \mathbf{A}(\mathbf{r}_\alpha)$ is of course a linear functional. (For mathematicians, this property *defines* the δ -function.) To proceed, we use the usual rules of differential calculus and get

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})} \sqrt{[\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha)]^2 c^2 + m^2 c^4} = \delta(\mathbf{r}_\alpha - \mathbf{x}) \frac{e_\alpha (\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha)) c^2}{\sqrt{[\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha)]^2 c^2 + m^2 c^4}} \quad (2.91)$$

Performing the same calculations as for the particles’ equations of motion, this can be written as the current density $\mathbf{j}(\mathbf{x})$.

The last term now involves the derivative

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})} \frac{1}{2\mu_0} \int d^3x (\nabla \times \mathbf{A})^2 \quad (2.92)$$

that we handle with the mathematical definition (2.84). Consider a small change $\mathbf{a}(\mathbf{x})$ of the vector potential. To linear order, this gives a change

$$\begin{aligned} (\nabla \times (\mathbf{A} + \mathbf{a}))^2 - (\nabla \times \mathbf{A})^2 &\approx 2(\nabla \times \mathbf{a}) \cdot (\nabla \times \mathbf{A}) \\ &= 2\nabla \cdot [\mathbf{a} \times (\nabla \times \mathbf{A})] + 2\mathbf{a} \cdot [\nabla \times (\nabla \times \mathbf{A})] \end{aligned} \quad (2.93)$$

the first term is a divergence and vanishes after integrating over all space. The second one contains a multiplied with a weighting function so that we get

$$-\frac{1}{2\mu_0} \frac{\delta}{\delta \mathbf{A}(\mathbf{x})} \int d^3x (\nabla \times \mathbf{A})^2 = -\frac{1}{\mu_0} \nabla \times (\nabla \times \mathbf{A}) \quad (2.94)$$

Putting everything together, we have for the equation of motion of the vector potential:

$$\dot{\mathbf{\Pi}} = \varepsilon_0 \ddot{\mathbf{A}} = \mathbf{j}(\mathbf{x}) - \frac{1}{\mu_0} \nabla \times (\nabla \times \mathbf{A}) \quad \dots \text{wrong} \quad (2.95)$$

which is nearly equivalent to the wave equation (2.7). The point is that the source term is the ‘full current’, not its transverse part. This is actually an error in our calculation because we did not take into account the fact that the vector potential is restricted to be transverse.

A simple way to repair this is to use \mathbf{A}_\perp in the Lagrangian (2.80) and the Hamiltonian (2.86). Now, the link between \mathbf{A}_\perp and the ‘full’ \mathbf{A} is a linear functional (actually, a linear projector).

This can be seen in the following way: consider an arbitrary \mathbf{A} and perform a gauge transformation (2.75) to remove the nonzero divergence. This fixes the ‘gauge function’ to satisfy

$$\nabla^2 \chi = -\nabla \cdot \mathbf{A} \quad (2.96)$$

whose solution (vanishing at infinity) is given by a ‘superposition of Coulomb potentials’:

$$\chi(\mathbf{x}) = \frac{1}{4\pi} \int d^3 x' \frac{\nabla' \cdot \mathbf{A}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \quad (2.97)$$

where ∇' means the gradient with respect to \mathbf{x}' . After the gauge transformation, the now transverse vector potential is given by

$$\mathbf{A}_\perp(\mathbf{x}) = \mathbf{A}(\mathbf{x}) + \frac{1}{4\pi} \int d^3 x' [\nabla' \cdot \mathbf{A}(\mathbf{x}')] \nabla \frac{1}{|\mathbf{x} - \mathbf{x}'|} \quad (2.98)$$

Now, $\nabla(1/r) = -\nabla'(1/r)$, and after one integration by parts we have

$$A_{\perp i}(\mathbf{x}) = \int d^3 x' \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') A_j(\mathbf{x}') \quad (2.99)$$

where the transverse δ -function appears for which we have just derived the following representation

$$\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') = \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') + \frac{1}{4\pi} \partial_j' \partial_i' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \quad (2.100)$$

A careful evaluation of the second derivatives yields the explicit result

$$\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') = \frac{2}{3} \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') - \frac{1}{4\pi} \left(\frac{\delta_{ij}}{r^3} - 3 \frac{r_i r_j}{r^5} \right), \quad \mathbf{r} = \mathbf{x} - \mathbf{x}' \quad (2.101)$$

By construction, the transverse δ -function acts like a usual δ -function on vector fields that are already transverse. We can interpret it as the ‘unit operator’ in the space of transverse vector fields.

Finally, if we write \mathbf{A}_\perp in the Hamiltonian, the equations of motion for $A_{\perp i}(\mathbf{x})$ lead to the following term

$$\int d^3 x' \frac{\delta H}{\delta \Pi_j(\mathbf{x}')} \frac{\delta A_{\perp i}(\mathbf{x})}{\delta A_j(\mathbf{x}')} = \int d^3 x' \frac{\delta H}{\delta \Pi_j(\mathbf{x}')} \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') = \left(\frac{\delta H}{\delta \Pi(\mathbf{x}')} \right)_{\perp i} \quad (2.102)$$

The functional derivative with respect to \mathbf{A} makes the transverse δ -function appear. The integral over \mathbf{x}' then projects the functional derivative with respect to Π into the transverse subspace. In this way, the time derivative of \mathbf{A}_\perp is transverse, as it should be in order to maintain the Coulomb gauge at all times.

The same procedure applies to the equation of motion for the field momentum: the bottom-line is that the source current \mathbf{j} is ‘transversalized’, leading to the correct wave equation (2.7).

2.4.4 Quantization

Mode expansion. The next step is to look for ‘normal modes’ of this field theory. We first identify some general requirements for the modes. The passage to plane waves is a little bit

tricky and is treated in detail in Sec. 2.1.2. Note that we ignore for the moment the matter-field coupling: we focus on the field Hamiltonian only.

We adopt the expansion

$$\begin{pmatrix} \mathbf{A}(\mathbf{x}, t) \\ \mathbf{\Pi}(\mathbf{x}, t) \end{pmatrix} = \sum_{\kappa} \mathbf{f}_{\kappa}(\mathbf{x}) \begin{pmatrix} q_{\kappa}(t) \\ p_{\kappa}(t) \end{pmatrix} \quad (2.103)$$

where the ‘mode functions’ $\mathbf{f}_{\kappa}(\mathbf{x})$ carry the space dependence and the ‘coordinates’ $q_{\kappa}(t)$ and ‘momenta’ $p_{\kappa}(t)$ the time-dependence.

The Coulomb gauge requires, of course, $\nabla \cdot \mathbf{f}_{\kappa}(\mathbf{x}) = 0$: the mode functions must be transverse.

We want the Hamiltonian to adopt a simple form using these modes. The space integral over $\mathbf{\Pi}^2$ becomes simple if we impose the modes to be orthogonal:

$$\int d^3x \mathbf{f}_{\kappa}(\mathbf{x}) \cdot \mathbf{f}_{\kappa'}(\mathbf{x}) = N_{\kappa} \delta_{\kappa\kappa'} \quad (2.104)$$

where N_{κ} is a normalization constant that we fix later. The momentum-part of the Hamiltonian then becomes

$$\frac{1}{2\varepsilon_0} \int d^3x \mathbf{\Pi}^2 = \sum_{\kappa} N_{\kappa} \frac{p_{\kappa}^2}{2\varepsilon_0} \quad (2.105)$$

Similarly, for the integral over $(\nabla \times \mathbf{A})^2$. Integrating by parts:

$$\begin{aligned} & \int d^3x (\nabla \times \mathbf{f}_{\kappa}) \cdot (\nabla \times \mathbf{f}_{\kappa'}) \\ &= \int d\mathbf{A} \cdot [\mathbf{f}_{\kappa} \times (\nabla \times \mathbf{f}_{\kappa'})] + \int d^3x \mathbf{f}_{\kappa} \cdot [\nabla \times (\nabla \times \mathbf{f}_{\kappa'})] \end{aligned} \quad (2.106)$$

The volume integral, strictly speaking, must be evaluated over a finite volume only, otherwise, we could not work with a discrete set of mode labels κ . The boundary term can nevertheless be made to vanish if either (i) the mode function \mathbf{f}_{κ} or its curl $(\nabla \times \mathbf{f}_{\kappa'})$ is required to vanish on the boundary of the volume or (ii) periodic boundary conditions on ‘opposite faces’ of a cubic volume are assumed. The case (i) is appropriate for modes in a cavity with perfectly conducting boundaries: then, \mathbf{f}_{κ} is proportional to the electric field, and the integrand in Eq.(2.106) vanishes because the field is normal to the boundary. The case (ii) is the favorite one for theorists because the mode functions can be taken as plane waves. Note that the eigenfrequencies of the two cavities are not the same. We ignore for the moment the complications of complex mode functions (see details below and the exercises) and continue.

The volume integral in (2.106) is reduced to the orthogonality relation if we require the mode functions to be eigenfunctions of the (vector) Helmholtz equation:

$$\nabla \times (\nabla \times \mathbf{f}_{\kappa}) = \varepsilon_0 \mu_0 \omega_{\kappa}^2 \mathbf{f}_{\kappa} \quad (2.107)$$

(This equation is actually equivalent to the scalar Helmholtz equation for all components of \mathbf{f}_{κ} because of transversality.)

With all these assumptions taken together, the Hamiltonian for the field takes the form

$$H_F = \sum_{\kappa} \left[\frac{N_{\kappa}}{2\varepsilon_0} p_{\kappa}^2 + \frac{\varepsilon_0}{2} N_{\kappa} \omega_{\kappa}^2 q_{\kappa}^2 \right] \quad (2.108)$$

We now fix the normalization to be $N_\kappa = 1$ and get a sum of harmonic oscillator Hamiltonians, one for each mode κ with ‘mass’ ε_0 and frequency ω_κ .

Note: the construction of field modes is a ‘classical problem’ of electrodynamics, it has nothing to do with quantum mechanics. The word ‘quantization volume’ that is sometimes used (to ensure that the mode index κ is discrete) is therefore misleading. Quantization is something different, as we shall see now.

Mode operators. Quantization proceeds by promoting the p_κ and q_κ to operators with the commutation relations

$$\frac{i}{\hbar} [p_\kappa, q_{\kappa'}] = \delta_{\kappa\kappa'} \quad (2.109)$$

The choice for this commutator is similar to the one for the particle coordinates and momenta in ordinary quantum mechanics. So in the end, field quantization is nothing else but ordinary quantization, once the dynamics of the field is reduced to a discrete set of ‘normal modes’. The procedure that we have followed was first laid out by Dirac. It is called ‘canonical quantization’.

The commutator between the fields becomes

$$\frac{i}{\hbar} [\Pi_i(\mathbf{x}), A_j(\mathbf{x}')] = \sum_\kappa f_{\kappa i}(\mathbf{x}) f_{\kappa j}(\mathbf{x}') \stackrel{!}{=} \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') \quad (2.110)$$

The last equality is obtained by applying the canonical quantization scheme directly to the fields, care being taken that the fields (operators) ‘live’ in the space of transverse vector fields (operators). It means that the mode functions $\mathbf{f}(\mathbf{x})$ form a *complete set* of functions in the transverse field space. To implement this equality, one takes in practice the limit of an infinitely large quantization volume where the sum degenerates into an integral. With discrete functions, one can actually represent only a ‘finite volume version’ of the transverse δ -function—the one that comes by applying the finite volume boundary conditions to the equation (2.96).

For the harmonic oscillator, creation and annihilation operators are a convenient tool to construct the Hilbert space of quantum states. In our context, these operators, a_κ^\dagger and a_κ , correspond to the ‘creation’ and ‘destruction’ of one ‘photon’. The mode coordinate and momentum operators are given by

$$q_\kappa = \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa}} (a_\kappa + a_\kappa^\dagger) \quad (2.111)$$

$$p_\kappa = \sqrt{\frac{\hbar\varepsilon_0\omega_\kappa}{2}} i (a_\kappa^\dagger - a_\kappa) \quad (2.112)$$

where we continue to write ε_0 for the oscillator mass and where the commutation relation is

$$[a_\kappa, a_{\kappa'}^\dagger] = \delta_{\kappa\kappa'} \quad (2.113)$$

The field Hamiltonian then takes the form

$$H_F = \sum_\kappa \frac{\hbar\omega_\kappa}{2} (a_\kappa a_\kappa^\dagger + a_\kappa^\dagger a_\kappa) = \sum_\kappa \hbar\omega_\kappa (a_\kappa^\dagger a_\kappa + \frac{1}{2}) \quad (2.114)$$

The last way of writing makes two essential things explicit:

- the energies (the energy eigenvalues!) of a given field mode are quantized in units of $\hbar\omega_\kappa$ (a ‘photon energy’) and the ‘number of photons’ is represented by the operator $a_\kappa^\dagger a_\kappa$.
- The ground state of the field corresponds to the state $|\text{vac}\rangle$ such that $a_\kappa|\text{vac}\rangle = 0$ for all κ . This is an energy eigenstate whose energy is infinite, $\frac{1}{2} \sum_\kappa \hbar\omega_\kappa$, the sum over the ‘zero-point energies’ of all the modes.

To summarize, we give the mode expansions of the vector potential that we have found

$$\mathbf{A}(\mathbf{x}, t) = \sum_\kappa \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa}} \mathbf{f}_\kappa(\mathbf{x}) (a_\kappa e^{-i\omega_\kappa t} + a_\kappa^\dagger e^{i\omega_\kappa t}). \quad (2.115)$$

We have used here the Heisenberg picture for the vector potential operator. From the Hamiltonian (2.114), it is easy to show that the operator $a_\kappa(t)$ evolves with a complex exponential $e^{-i\omega_\kappa t}$. This is also called a ‘positive frequency operator’. It can be shown that operators that destroy particles and lower the energy of a quantum state are always positive frequency operators.

Plane wave modes. For completeness, we give here the plane-wave expansion for the field mode functions. These are complex, and therefore they are normalized according to

$$\int d^3x \mathbf{f}_\kappa^*(\mathbf{x}) \cdot \mathbf{f}_{\kappa'}(\mathbf{x}) = \delta_{\kappa\kappa'} \quad (2.116)$$

instead of Eq.(2.104). This can be ensured with the choice

$$\mathbf{f}_\kappa(\mathbf{x}) = \frac{1}{\sqrt{V}} \mathbf{e}_\kappa e^{i\mathbf{k}\cdot\mathbf{x}} \quad (2.117)$$

where V is the volume of the box with periodic boundary conditions, \mathbf{k} is a discrete wave vector: it increases in steps of $2\pi/V^{1/3}$ for a cubic box. And \mathbf{e}_κ is a ‘transverse’ polarization vector with the property $\mathbf{k} \cdot \mathbf{e}_\kappa = 0$. There are two mutually orthogonal choices of polarization for a given \mathbf{k} . (These can be complex, describing circular polarization.) The frequency of this mode is $\omega_\kappa = |\mathbf{k}|/\sqrt{\varepsilon_0\mu_0} = c|\mathbf{k}|$, as can be seen from the Helmholtz equation (2.107). The magnetic field is oriented along $\mathbf{k} \times \mathbf{e}_\kappa \equiv (\omega_\kappa/c)\mathbf{b}_\kappa$.

Finally, the quantized vector potential, electric and magnetic fields are given in terms of the following plane wave expansion

$$\mathbf{A}_\perp(\mathbf{x}, t) = \sum_\kappa \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa V}} \left(\mathbf{e}_\kappa e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_\kappa t)} a_\kappa + \text{h.c.} \right). \quad (2.118)$$

$$\mathbf{E}_\perp(\mathbf{x}, t) = \sum_\kappa \sqrt{\frac{\hbar\omega_\kappa}{2\varepsilon_0 V}} \left(i\mathbf{e}_\kappa e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_\kappa t)} a_\kappa + \text{h.c.} \right). \quad (2.119)$$

$$\mathbf{B}(\mathbf{x}, t) = \sum_\kappa \sqrt{\frac{\hbar\omega_\kappa\mu_0}{2V}} \left(i\mathbf{b}_\kappa e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_\kappa t)} a_\kappa + \text{h.c.} \right). \quad (2.120)$$

Sometimes, you may encounter these formulas without the factor i . Then the operators $ia_{\mathbf{k}\lambda}$ are being used instead, but they have the same commutation relations. Note that Eq.(2.119) gives only the ‘transverse’ part of the electric field. The ‘longitudinal’ part, $-\nabla\phi$, is determined according to (2.5) by the charge density.

Note: A useful shortcut to derive the prefactors is the following: for each mode, match the energy density $\frac{1}{2}\epsilon_0\mathbf{E}^2 + (1/2\mu_0)\mathbf{B}^2$ to the photon energy per quantization volume, $(\hbar\omega_\kappa/V)(a_\kappa^\dagger a_\kappa + \frac{1}{2})$. In free space, the electric and magnetic energy densities are equal. Average over the spatial oscillations in \mathbf{E}^2 for simplicity.

Exercise. Show that the momentum of the field can be written as a sum over modes as well. With plane wave modes, the momentum per mode is quantized in units of $\hbar\mathbf{k}$, as expected. Arbitrary cavity modes involving sin or cos functions are not eigenfunctions of the momentum operators, therefore their momentum is not well-defined. A ‘cavity photon’ therefore does not have a well-defined momentum.

Exercise. Write the equation of motion for a mode operator a_κ and include the source current. Solve it for known time-dependence of current.

Chapter 3

Applications

3.1 Photodetection

square-law detector signal (Glauber, 1960s)

$$I(t) = \langle \hat{I}(t) \rangle = \langle \hat{\mathcal{E}}^\dagger(t) \hat{\mathcal{E}}(t) \rangle \quad (3.1)$$

where the operator $\hat{\mathcal{E}}(t)$ gives the *positive frequency component* of the electric field, evaluated at the detector position and projected onto a polarization vector that reaches the detector. The positive frequency component of a free field operator contains all annihilation operators a_{κ} . These evolve in time as $e^{-i\omega_{\kappa}t}$, this motivates the name “positive frequency”. The conjugate operator $\hat{\mathcal{E}}^\dagger(t)$ is called the negative frequency component. Sometimes the notation $\hat{E}^{(-)}(t)\hat{E}^{(+)}(t)$ for the intensity operator is used.

Key feature: detector signal is nonzero only when photons are present, not in the vacuum state.

To remember: this is a “slow detector” – the derivation makes use of time-dependent perturbation theory and to get a sizable signal, one has to “wait” for many optical periods (to create a free electron, for example). This is the technical reason why the mixed product of negative/positive frequency operators appears and not the ordinary electric energy density, for example. Hence: Glauber’s theory does not work for “very fast” detectors (on the fs scale in the visible).

Reduced state, decoherence, recoil momentum.

3.2 Quantum optics of the beamsplitter

recall scattering theory

transformation rules for mode operators, for quantum states

split a single photon (generate entanglement)

two-photon interference: Hong–Ou–Mandel experiment

homodyne measurement (local oscillator)

More details on multi-mode quantum fields can be found in Sec. 3.6.

3.2.1 State transformation

A beamsplitter is the most simple way to mix two modes, see Figure 3.1. From

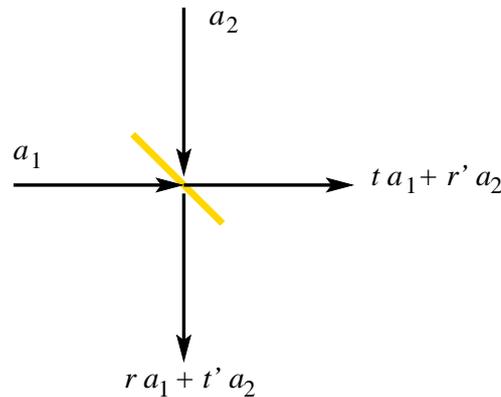


Figure 3.1: Mixing of two modes by a beam splitter.

classical electrodynamics, one gets the following amplitudes for the outgoing modes:

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}^{\text{in}} \mapsto \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}^{\text{out}} = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}^{\text{in}}. \quad (3.2)$$

The recipe for quantization is now: ‘replace the classical amplitudes by annihilation operators’. If the outgoing modes are still to be useful for the quantum theory, they have to satisfy the commutation relations:

$$[a_i(\text{out}), a_j^\dagger(\text{out})] = \delta_{ij}. \quad (3.3)$$

These conditions give constraints on the reflection and transmission amplitudes, for example $|t|^2 + |r'|^2 = 1$. Note that this is *not* identical to energy conservation for the incoming mode $a_1(\text{in})$ [that would read $|t|^2 + |r|^2 = 1$]. But

a sufficient condition is that the classical ‘reciprocity relation’ (*Umkehrung des Strahlengangs*) holds: $t = t'$.

We are now looking for a unitary operator S [the S-matrix] that implements this beamsplitter transformation in the following sense:

$$a'_i = S^\dagger a_i S, \quad i = 1, 2 \quad (3.4)$$

From this operator, we can also compute the transformation of the states: $|\text{out}\rangle = S|\text{in}\rangle$. Let us start from the general transformation

$$a_i \mapsto A_i = M_{ij} a_j \quad \text{or} \quad \vec{a} \mapsto \vec{A} = \mathbf{M} \vec{a} \quad (3.5)$$

where we have introduced matrix and vector notation. For the unitary transformation, we make the *Ansatz*

$$S(\theta) = \exp\left(i\theta B_{jk} a_j^\dagger a_k\right) \quad (3.6)$$

with B_{jk} a hermitean matrix (ensuring unitarity). The action of this unitary on the photon mode operators is now required to reduce to

$$a_i \mapsto A_i(\theta) \equiv S^\dagger(\theta) a_i S(\theta) \stackrel{!}{=} M_{ij} a_j. \quad (3.7)$$

We compute this ‘conjugated operator’ with a trick using a differential equation:

$$\frac{d}{d\theta} A_i(\theta) = -i B_{jk} S^\dagger(\theta) [a_j^\dagger a_k, a_i] S(\theta) \quad (3.8)$$

$$= -i B_{jk} S^\dagger(\theta) (-\delta_{ij} a_k) S(\theta) \quad (3.9)$$

$$= i B_{ik} A_k(\theta). \quad (3.10)$$

This is a system of linear differential equations with constant coefficients, so that we get as solution

$$\vec{A}(\theta) = \exp(i\theta \mathbf{B}) \vec{A}(0) = \exp(i\theta \mathbf{B}) \vec{a}. \quad (3.11)$$

We thus conclude that the matrix \mathbf{B} is fixed by

$$\mathbf{M} = \exp(i\theta \mathbf{B}). \quad (3.12)$$

If the transformation \mathbf{M} is part of a continuous group and depends on θ as a parameter, we can expand it around unity. Doing the same for the matrix exponential, we get

$$\mathbf{M} \approx \mathbb{1} + i\theta \mathbf{B} + \dots$$

Here, B is called the *generator* of the set of matrices $M = M(\theta)$. The unitary transformation is thus determined via the same generator B .

For the two-mode beam splitter, an admissible transformation is given by

$$M = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}. \quad (3.13)$$

Expanding for small θ , the generator is

$$B = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_2 \quad (3.14)$$

so that the corresponding unitary operator reads

$$S(\theta) = \exp \left[i\theta(-ia_1^\dagger a_2 + ia_2^\dagger a_1) \right] = \exp \left[\theta(a_1^\dagger a_2 - a_2^\dagger a_1) \right]. \quad (3.15)$$

Note that indeed, one has the identity

$$\exp(i\theta\sigma_2) = \cos \theta + i\sigma_2 \sin \theta = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad (3.16)$$

Example: splitting a single photon state

What is the state of the two-mode system if one photon is incident in mode 1 on the beam splitter? Initial state $|\text{in}\rangle = |1, 0\rangle = a_1^\dagger |\text{vac}\rangle$. The final state is then, using Eq.(3.15) for small θ

$$\begin{aligned} |\text{out}\rangle &= S|1, 0\rangle \approx |1, 0\rangle + \theta(a_1^\dagger a_2 - a_2^\dagger a_1)|1, 0\rangle \\ &= |1, 0\rangle - \theta|0, 1\rangle. \end{aligned} \quad (3.17)$$

For finite θ , the higher powers also contribute. The calculation gets easy with the beam splitter transformation of the creation operators.

$$\begin{aligned} |\text{out}\rangle &= Sa_1^\dagger |\text{vac}\rangle \\ &\stackrel{(1)}{=} Sa_1^\dagger S^\dagger |\text{vac}\rangle \\ &\stackrel{(2)}{=} (a_1^\dagger \cos \theta - a_2^\dagger \sin \theta) |\text{vac}\rangle \\ &= \cos \theta |1, 0\rangle - \sin \theta |0, 1\rangle \end{aligned} \quad (3.18)$$

In step (1), we have used that the unitary operator leaves the vacuum state unchanged. (This is because we have written the exponent in normal order.)

In step (2), we have used that S implements the transformation inverse to S^\dagger (unitarity). Re-introducing the transmission amplitudes, we find

$$|1, 0\rangle \mapsto t|1, 0\rangle + r|0, 1\rangle \quad (3.19)$$

so that the probability amplitudes to find the photon in either output mode correspond exactly, for this incident one-photon state, to the classical transmission and reflection amplitudes.

It is quite complicated to show in the same way the following property of a ‘bi-coherent state’

$$S|\alpha, \beta\rangle = |\alpha', \beta'\rangle, \quad \begin{pmatrix} \alpha' \\ \beta' \end{pmatrix} = M \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (3.20)$$

that remains bi-coherent after the beam splitter. But the proof is quite simple with the unitary transformation of the mode operators.

Example: splitting a two-photon state (Hong, Ou, Mandel)

Two-photon states do not behave as ‘intuitively’. Let us consider two single-photon states incident on the same beam splitter as before, $|\text{in}\rangle = |1, 1\rangle$. Then, by the same trick,

$$\begin{aligned} |\text{out}\rangle &= S|\text{in}\rangle = S a_1^\dagger S^\dagger S a_2^\dagger S^\dagger |0, 0\rangle \\ &= (a_1^\dagger \cos \theta - a_2^\dagger \sin \theta)(a_2^\dagger \cos \theta + a_1^\dagger \sin \theta) |\text{vac}\rangle \\ &= (|2, 0\rangle - |0, 2\rangle) \frac{\sin 2\theta}{2} + |1, 1\rangle \cos 2\theta \end{aligned} \quad (3.21)$$

Hence, for a 50/50 beam splitter ($\cos \theta = \sin \theta$ or $\theta = 45^\circ$), the last term cancels and the photons are transmitted in ‘bunches’: they come out together at either output port. There are zero ‘coincidences’ of one photon in port a_1' and the other in a_2' . This is due to a destructive interference between two indistinguishable histories for the two photons from source to detector – this is called the ‘Hong-Ou-Mandel dip’. The dip in the coincidence signal can be observed by tuning a parameter (like a delay time) that makes the two photons (in)distinguishable.

3.2.2 Homodyne detection

Introduce coherent state $|\beta\rangle$, simplest model for an intense laser beam.

Discuss output operators $a \pm \beta$ after a beam splitter: “mixing” of signal with “local oscillator” (= laser beam). The quadratures X_θ appear in the “beating” (interference) when a signal mode $a \mapsto a + \beta$ is mixed on a beam splitter with a large-amplitude coherent state $|\beta\rangle$ (“local oscillator”, “reference beam”). The quadrature phase can be chosen from the phase of β , in other words, the quadratures of a are measured relative to the phase of the local oscillator. (“Only relative phases are measurable.”)

Picture of quadratures in phase space plane for different states for signal mode a : vacuum state, number state, coherent state.

3.3 Quantum states of a single mode

In the WS 2013/14 lecture, this section was presented only as an overview.

3.3.1 How to identify a single mode

The quantized light field can be in different states. We start here with a single mode of the field. This may be a oversimplification, but single-mode fields have become part of the experimental reality with the advent of high-quality optical cavities. These devices give an electromagnetic field whose amplitude, in the region between two well-reflecting mirrors, is much higher at some resonant frequencies. The ‘mode function’ is in this case not a plane wave, of course, but a standing wave. In the transverse directions, one often has a gaussian profile. Around a cavity resonance, it is a frequent approximation to treat the full field as if it contained only a single mode. The coupling to other modes may be taken into account as a loss.

The electric field is given by

$$\mathbf{E}(\mathbf{x}, t) = E_1 \boldsymbol{\varepsilon} \left(a(t) + a^\dagger(t) \right) \sin kz \quad (3.22)$$

where z is the coordinate along the cavity axis and $k = n_z \pi / L$. The factor E_1 can be called the ‘electric field per photon’. From the multimode expansion, E_1 is given by the prefactor $E_k = (\hbar \omega_k / 2 \varepsilon_0 V)^{1/2}$. The corresponding ‘intensity’ is

$$I_{1\text{ph}} = \varepsilon_0 c E_k^2 = \frac{\hbar \omega_k c}{2V}. \quad (3.23)$$

In a cavity, we can take for V the volume ‘filled’ by the mode. For a transverse mode size of 1 micrometer and a cavity length of 1 cm, we get $I_{1\text{ph}} \sim 10^3 \text{ mW/cm}^2$ which is not really small. The total power, however, is quite small:

about 10^{-8} W. Note also that these numbers are based on very ‘tight’ (diffraction-limited) focussing — beams with larger cross-section have a smaller ‘field per photon’.

In the Heisenberg picture, the field operator evolves as

$$\mathbf{E}(\mathbf{x}, t) = E_1 \boldsymbol{\varepsilon} \left(a e^{-i\omega t} + a^\dagger e^{i\omega t} \right) \sin kz \quad (3.24)$$

A combination of annihilation and creation operators like the one in parentheses is called a ‘quadrature’. Quadratures always come in pairs. One can find a second quadrature variable by shifting the origin of time by one quarter period: $\propto -i a e^{-i\omega t} + i a^\dagger e^{i\omega t}$. This corresponds to the magnetic field [compare eqs. (2.119) and (2.120)]. In analogy to the harmonic oscillator, one often uses the following quadrature variables

$$X = \frac{a + a^\dagger}{\sqrt{2}} \quad P = \frac{a - a^\dagger}{\sqrt{2}i} \quad (3.25)$$

or more generally

$$X_\theta = \frac{a e^{-i\theta} + a^\dagger e^{i\theta}}{\sqrt{2}} \quad (3.26)$$

with $X_0 = X$ and $X_{\pi/2} = P$.

The ground state of the field mode is called the ‘vacuum’ (no photon, i.e., no excitation present). It is found by looking for the state that is annihilated by the annihilation operator: $a|\text{vac}\rangle = 0$. Obviously, this is also an eigenstate of the photon number operator with zero photons: $|\text{vac}\rangle = |0\rangle$. In the vacuum state, the electric field is also zero on average, of course.

But there are fluctuations around this average, called ‘quantum noise’. In the vacuum state of the single mode (3.22), e.g., we get

$$\langle \mathbf{E}(\mathbf{x}, t)^2 \rangle_0 = E_1^2 \sin^2 kz \langle 0 | \left(a(t) + a^\dagger(t) \right) \left(a(t) + a^\dagger(t) \right) | 0 \rangle \quad (3.27)$$

and this combination of operators gives an average

$$\langle 0 | \left(a(t) + a^\dagger(t) \right) \left(a(t) + a^\dagger(t) \right) | 0 \rangle = \langle 0 | a(t) a^\dagger(t) | 0 \rangle = 1 \quad (3.28)$$

The ‘vacuum noise’ in our mode is thus given by the squared single photon field $E_1^2 \sin^2 kz$. Similarly, the other quadrature variable $a(t) - a^\dagger(t)$ shows a noise strength of unity. This is in accordance with Heisenberg’s indeterminacy relation, since

$$\left[a(t) + a^\dagger(t), a(t) - a^\dagger(t) \right] = -2. \quad (3.29)$$

name	person	notation	eigenstate of	$\langle \hat{n} \rangle$	preparation
number	Fock	$ n\rangle$	$\hat{n} = \hat{a}^\dagger \hat{a}$	n	micromaser (difficult!)
thermal	Boltzmann	ρ_T	?	$\bar{n}(T)$ (BE)	contact with thermal bath
coherent	Glauber	$ \alpha\rangle = \hat{D}(\alpha) 0\rangle$	$\hat{a} \alpha\rangle = \alpha \alpha\rangle$	$ \alpha ^2$	classical source
squeezed	?	$ \xi\rangle = \hat{S}(\xi) 0\rangle$	$(\mu a - \nu a^\dagger) \xi\rangle = 0$	$ \nu ^2$	non-linear medium, parametric resonance

Table 3.1: Quantum states of a single mode (annihilation operator a). The operator $\hat{D}(\alpha) = \exp(\alpha a^\dagger - \alpha^* a)$ is called displacement operator. Similarly, $\hat{S}(\xi) = \exp(\xi a^{\dagger 2} - \xi^* a^2)$ for the squeezing operator. Parametrization $\xi = (r/2)e^{i\phi}$ with $\mu = \cosh r$, $\nu = e^{i\phi} \sinh r$. (Check factor 1/2.)

Overview

An overview on the “typical” quantum states that appear in the quantum optics context is given in Table 3.1. Note that these states apply to any physical system described by a harmonic oscillator, this is a larger class than just modes of the electromagnetic field.

3.3.2 Number (Fock) states

The simplest quantum states of the single mode field are given by the well-known stationary states of the harmonic oscillator. These quantum states are called ‘Fock states’ or ‘number states’ $|n\rangle$. They are eigenstates of the ‘photon number operator’

$$\hat{n} = a^\dagger a = aa^\dagger - 1 \quad (3.30)$$

and are generated by applying the creation operator to the ground state of the oscillator:

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle \quad (3.31)$$

The expectation value of the annihilation operator is zero in a number state:

$$\langle a \rangle_n = \langle n|a|n\rangle = \sqrt{n} \langle n|n-1\rangle = 0 \quad (3.32)$$

The same is true for the creation operator. It follows that the electric field average vanishes not only in the vacuum state, but in any Fock state:

$$\langle n|\mathbf{E}(\mathbf{x}, t)|n\rangle = 0 \quad (3.33)$$

In the exercises, you are asked to compute the variances of the quadrature operators X_θ in an arbitrary number state $|n\rangle$.

The quantum numbers n give an intuitive interpretation to the creation and annihilation operators: they connect states whose photon numbers differ by one. In this sense, the ‘creation operator’ a^\dagger creates one photon since for example

$$\langle 1|a^\dagger|0\rangle = 1. \quad (3.34)$$

This matrix element plays an important role when one computed the probability amplitude that an excited atomic state emits a photon. For stimulated emission, one needs $\langle n+1|a^\dagger|n\rangle = \sqrt{n+1}$. Similarly, the ‘annihilator’ a destroys one photon:

$$\langle 0|a|1\rangle = 1. \quad (3.35)$$

This matrix element is needed to compute absorption, and in the general case, $\langle n-1|a|n\rangle = \sqrt{n}$.

- Experimentally, Fock (number) states are the most difficult to prepare. One has to avoid the loss of photons that makes the photon number uncertain. In addition, the preparation has to target precisely the photon number. One possible scheme works with a variant of the Jaynes-Cummings-Paul model: an excited two-level atom interacts with the single-mode cavity over a precisely tuned interaction time τ such that $g\sqrt{n+1}\tau$ is a multiple of 2π . According to Eq.(??), the atom then performs a full Rabi cycle and ends again in the excited state. If the other conditions are well-chosen, the state $|n\rangle$ of the cavity can be a stable equilibrium state for this pumped system. Of course, one has to inject atoms regularly to compensate for the loss.

3.3.3 Thermal states

This class of field states is more general than the ‘pure’ states described before. Strictly speaking, they are not “states”, but density operators. The thermal state is the first example where one has to use both classical and quantum statistics, and this is achieved with the concept of *density operator* that combines the two.

Density operators

A *density operator* is a hermitean operator $\hat{\rho}$ on the Hilbert space \mathcal{H} of the quantum system under consideration, with the properties

- ρ is positive, i.e., $\langle \psi | \hat{\rho} | \psi \rangle \geq 0$ for all $\psi \in \mathcal{H}$
- ρ is a trace class operator, i.e., $\text{tr } \hat{\rho} = \sum_n \langle n | \hat{\rho} | n \rangle = 1$ where the vectors $|n\rangle$ form a basis of \mathcal{H} .

It is easy to see the inequality $0 \leq \langle \psi | \hat{\rho} | \psi \rangle \leq 1$ for a normalized state vector. Physically, this means that this the real number can be interpreted as a probability: it is the probability to find the system in the state $|\psi\rangle$ when performing a measurement.

The expectation value of an operator A is now given by the rule

$$\langle A \rangle_{\hat{\rho}} = \text{tr}(A\hat{\rho}) = \text{tr}(\hat{\rho}A) \quad (3.36)$$

where the order under the trace can be changed because of cyclic permutations.

In a sense, thermal quantum states are a natural generalization of classical thermodynamics to the quantum world. One uses stationary states, hence the number states we found first, and imposes Boltzmann statistics to describe the field at thermal equilibrium.

For the single field mode we are discussing here, stationary states are the number states $|n\rangle$; they occur with a classical probability proportional to the Boltzmann factor $e^{-n\hbar\omega/k_B T}$. The density operator is given by

$$\hat{\rho} = \frac{1}{Z} \exp[-\hbar\omega\hat{n}/k_B T] = \frac{1}{Z} \sum_{n=0}^{\infty} e^{-n\hbar\omega/k_B T} |n\rangle\langle n| \quad (3.37)$$

The normalization factor Z is found by requiring that the trace of this operator be unity:

$$Z = \text{tr} \left(\sum_{n=0}^{\infty} e^{-n\hbar\omega/k_B T} |n\rangle\langle n| \right) = \sum_{n=0}^{\infty} e^{-n\hbar\omega/k_B T} = \frac{1}{1 - e^{-\hbar\omega/k_B T}}, \quad (3.38)$$

where a geometric series has been summed. You know this sum from classical thermodynamics as ‘partition function’ (*Zustandssumme*). The normalized probabilities

$$p_n(T) = (1 - e^{-\hbar\omega/k_B T}) e^{-n\hbar\omega/k_B T} \quad (3.39)$$

are simply the classical probability that the stationary state $|n\rangle$ is realized in the canonical ensemble.

We note that the terms $|n\rangle\langle n|$ in the sum (3.37) are also density operators: they are obviously positive and have trace unity. (In fact, the trace boils down to the norm squared of the state $|n\rangle$.) The thermal density operator is thus a

probability-weighted, convex sum of density operators.¹ This convex summation is, in general, an allowed linear operation on the space of density operators.

The density operators $|n\rangle\langle n|$ are special because they are made up of a single state. These quantum states are called *pure*. A formal definition:

- A density operator $\hat{\rho}$ describes a *pure state* if $\hat{\rho}^2 = \hat{\rho}$.

In mathematics, operators with this property are called *projectors*. This is also what is suggested by the Dirac notation $|\psi\rangle\langle\psi|$: this operator acts on the Hilbert space by first projecting onto the state $|\psi\rangle$ and then gives back a vector proportional to $|\psi\rangle$, just what happens in geometry for the projection onto a vector.

Purity

States that are not pure are called ‘mixed’. This can be made more quantitative:

- The *purity* of a density operator $\hat{\rho}$ is defined by

$$\text{Pu}(\hat{\rho}) = \text{tr}(\hat{\rho}^2 - \hat{\rho}) + 1 = \text{tr} \hat{\rho}^2 \quad (3.40)$$

where the two definitions are equal if $\hat{\rho}$ is trace-normalized.

The purity is normalized such that for pure states, $\text{Pu}(\hat{\rho}) = 1$. It is easy to see that the first term in (3.40), $\text{tr}(\hat{\rho}^2 - \hat{\rho})$ is negative for mixed states. One can also show that all states with $\text{Pu}(\hat{\rho}) = 1$ are necessarily pure.

To show these properties, evaluate the trace of $\hat{\rho}^2$ in the eigenbasis of $\hat{\rho}$. All eigenvalues are in the interval $[0, 1]$.

A thermal field mode

At optical frequencies and room temperature, the Boltzmann factor $\exp(-n\hbar\omega/k_B T)$ has a large negative argument for $n \geq 1$ so that the field is essentially at zero temperature. This is different for microwave radiation, e.g., or for star atmospheres.

Simple exercise: mean photon number. Let us apply the general rule (3.36):

$$\langle \hat{n} \rangle_T = \text{tr}(\hat{n}\hat{\rho}_T) = \frac{1}{Z} \sum_{n=0}^{\infty} \langle n | \hat{n} \exp(-\hbar\omega\hat{n}/k_B T) | n \rangle \quad (3.41)$$

¹One talks about a *convex sum* if all coefficients are real numbers between zero and one.

The number operators and the Boltzmann ‘operator’ act on their eigenvectors, hence

$$\langle \hat{n} \rangle_T = \frac{1}{Z} \sum_{n=0}^{\infty} n \exp(-\hbar\omega n/k_B T) = \frac{1}{e^{\hbar\omega/k_B T} - 1}. \quad (3.42)$$

Exercise: photon number variance. Result:

$$(\Delta n)_T^2 = \frac{e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T} - 1)^2} = \frac{1}{4 \sinh^2(\hbar\omega/2k_B T)}. \quad (3.43)$$

Exercise: discuss the purity $\text{Pu}(T) = \text{Pu}(\hat{\rho}_T)$. It is a function that goes to zero linearly when $\omega/T \rightarrow 0$ (‘hot’ or ‘classical’ limit) and reaches asymptotically unity for $\omega/T \rightarrow \infty$ (‘cold’ or ‘quantum’ limit).

Electric field fluctuations in a single mode at finite temperature:

$$\langle \mathbf{E}^2(\mathbf{x}, t) \rangle_T = E_1^2 \sin^2 kz \langle a(t)a^\dagger(t) + a^\dagger(t)a(t) \rangle_T = E_1^2 \sin^2 kz (2\langle \hat{n} \rangle_T + 1) \quad (3.44)$$

they are enhanced by a factor $2\langle \hat{n} \rangle_T + 1 = \coth(\hbar\omega/2k_B T)$ compared to zero temperature.

Three remarks on the advantages of the density operator formalism:

- the traces that are required for expectation values can be taken in any basis. One can choose a basis adapted to the operator whose average one is interested in.
- Second, the presence of the density operator $\hat{\rho}$ under the trace ensures that the trace exists even if the operator A has ‘large matrix elements’ (like the photon number operator). Well, this is in fact just a restriction on the observables and states that are mathematically allowed. Thermal states have the advantage that the expectation values exist for a broad class of observables because the matrix elements of the density operator become rapidly small for large n .
- The third advantage of using a density operator approach is that it gives a suitable description of a quantum system whose dynamics is not completely known and can only be specified by probabilities. In that case, one formulates an equation of motion for the density matrix from the solution of which the averages of all interesting quantities can be calculated.

Preparation of a thermal state with rate equations

As an example of the last remark, we sketch here a ‘preparation scheme’ for a thermal state. We are going to use ‘rate equations’: differential equations for the diagonal elements $p_n(t) = \langle n | \hat{\rho}(t) | n \rangle$:

$$\frac{dp_n}{dt} = -\kappa n p_n + \kappa' n p_{n-1} - \kappa' (n+1) p_n + \kappa (n+1) p_{n+1} \quad (3.45)$$

The constants κ and κ' can be interpreted as transition rates between states: the transition $|n\rangle \rightarrow |n-1\rangle$ happens with the rate κn (this rate appears as a negative term in \dot{p}_n and as a positive term in \dot{p}_{n-1}). This process can be interpreted physically as the loss of one of the n photons. This photon goes into a ‘thermostat’ or ‘environment’ and is absorbed there. Similarly, the system described by $\hat{\rho}$ can absorb one photon from the thermostat – this happens with a ‘Bose stimulation factor’ because for the transition $|n-1\rangle \rightarrow |n\rangle$, the rate is $\kappa' n$. (To be read off from the second and third terms in Eq.(3.45).) Even the vacuum state can absorb a photon, hence not $n-1$, but n appears here.

If one waits long enough, the density matrix (more precisely, its diagonal elements) relaxes into a steady state given by the equations of ‘detailed balance’

$$0 = -\kappa n p_n^{(ss)} + \kappa' n p_{n-1}^{(ss)} \quad (3.46)$$

This equation implies that $\dot{p}_n = 0$ in Eq.(3.45), but is slightly stronger. (One can probably show it by induction, starting from $n = 0$.) Eq.(3.46) gives a recurrence relation that links $p_n^{(ss)}$ to $p_{n-1}^{(ss)}$, whose solution is

$$p_n^{(ss)} \sim \left(\frac{\kappa'}{\kappa} \right)^n =: e^{-n\hbar\omega/k_B T} \quad (3.47)$$

where we can identify the temperature T from the ratio of the rate constants κ'/κ . (One needs $\kappa' < \kappa$, otherwise, no stable equilibrium state is found.) Of course, this definition of temperature is linked to assigning an energy $n\hbar\omega$ to the state $|n\rangle$.

3.3.4 Coherent states

Definition and properties

The coherent state $|\alpha\rangle$ is an eigenstate of the annihilation operator:

$$a|\alpha\rangle = \alpha|\alpha\rangle \quad (3.48)$$

Since a is not an hermitean operator, α can be complex. In a coherent state, the average electric field is nonzero:

$$\langle \mathbf{E}(\mathbf{x}, t) \rangle_\alpha = E_1 \sin kz \langle \alpha | (a(t) + a^\dagger(t)) | \alpha \rangle = E_1 \sin kz (\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}). \quad (3.49)$$

We have assumed the field in a coherent state of the initial annihilator a . This expression is the same that we have used in chapter 1 for a classical, monochromatic field. The magnetic field quadrature also has on average its classical value in a coherent state. Coherent states are thus very useful to represent laser fields. We see that α measures the electric field strength in units of the ‘single photon field’ E_1 . If we compute the average photon number in a coherent state, we get

$$\langle \hat{n} \rangle_\alpha = \langle a | a^\dagger a | \alpha \rangle = |\alpha|^2, \quad (3.50)$$

so that as an order of magnitude $\langle E \rangle \approx E_1 \langle \hat{n} \rangle^{1/2}$ (note the nonlinear dependence).

Coherent states are not stationary, but rotate in the complex α -plane: if $|\psi(0)\rangle = |\alpha\rangle$, then $|\psi(t)\rangle = |\alpha e^{-i\omega t}\rangle$. This can be shown using the expansion of a coherent state in terms of number states:

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (3.51)$$

Note that number states with arbitrarily high photon numbers are present in a coherent state. More specifically, we can introduce the probability $p_n(\alpha)$ of finding n photons in a coherent state:

$$p_n(\alpha) = |\langle n | \alpha \rangle|^2 = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!} \quad (3.52)$$

which is a ‘Poisson distribution’ (the probability distribution of the sum of independent random bits). In the exercises, you are asked to compute the average photon number and its fluctuations (variance) in a coherent state.

The field quadratures also show quantum fluctuations around their classical average in a coherent state. This is inevitable because of the Heisenberg inequality. In the exercises, you are asked to show that these are equal to the quantum noise in the vacuum state (which is in fact a particular coherent state with $\alpha = 0$). This result can be displayed graphically in the complex α -plane by the sketch shown in fig. 3.2. We shall see that this plot gives the so-called Q-function (or Husimi function) of the state, see Eq.(3.99) below. This function provides a way to illustrate a quantum state by the analogy to the classical

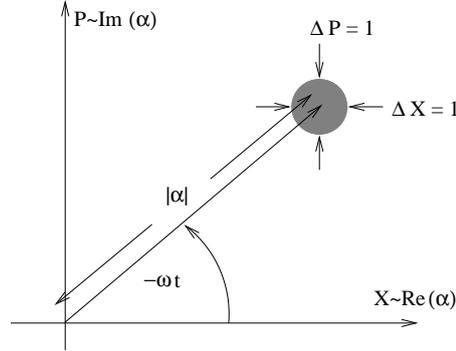


Figure 3.2: Representation of a coherent state in phase space.

phase space. Note that since $a = (X + iP)/\sqrt{2}$, we may identify the α -plane with the classical phase space of a harmonic oscillator. The gray area in this sketch indicates values for the position and momentum quadratures that are probable outcomes of measurements. This representation is of course schematic since X and P cannot be measured simultaneously. We shall give it a precise meaning in section 3.5 where we show how coherent states can be used to expand any field state. (There are some subtleties related to the fact that they are not eigenstates of an hermitean operator.)

Finally, coherent states are not orthogonal. This is again a consequence of being the eigenstate of a non-hermitean operator. Let us calculate the overlap

$$\begin{aligned}
 \langle \alpha | \beta \rangle &= \sum_n e^{-|\alpha|^2/2 - |\beta|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^{*n} \beta^n}{n!} \\
 &= \exp \left[-\frac{1}{2} \left(|\alpha|^2 + |\beta|^2 - \alpha^* \beta - \alpha \beta^* - \alpha^* \beta + \alpha \beta^* \right) \right] \\
 &= \exp \left[-\frac{1}{2} |\alpha - \beta|^2 + i \operatorname{Im} \alpha^* \beta \right] \tag{3.53}
 \end{aligned}$$

Here, we have split the complex overlap into its magnitude: a Gaussian with maximum at $\beta = \alpha$ and a phase factor. If we consider the Gaussian as a function of α , we get a peaked function in the phase space plane, with a typical width (the same in all directions) of the order of $\frac{1}{2}$ or 1.

Coherent states can be prepared by feeding the field mode with a “classical source”. This could be a classical oscillating dipole, as it happens in a so-called “free electron laser”. Or the field of a intense laser which is often approximated by a classical field. More details including the calculation of the time evolution operator for a classical source follow now.

Preparation: displacement operator

How is it possible to generate a coherent state physically? One possible answer is ‘never’ because to this end, one must be able to control the phase of the complex number α , or equivalently, the origin of time (recall the discussion before Eq.(3.51)). In practice, however, it is at least useful, if not necessary, to think ‘as if’ the phase of a light field were controlled, for example in a laser field. For an instructive discussion, see two papers by Klaus Mølmer (1997) where he talks about a ‘convenient fiction’. A physical example where it is plausible that the phase of a light field can be controlled is the ‘free electron laser’ where a beam of electrons is modulated in a controlled way (in a ‘wiggler’ element of an accelerator ring). The accelerated electrons are emitting photons that are injected into a laser cavity.

This example comes close to the following single-mode Hamiltonian

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) + i\hbar \left(e^{-i\omega_s t} g a^\dagger - e^{i\omega_s t} g^* a \right) \quad (3.54)$$

where the first term is the energy of our mode and the second term describes

- the coupling of a classical dipole oscillator at frequency ω_s with the field mode (in the electric-dipole interaction, replace the dipole operators σ_\pm by c-numbers),
- or the coupling of a classical current density $\mathbf{j}(x, t)$ with the vector potential of the mode (via the minimal coupling interaction).

We are going to see that *classical sources generate coherent states*.

In the interaction representation, the first term of the Hamiltonian (3.54) is transformed away and the exponentials are replaced by $e^{\pm i(\omega - \omega_s)t}$. If we choose resonant conditions, $\omega_s = \omega$, we thus get a Schrödinger equation with a time-independent Hamiltonian. The solution is easy (still in the interaction picture)

$$|\tilde{\psi}(t)\rangle = \exp[t(ga^\dagger - g^*a)]|\tilde{\psi}(0)\rangle = \hat{D}(gt)|\tilde{\psi}(0)\rangle \quad (3.55)$$

where $\hat{D}(\alpha)$ is the so-called *displacement operator*

$$\hat{D}(\alpha) = \exp(\alpha a^\dagger - \alpha^* a) \quad (3.56)$$

Let us assume that the mode starts in the vacuum state, we thus find using the Baker-Campbell-Hausdorff identity²

$$|\psi(t)\rangle = \exp[t(ga^\dagger - g^*a)]|0\rangle = e^{-|g|^2 t^2/2} e^{gt a^\dagger} e^{-g^* t a}|0\rangle \quad (3.57)$$

² If the commutator $[A, B]$ commutes with A and B : $e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$.

Now the annihilation operator gives 0 when acting on the vacuum state, so that its exponential reduces to unity here. Expanding the exponential with the creation operator in a power series, we find

$$|\psi(t)\rangle = e^{-g^2 t^2/2} \sum_{n=0}^{\infty} \frac{(gt a^\dagger)^n}{n!} |0\rangle = |gt\rangle \quad (3.58)$$

This interaction thus generates a coherent state with amplitude $\alpha = gt$ that grows linearly in time. To obtain a stationary result, either the ‘oscillator amplitude’ g can be made time-dependent, or loss processes have to be added.

We have just shown that coherent states can be obtained by applying a ‘displacement operator’ to the vacuum state:

$$|\alpha\rangle = D(\alpha)|0\rangle \quad D(\alpha) = \exp\{\alpha a^\dagger - \alpha^* a\} \quad (3.59)$$

This unitary operator also displaces the creation and annihilation operators as follows (to prove by deriving a differential equation in the ‘Heisenberg picture’, setting $\alpha = gt$)

$$D^\dagger(\alpha) a D(\alpha) = a + \alpha \quad (3.60)$$

$$D^\dagger(\alpha) a^\dagger D(\alpha) = a^\dagger + \alpha^*. \quad (3.61)$$

This identity is useful to show that the field quadrature fluctuations in a coherent state are those of the vacuum state.

The displacement operators provide a mapping from the complex numbers into unitary operators on the single-mode Hilbert space. Complex numbers can be added, and operators be applied sequentially. So how do the two operations compare? The answer lies in the equation

$$D(\alpha)D(\beta) = e^{i\text{Im}(\alpha\beta^*)} D(\alpha + \beta) \quad (3.62)$$

that can be easily proven with the Baker-Campbell-Hausdorff formula (footnote 2). If the phase factor were not there, this equation would make the mapping $\alpha \mapsto \hat{D}(\alpha)$ a *representation* (*Darstellung*) of the additive group in \mathbb{C} in the space of unitary operators $\mathcal{U}(\mathcal{H})$ over the (infinite-dimensional) Hilbert space \mathcal{H} of the single mode: either one applies the displacement operators one after the other (left-hand side) or one adds the complex numbers and applies a single displacement (right-hand side), one gets the same result.

Now, there is a phase factor, involving $\text{Im}(\alpha\beta^*)$. The mapping $\alpha \mapsto \hat{D}(\alpha)$ is then not a (‘proper’) representation, but only a *projective representation*. This

must be so because the additive group in \mathbb{C} is finite-dimensional and commutative, while the unitary operators $D(\alpha)$ form a non-commutative and infinite-dimensional group. And more precisely, the *generators* of the two groups do not have the same algebra (a Lie algebra formed by their commutators). For the additive group and its action on \mathbb{C} itself, the generators can be taken as unit vectors parallel to the x and p axes. The addition of these vectors is, of course, commutative. For the ‘image’ formed by the $D(\alpha)$, acting on the Hilbert space of state vectors, the corresponding generators are (expand for small $\alpha = x + ip$ with real parameters x and p)

$$D(\alpha) \approx \mathbb{1} + x(a^\dagger - a) + ip(a^\dagger + a) \quad (3.63)$$

so we identify the generators $(a^\dagger - a)/i$ and $(a^\dagger + a)$ whose commutator is twice $i\mathbb{1}$. (One likes to choose hermitean generators, this explains the factors i . The commutator is hermitean after multiplication with i as well.) This means that the group structure is fundamentally different: the algebra spanned by the generators does not close, and a proper representation is not possible. In fact, the additional phase factor that appears in the formula for the projective representation can be understood by enlarging the Lie algebra (and the group) to include also the unit operator.

To conclude, the phase factor appearing in Eq.(3.62) could be argued to have no physical significance: after all, changing a state vector by a (‘global’) phase does not change the quantum-mechanical predictions. But if a superposition can be constructed where the phase appears only in one term, then the phase becomes observable. A typical example is the ‘geometric Berry phase’. We are not aware whether there is a link between this concept and the projective phase for the displacement operators.

3.3.5 Squeezed states

You should have got the feeling up to now that the quantized field essentially differs from a classical field by its (‘quantum’) fluctuations. So people have thought whether it is possible to reduce the quantum noise in a field quadrature to get something even ‘more classical’ – or having less noise. This can be achieved in part, to 50%, say. Of course, one cannot beat the Heisenberg inequality, and the reduced fluctuations in one quadrature have to be paid by enhanced noise in the other one.

Let us consider the following unitary operator

$$S(\xi) = \exp(\xi a^{\dagger 2} - \xi^* a^2) \quad (3.64)$$

Its action on the operators a and a^\dagger is the following linear transformation (also called Bogoliubov or squeezing transformation)

$$\begin{aligned} a &\mapsto S(\xi) a S^\dagger(\xi) = \mu a - \nu a^\dagger \\ a^\dagger &\mapsto S(\xi) a^\dagger S^\dagger(\xi) = \mu a^\dagger - \nu^* a \end{aligned} \quad (3.65)$$

where the squeezing parameters are

$$\mu = \cosh(2|\xi|), \quad \nu = e^{i\phi} \sinh(2|\xi|), \quad \phi = \arg(\xi) \quad (3.66)$$

To prove Eq.(3.65), one makes the replacement $\xi \mapsto \xi t$ and derives a differential equation with respect to the parameter t . (Mathematically: one studies the one-parameter family of squeezing operators $S(\xi t)$, a subgroup in the group of unitary transformations.)

The squeezed state $|\xi\rangle$ is now defined as the ‘vacuum state’ with respect to the transformed annihilation operator:

$$0 = S(\xi) a S^\dagger(\xi) |\xi\rangle = (\mu a - \nu a^\dagger) |\xi\rangle \quad (3.67)$$

This equation combined with the assumption that the vacuum state defined by $a|\text{vac}\rangle = 0$ is unique, gives $|\text{vac}\rangle = S^\dagger(\xi) |\xi\rangle$ after fixing a phase reference and therefore

$$|\xi\rangle = S(\xi) |\text{vac}\rangle \quad (3.68)$$

because S^\dagger is inverse to the unitary operator S . We thus get the squeezed state by applying the squeezing operator to the vacuum state.

One can also discuss more general cases, for example a squeezed coherent state $|\xi, \alpha\rangle = S(\xi) |\alpha\rangle = S(\xi) D(\alpha) |\text{vac}\rangle$. See the book by Vogel & al. (2001) for more details.

The squeezed state has a mean photon number

$$\langle \xi | a^\dagger a | \xi \rangle = \langle \text{vac} | S^\dagger(\xi) a^\dagger a S(\xi) | \text{vac} \rangle = \dots = |\nu|^2 \quad (3.69)$$

as can be shown by applying the transformation inverse to Eq.(3.65) (replace ξ by $-\xi$).

The photon number distribution reveals more interesting features. Consider first the case of a small squeezing parameter ξ . The expansion of Eq.(3.68) yields

$$|\xi\rangle = (\mathbb{1} + \xi a^{\dagger 2} - \xi^* a^2 + \dots) |\text{vac}\rangle = |\text{vac}\rangle + \sqrt{2} \xi |2\rangle + \dots \quad (3.70)$$

so that in addition to the ordinary vacuum, a state with a photon pair appears. This is a general feature: the squeezed (vacuum) state $|\xi\rangle$ contains pairs of photons, $|2\rangle$, $|4\rangle$, \dots . We shall see below that this can be interpreted as the result of a nonlinear process where a “pump photon” (of blue color, say) is “down-converted” into a pair of red photons. The unusual feature of this “photon pair state” is that the pair appears in a superposition with the vacuum state, with a relative phase fixed by the complex squeezing parameter ξ .

The expansion of the ‘squeezed vacuum’ $S(\xi)|0\rangle$ in the Fock (number state) basis gives for even photon numbers the amplitudes

$$c_{2m} = \frac{(2m-1)!!}{\sqrt{(2m)!}} e^{im\phi} \frac{\tanh^m(2|\xi|)}{\cosh^{1/2}(2|\xi|)}$$

where ϕ is again the phase of ξ , and $n!!$ is the product $n(n-2)\dots$ of all positive numbers with the same parity up to n .

The mean value of the complex field amplitude is zero in the squeezed state, as a calculation similar to Eq.(3.69) easily shows: $\langle \xi|a|\xi\rangle = 0$. In the phase-space plane introduced in Fig. 3.2, the squeezed state $|\xi\rangle$ would therefore be represented by a “blob” centered at zero.

The “squeezing” becomes apparent if one asks for the quantum fluctuations around the mean value. Let us introduce the general quadrature operator

$$X_\theta = \frac{a e^{-i\theta} + a^\dagger e^{i\theta}}{\sqrt{2}} \quad (3.71)$$

The familiar position and momentum quadratures X , P correspond to phases $\theta = 0, \pi/2$. But more generally, two ‘orthogonal’ quadratures are given by X_θ and $X_{\theta+\pi/2}$. The squeezed state now has fluctuations around the vacuum state such that *one quadrature component has quantum noise below the Heisenberg limit* $1/2$. A straightforward calculation gives the following quadrature uncertainty

$$\langle \xi|\Delta X_\theta^2|\xi\rangle = \frac{|\mu + \nu e^{-2i\theta}|^2}{2} \quad (3.72)$$

If we take $2\theta = \phi$ (the phase of the squeezing parameter), we have $\mu + \nu e^{-2i\theta} = \cosh(2|\xi|) + \sinh(2|\xi|) = e^{+2|\xi|}$ which becomes exponentially large as the magnitude of ξ increases. For the orthogonal quadrature, one finds an exponential reduction of the fluctuations:

$$\Delta X_{\phi/2}^2 = \frac{e^{+2|\xi|}}{2}, \quad \Delta X_{(\phi+\pi)/2}^2 = \frac{e^{-2|\xi|}}{2}. \quad (3.73)$$

This is the hallmark of a squeezed state. Note that the uncertainty product is unchanged: this could have been expected as $|\xi\rangle$ remains a pure state.

A graphical representation is shown in Fig. 3.3 where the squeezed state is the ellipse around the origin. As discussed for Fig. 3.2, this picture can be made more quantitative by calculating certain phase-space distribution functions for the different states discussed so far. This topic will be discussed in detail in part II of the lecture, the main results appear in Sec. 3.5 below.

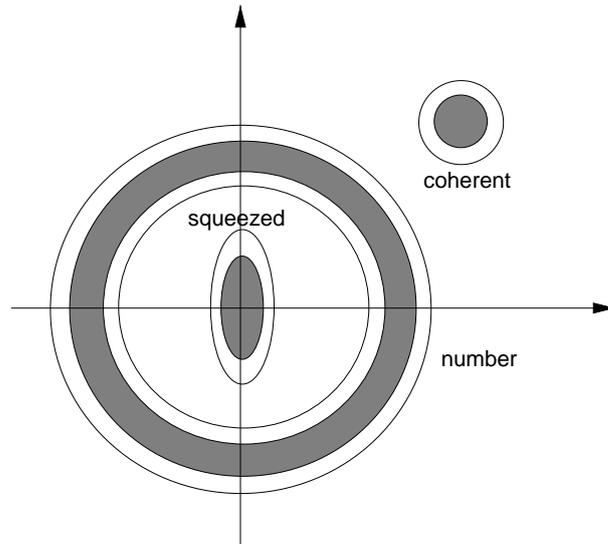


Figure 3.3: Quantum states of the radiation field, schematically represented in the phase space plane.

Preparation of a squeezed state

How can one prepare a squeezed state? The “cheating way of it” is just a re-scaling of the position and momentum quadratures:

$$X' = \eta X, \quad P' = \eta^{-1} P \quad (3.74)$$

This generates operators X' and P' that obey the same commutation relations. However, the energy of the field mode will not be proportional to $a'^{\dagger} a' \sim X'^2 + P'^2$, but involve terms of the form $(a')^2$ and $(a'^{\dagger})^2$. So the “ground state” $|\psi\rangle$ defined by $a'|\psi\rangle = 0$ will not be a stationary state of this Hamiltonian. This example illustrates, however, that (i) squeezed states evolve in time and are not stationary and (ii) that the quadratic terms $(a')^2$ and $(a'^{\dagger})^2$ play a key role.

The second way is to find a way to add these terms to the Hamiltonian. This can be done with a nonlinear medium. The ‘squeezing’ operator (3.64) can be realized with the interaction Hamiltonian

$$H_{\text{int}} = i\hbar \left(g e^{-2i\omega t} a^{\dagger 2} - g^* e^{2i\omega t} a^2 \right) \quad (3.75)$$

with the squeezing parameter given by $\xi = \int dt g(t)$. This interaction occurs in nonlinear optics. To get a qualitative understanding, imagine a medium with a field-dependent dielectric constant (‘ $\chi^{(2)}$ nonlinearity’). This is usually forbidden for symmetry reasons, but it happens in some special cases. In the electromagnetic energy density, one has

$$u = \frac{\varepsilon(|\mathbf{E}|)}{2} \mathbf{E}^2 + \frac{1}{2\mu_0} \mathbf{B}^2 \quad (3.76)$$

where the linearization

$$\varepsilon(|\mathbf{E}|) = \varepsilon_0 (1 + n_2 |\mathbf{E}|^2) \approx \varepsilon_0 (1 + 2n_2 |\mathbf{E}|^2)$$

is often appropriate. In the quantum picture, this gives a contribution to the Hamiltonian with a term of third order in the field:

$$H_3 = \varepsilon_0 n_2 \int_V d^3x |\mathbf{E}(\mathbf{x}, t)|^3 \quad (3.77)$$

Let us now pick out two spatial modes of the field and put one of it into a coherent state $|\alpha e^{-i\omega_p t}\rangle$ with a ‘large’ amplitude $|\alpha| \gg 1$. The index ‘p’ is for ‘pump field’. Let us call the other mode (the ‘quantum’ one) the ‘signal’. The electric field is then

$$\mathbf{E}(\mathbf{x}, t) = E_p a_p \boldsymbol{\varepsilon}_p e^{-i(\omega_p t - \mathbf{k}_p \cdot \mathbf{x})} + E_1 \boldsymbol{\varepsilon}_1 a(t) e^{i\mathbf{k} \cdot \mathbf{x}} + \text{h.c.} \quad (3.78)$$

The interaction Hamiltonian thus generates cross terms of the form³

$$H_{\text{int}} = \dots + \hbar \left(g e^{-i\omega_p t} a_p a^{\dagger 2} + g^* e^{i\omega_p t} a_p^\dagger a^2 \right) \quad (3.79)$$

$$\hbar g = 3\varepsilon_0 n_2 E_p E_1 \boldsymbol{\varepsilon}_p \cdot \boldsymbol{\varepsilon}^* \int_V d^3x e^{i(\mathbf{k}_p - 2\mathbf{k}) \cdot \mathbf{x}} \quad (3.80)$$

One often ignores the quantum fluctuations of the pump mode and replaces its annihilation operator a_p by the coherent state amplitude α . The interaction (3.79) then looks quite like our model Hamiltonian (3.75).

³We are actually cheating with the polarization vector $\boldsymbol{\varepsilon}$. An accurate description replaces n_2 by a third-rank tensor that produces a scalar out of three vectors.

The nonlinear squeezing parameter $g\alpha$ is nonzero when the pump and signal modes are ‘phase matched’, i.e., $\mathbf{k}_p = 2\mathbf{k}$. For collinear modes, this is achieved by taking $\omega_p = 2\omega$. The spatial integral actually runs only over the region where the nonlinear index n_2 is different from zero. We also see from (3.79) that one ‘pump photon’ with energy $\hbar\omega_p = 2\hbar\omega$ can ‘decay’ into a pair of signal photons. We already anticipated this behaviour in the number state expansion (??).

We finally get a time-independent Hamiltonian by assuming that the pump mode is in a coherent state, $a_p \mapsto \alpha_p$ and by going into a rotating frame at half the pump frequency, $a(t) = e^{-i\omega_p t/2} \tilde{a}(t)$. If one works in addition at exact resonance, the time evolution operator is $U(t) = S(\xi)$ with $\xi = g\alpha_p t$. In practice, one does not get infinite squeezing as $t \rightarrow \infty$ because of damping.

Two-mode squeezing

What we have seen so far is “one-mode squeezing”. The squeezed state can be used to create non-classical correlations between two bright beams.

Consider the output $a_{1,2} = (a \pm b)/\sqrt{2}$ of a balanced beamsplitter with squeezed vacuum state in mode a . This gives for suitable position and momentum quadratures the uncertainty product

$$\Delta(X_1 - X_2)\Delta(P_1 + P_2) < 1 \quad (3.81)$$

because the variance of the difference, $\Delta(X_1 - X_2)$, is just related to the squeezed variance $\Delta X < 1/\sqrt{2}$ of the input mode a . The other variable $P_1 + P_2$ has a variance related to the state of input mode b , it can be brought to a minimum uncertainty of order 1 with a coherent state in mode b . The inequality (3.90) is not inconsistent with the Heisenberg relations because the sum $P_1 + P_2$ and the difference $X_1 - X_2$ are commuting operators.

In other words, Eq.(3.90) tells us that the combination “squeezed vacuum + coherent state” sent onto a beam splitter provides two beams whose X -quadratures are correlated better than what is allowed by the standard vacuum fluctuations (or the fluctuations around a coherent = quasi-classical state). This is the criterion for a non-classical correlation.

Einstein, Podolski, and Rosen (1935) or “EPR” have discussed this arrangement in a slightly different form and came to the conclusion that quantum mechanics must be an incomplete theory. They mixed up, however, that the correlations we have here do not require some “instantaneous action at a distance” between the systems A and B (the two output beams after the beam splitter).

Nonlocal correlations of this kind already appear in classical physics: hide a red and a blue ball in two boxes, move one box to the moon and open it. You know immediately the color of the other box, wherever it is. This correlation cannot be used to transmit information, however.

Unitary operator that generates two-mode squeezing:

$$S_{ab}(\xi) = \exp(\xi a^\dagger b^\dagger - \xi^* ab) \quad (3.82)$$

Exercise: check with single-mode squeezer (3.64) and beam splitter transformation (3.15). Appears in many different situations:

- non-degenerate nonlinear media (production of correlated photon pairs)
- normal modes of a degenerate, weakly interacting Bose gas (Bogoliubov quasi-particles)
- quantum field theory in classical background fields (Klein paradox, Hawking radiation, Unruh radiation), leading to “unstable vacuum states”

3.4 Nonclassical states, correlations, and entanglement

The material of Secs. 3.4, 3.5, 3.6 was not presented in the WS 2011/12 lecture.

3.4.1 Nonclassical states

Long tradition in this area: *Arbeitsgruppe Nichtklassische Strahlung* led by Harry Paul at HU Berlin.

- more information about phase-space distribution functions in Sec. 3.5.

Definition of Sudarshan (1963): any state whose P-function is regular (not more singular than a δ -function) has a classical interpretation. Conversely: a state is ‘non-classical’ if its P-function is singular (i.e., more singular than a δ -function).

Related to representation of normally ordered averages as integrals over the P-function, for example:

$$\langle a^\dagger a \rangle = \dots = \int d^2\alpha \alpha^* \alpha P(\alpha) \quad (3.83)$$

If $P(\alpha) \geq 0$ and not more singular than a δ -function, we can read this integral as a classical average over “existing values” α and α^* for the operators a and a^\dagger . This works

only if the operators are in normal order, of course. This is not a real restriction, however, since any observable can be brought into normal order using the commutation relations.

An alternative criterion which is “easier” to verify experimentally: a state is non-classical if for some point α in the phase space plane, the Wigner function is negative, $W(\alpha) < 0$. (This definition may not be equivalent to the previous one.) The Wigner function is related to the P-function by a gaussian convolution

$$W(\alpha) = \int \frac{d^2\beta}{\pi} e^{-\frac{1}{2}|\alpha-\beta|^2} P(\beta) \quad (3.84)$$

(Convolution: smoothen a photo and make it less “sharp”.) The singular features of a non-classical P-function are smoothened by this convolution because the Wigner function $W(\alpha)$ is a continuous function. But the non-classical singularities do not appear completely, because $W(\alpha)$ can be negative.

Wigner function: provides a statistical interpretation of symmetrically ordered averages, for example

$$\frac{1}{2}\langle aa^\dagger + a^\dagger a \rangle = \int d^2\alpha \frac{\alpha\alpha^* + \alpha^*\alpha}{2} W(\alpha) \quad (3.85)$$

For the vacuum state, this is not zero because the Wigner function has a finite width around $\alpha = 0$ (a disk of “vacuum fluctuations”). In Eq.(3.83) for the P-function, the result is zero because $P(\alpha)$ is a δ -peak centered at zero for the vacuum state (“no fluctuations”).

3.4.2 Quasi-probabilities

Characteristic functions (moment generating functions), marked by tilde. Related to distribution functions by Fourier transform in the phase-space plane, i.e. for the P-function

$$P(\alpha) = \int \frac{d^2\beta}{\pi^2} e^{\alpha\beta^* - \alpha^*\beta} \tilde{P}(\beta) \quad (3.86)$$

The quantity $\alpha\beta^* - \alpha^*\beta$ is imaginary and gives the natural phase factor for the Fourier transform. The distribution functions differ to the extent this integral exists as an ordinary function or must be re-interpreted as a more or less singular distribution.

For the P-function, the characteristic function involves the normally ordered form of displacement operator

$$\tilde{P}(\alpha) = \langle : \hat{D}(\alpha) : \rangle = \langle e^{\alpha a^\dagger} e^{-\alpha^* a} \rangle \quad (3.87)$$

where $:\dots:$ means: write all operator products in \dots in normally ordered form, ignoring commutators.⁴ Expansion in powers of α and α^* gives normally ordered operator products. Inverse Fourier transform from $\tilde{P}(\alpha)$ gives the P-function [Eq.(3.86)], the same relation that is used for the characteristic function in classical statistics.

⁴This is a subtle issue. Example: $:a^\dagger a: = :aa^\dagger: = a^\dagger a$.

Similarly for the Wigner function: generating function for symmetrically ordered products is the displacement operator itself

$$\tilde{W}(\alpha) = \langle \hat{D}(\alpha) \rangle \quad (3.88)$$

The Campbell-Baker-Hausdorff formula allows to re-order the operators in $\hat{D}(\alpha)$ and to bring it in normal order, see Eq.(3.57). This gives the relation

$$\tilde{Q}(\alpha) = e^{-\frac{1}{2}|\alpha|^2} \tilde{W}(\alpha) = e^{-|\alpha|^2} \tilde{P}(\alpha) \quad (3.89)$$

The characteristic functions of the Wigner and Q-functions are therefore smaller for large values of α . This implies for their Fourier transforms (the Wigner and Q-functions) that they are “smoother” (a picture with few high k -vectors is blurred, out of focus, *unschärf*). From a mathematical viewpoint, this means that the Fourier transforms exist as ordinary functions for Wigner and Q, but that the P-function does not necessarily exist (as an ordinary function). One must then take recourse to the singular functions of distribution theory.

3.4.3 Entanglement and correlations

Entanglement is a property of two observables A and B or of two subsystems described by A and B . The two subsystems are called *entangled* when A and B show “non-classical correlations”, i.e., correlations that cannot be explained by classical statistics.

This formulation is similar to the negative (or singular) values of certain quasi-probabilities. When these cannot be interpreted as classical probabilities, we encounter non-classical states. The examples discussed below illustrate for example that squeezing in one mode can be used to entangle two modes – the “non-classicality” of one input state is a “resource” that provides “entangling power”.

EPR correlations

Section appears already earlier, in Sec. 3.3.5.

Output $a_{1,2} = (a \pm b)/\sqrt{2}$ of a balanced beamsplitter with squeezed vacuum state in mode a . This gives for suitable position and momentum uncertainties

$$\Delta(X_1 - X_2)\Delta(P_1 + P_2) < 1 \quad (3.90)$$

because the variance of the difference, $\Delta(X_1 - X_2)$, is just related to the squeezed variance $\Delta X < 1/\sqrt{2}$ of the input mode a . The other variable $P_1 + P_2$ has a variance related to the state of input mode b , it can be brought to a minimum uncertainty of order

1 with a coherent state. The inequality (3.90) is not inconsistent with the Heisenberg relations because the sum $P_1 + P_2$ and the difference $X_1 - X_2$ are commuting operators.

In other words, Eq.(3.90) tells us that the combination “squeezed vacuum + coherent state” sent onto a beam splitter provides two beams whose X -quadratures are correlated better than what is allowed by the standard vacuum fluctuations (or the fluctuations around a coherent = quasi-classical state). This is the criterion for a non-classical correlation.

Einstein, Podolski, and Rosen (1935) or “EPR” have discussed this arrangement in a slightly different form and came to the conclusion that quantum mechanics must be an incomplete theory. They mixed up, however, that the correlations we have here do not require some “instantaneous action at a distance” between the systems A and B (the two output beams after the beam splitter). Nonlocal correlations of this kind already appear in classical physics: hide a red and a blue ball in two boxes, move one box to the moon and open it. You know immediately the color of the other box, wherever it is. This correlation cannot be used to transmit information, however.

Bell correlations

The reasoning of EPR has been made more precise by John Bell (1987) who invented a systematic way of deriving inequalities (upper limits) to correlations between observables A and B . The “classical” assumption is that these take definite values (those that appear as outcomes of single measurements), but determined by some other “hidden variables” that obey classical statistics. If these “hidden variable theories” are formulated in a non-local way, any quantum correlation can be reproduced. But this would require assumptions that are not natural from the “local” viewpoint that has become familiar to us from relativity. An example of a local hidden variable theory provides an upper limit to spin correlations measured on two two-level systems with spin operators $\sigma \otimes \mathbb{1}$ (system A) and $\mathbb{1} \otimes \sigma$ (system B). More precisely, let us take four unit vectors: \mathbf{n}, \mathbf{n}' (for system A) and \mathbf{m}, \mathbf{m}' (for system b). One assumes that all the observables $\mathbf{n} \cdot \sigma$ have determined (although unknown) values ± 1 corresponding to the possible outcomes of measurements (the eigenvalues ± 1). Then the following inequality holds for a hidden variable theory (Clauser, Horne, Shimony, and Holt 1969)

$$|\langle \mathbf{n} \cdot \sigma \otimes \mathbf{m} \cdot \sigma \rangle + \langle \mathbf{n}' \cdot \sigma \otimes \mathbf{m} \cdot \sigma \rangle + \langle \mathbf{n}' \cdot \sigma \otimes \mathbf{m}' \cdot \sigma \rangle - \langle \mathbf{n} \cdot \sigma \otimes \mathbf{m}' \cdot \sigma \rangle| \leq 2 \quad (3.91)$$

where the pattern of signs is to be noted. One central idea in the proof is that one can “locally choose” between \mathbf{n} and \mathbf{n}' (i.e. two different components of the Bloch vector for system A), and that the outcome for system B is not affected by this choice (this is a “local theory of hidden variables”).

A classical, perfect correlation can always be achieved between detectors in a fixed direction, $\mathbf{n} = \mathbf{m}$, say. This is within the scope of the CHSH inequality (3.91), however.

Take for example $\mathbf{n} \cdot \boldsymbol{\sigma} = \sigma_3$ with eigenstates $|e\rangle, |g\rangle$ and consider the statistical mixture

$$\rho = \frac{1}{2} (|e, g\rangle\langle e, g| + |g, e\rangle\langle g, e|) \quad (3.92)$$

Then perfect anti-correlation holds $\langle \sigma_3 \otimes \sigma_3 \rangle = \text{tr}[(\sigma_3 \otimes \sigma_3) \rho] = -1$. This does not produce any correlations for the Bloch components $\sigma_{1,2}$, however. Check that one gets for the CHSH correlation

$$\begin{aligned} \text{CHSH} &= -n_3 m_3 - n'_3 m_3 - n'_3 m'_3 + n_3 m'_3 \\ &= -(n_3 + n'_3) m_3 - (n'_3 - n_3) m'_3 \end{aligned} \quad (3.93)$$

Let us look for the maximum value of this expression. The components of the unit vectors are in the range $-1 \dots +1$. For $-1 \leq n_3 < n'_3 < 0$, both parentheses are negative, and we get a maximum by choosing $m_3 = m'_3 = 1$. But then, $\text{CHSH} = -2n'_3 \leq 2$. Along similar lines, one can prove the inequality (3.91).

The power of this reasoning is that the inequality applies to any choice of state, i.e., of choice of “hidden variables” or classical correlations between the outcomes.

Quantum mechanics gives a different answer, however, sometimes. Take the “maximally entangled state”

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|e, g\rangle - |g, e\rangle) \quad (3.94)$$

whose density operator $|\psi\rangle\langle\psi|$ differs from Eq.(3.92) because of the off-diagonal terms $|e, g\rangle\langle g, e|$. In this state, one has the perfect anti-correlation

$$\langle\psi|\mathbf{n} \cdot \boldsymbol{\sigma} \otimes \mathbf{n} \cdot \boldsymbol{\sigma}|\psi\rangle = -1 \quad (3.95)$$

in any choice of basis \mathbf{n} . (This is related to the “singlet” or zero total spin character of the state $|\psi\rangle$.)⁵ For two different orientations at A and B , one gets the result

$$\langle\psi|\mathbf{n} \cdot \boldsymbol{\sigma} \otimes \mathbf{m} \cdot \boldsymbol{\sigma}|\psi\rangle = -\mathbf{n} \cdot \mathbf{m} \quad (3.96)$$

where $\mathbf{n} \cdot \mathbf{m}$ is the standard scalar product. The CHSH correlation then becomes

$$\text{CHSH} = -(\mathbf{n} + \mathbf{n}') \cdot \mathbf{m} - (\mathbf{n}' - \mathbf{n}) \cdot \mathbf{m}' \quad (3.97)$$

which can be maximized by choosing a suitable “tetrad” of unit vectors⁶ up to a value $2\sqrt{2}$. The range of CHSH correlations

$$2 < |\text{CHSH}| \leq 2\sqrt{2} \quad \text{Bell inequality violated} \quad (3.98)$$

⁵The form of the state $|\psi\rangle$ in a different cartesian basis for the spin vectors $\boldsymbol{\sigma}$ is generated by the three operators $\sigma_i \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_i$ ($i = 1, 2, 3$). However, their action on $|\psi\rangle$ gives zero: hence $|\psi\rangle$ is invariant under rotation (a “singlet state”). Hence the perfect anticorrelation for the components $\sigma_3 \otimes \sigma_3$ carries over onto any direction.

⁶Exercise: choose \mathbf{m} and \mathbf{m}' opposite to the directions of $\mathbf{n} \pm \mathbf{n}'$, respectively. Then $\text{CHSH} = \sqrt{2 + 2\cos\theta} + \sqrt{2 - 2\cos\theta}$ with $\cos\theta = \mathbf{n} \cdot \mathbf{n}'$. This quantity varies between 2 and $2\sqrt{2}$. The maxima are obtained for $\cos\theta = 0$, hence orthogonal directions \mathbf{n} and \mathbf{n}' . The directions \mathbf{m} and \mathbf{m}' are then orthogonal as well, and one bisects that angle between \mathbf{n} and \mathbf{n}' .

is therefore called the “non-classical” domain which cannot be interpreted in terms of a classical theory (more precisely: a local hidden variable model). The number $|\text{CHSH}| - 2$ can be taken as a quantitative measure of entanglement between system A and B : it quantifies the degree of “non-classicality” of the correlations between A and B .

Further reading

On entanglement between quadratures or position and momentum variables in general (so-called “continuous variables”): Eisert & Plenio (2003) and Plenio & Virmani (2007). An introduction to the EPR paradox and applications: Reid & al. (2009).

3.5 Phase space distribution functions

The quantum states of the radiation field can be characterized by their behaviour in phase space. Fig. 3.2 is one example for a coherent state, other states have been illustrated in Fig. 3.3. Can a similar picture be also constructed for the vacuum state? Yes: the vacuum is a special coherent state, $|\text{vac}\rangle = |0\rangle$. What about number states or thermal states?

3.5.1 Overview

There are several possibilities to construct distribution functions on the ‘phase space’ spanned by the quadratures X and P . This is rooted in the fact that these are non-commuting operators.

The Q-function

The overlap we calculated (3.53) motivates the following function to characterize a quantum state the *Husimi or Q-function*

$$Q(\alpha) = \frac{1}{\pi} \langle \alpha | \hat{\rho} | \alpha \rangle \quad (3.99)$$

where the meaning of the prefactor $1/\pi$ will become clear soon. Each density operator $\hat{\rho}$ defines a Q-function and more generally, the Q-function just provides an alternative characterization of the quantum state.

The Q-function has the following nice property: it is positive $Q(\alpha) \geq 0$ for all α and any density operator $\hat{\rho}$. This directly follows from $\hat{\rho}$ being a density operator and the coherent state $|\alpha\rangle$ being a normalizable Hilbert space vector.

For a pure coherent state, $\hat{\rho} = |\beta\rangle\langle\beta|$, the Q-function is a Gaussian centered at $\alpha = \beta$ and a spread of order unity, see (3.53).

Exercise: for a thermal state, $Q_T(\alpha)$ is a Gaussian centered at $\alpha = 0$ with a width of order $[\langle \hat{n} \rangle_T + 1]^{1/2}$.

How would the Q-function look for a number state? A first guess is a ‘ring’, since the photon number (or energy) is fixed and shows no fluctuations. This is not far from the precise answer that we have already calculated:

$$Q_n(\alpha) = |\langle \alpha | n \rangle|^2 = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!} \quad (3.100)$$

where now the Poisson distribution has to be read as a function of α . It is manifestly isotropic, increases like a power law $|\alpha|^{2n}$ near the origin and decays in a gaussian manner for large α . The maximum indeed occurs for $|\alpha|^2 \approx n$. The rim of this ‘volcano distribution’ becomes narrower and narrower as n increases.

The P-function

This function, also called Glauber-Sudarshan distribution provides an expansion of the density operator in the basis of coherent states. There are two variants: the (‘simple’) P-function (Sudarshan, 1963)

$$\hat{\rho} = \int d^2\alpha P(\alpha) |\alpha\rangle \langle \alpha| \quad (3.101)$$

(the integration measure is $d^2\alpha = d(\text{Re } \alpha) d(\text{Im } \alpha)$) and the ‘positive P-function’ (Glauber, 1963)

$$\hat{\rho} = \int d^2\alpha d^2\beta P(\alpha, \beta^*) |\alpha\rangle \langle \beta| \quad (3.102)$$

It is actually surprising that any density operator (well, there are some restrictions) can be represented as a sum of projectors $|\alpha\rangle \langle \alpha|$ on coherent states. This is related to the coherent states being not orthogonal. The price to pay is also that the P-function can be a quite singular distribution, containing δ -functions and derivatives of δ -functions.

Example: for a coherent state,

$$\hat{\rho} = |\beta\rangle \langle \beta| : \quad P_{\hat{\rho}}(\alpha) = \delta(\alpha - \beta) \quad (3.103)$$

where the δ -function is defined with respect to the integration measure: $\delta(\alpha) = \delta(\text{Re } \alpha) \delta(\text{Im } \alpha)$.

It is easy to see, by taking the expectation value in a coherent state, that *the Q-function is a Gaussian convolution (Faltung) of the P-function*:

$$Q(\alpha) = \int d^2\beta P(\beta) \exp(-\frac{1}{2}|\alpha - \beta|^2) \quad (3.104)$$

This explains why the Q-function behaves always ‘less singularly’ than the P-function.

3.6 Two modes, many modes

3.6.1 Multi-mode Hilbert space and observables

The state space of a two-mode field is the tensor product of the Fock spaces of two harmonic oscillators. In terms of number states, the basis vectors of this space can be written

$$|n_1; n_2\rangle = |n_1\rangle_{\text{mode 1}} \otimes |n_2\rangle_{\text{mode 2}}$$

where the first mode contains n_1 and the second mode n_2 photons. These states are called ‘product states’. That have expectation values of products of operators pertaining to mode 1 and 2, that factorize, e.g.,

$$\langle \hat{n}_1 \hat{n}_2 \rangle = \langle \hat{n}_1 \rangle \langle \hat{n}_2 \rangle.$$

But due to the possibility of forming superpositions, there is much more ‘space’ in the multi-mode Hilbert space. For example, it is possible that two modes ‘share’ a single photon:

$$\frac{1}{\sqrt{2}} (|0; 1\rangle + |1; 0\rangle) \quad (3.105)$$

This state is called ‘entangled’ if no change of basis for the mode expansion exists such that the state is mapped onto a product state (this may be very difficult to check in practice).⁷ The state is by no means unphysical, however, since it is generated by

$$\frac{1}{\sqrt{2}} (a_1^\dagger + a_2^\dagger) |0; 0\rangle \quad (3.106)$$

where $|0; 0\rangle$ is the two-mode vacuum. Such sums of creation operators occur always in the mode expansion of the quantized field. The decay of an excited atomic state, for example, generates a continuous superposition of one-photon states where an infinite number of modes share a single photon.

Many-mode single-photon states are also generated when an atom is illuminated by a single photon: the scattering of this photon by the atom generates, as in the classical electromagnetic theory, a continuous angular distribution of modes with a nonzero amplitude for one-photon excitations.

Finally, what about the density matrix for a multi-mode field? Let us start with the simple case of two modes of the same frequency in thermal equilibrium. According to the general rule, the density matrix is a sum of projectors onto the stationary states $|n_1; n_2\rangle$ of the two-mode system, each weighted with a probability proportional to $e^{-\beta(n_1+n_2)}$.

⁷It is simple to see, however, that the expectation value of $\hat{n}_1 \hat{n}_2$ does not factorize. Indeed, $\langle \hat{n}_1 \rangle = \frac{1}{2} = \langle \hat{n}_2 \rangle$ while $\langle \hat{n}_1 \hat{n}_2 \rangle = 0$ since in each component of the state (3.105), at least one mode has zero photons.

(Use $\beta = \hbar\omega/k_B T$.) Since the energy is made additively from single-mode energies, we can factorize this density operator:

$$\begin{aligned}
\hat{\rho} &= Z^{-1} \sum_{n_1, n_2} e^{-\beta(n_1+n_2)} |n_1; n_2\rangle\langle n_1; n_2| \\
&= Z \sum_{n_1} e^{-\beta n_1} |n_1\rangle\langle n_1| \otimes \sum_{n_2} e^{-\beta n_2} |n_2\rangle\langle n_2| \\
&= Z^{-1} \tilde{\rho}_1 \otimes \tilde{\rho}_2
\end{aligned} \tag{3.107}$$

where the $\tilde{\rho}_{1,2}$ are un-normalized density matrices. The tensor product of the projectors is defined by coming back to the tensor product of states

$$|n_1\rangle\langle n_1| \otimes |n_2\rangle\langle n_2| = (|n_1\rangle \otimes |n_2\rangle) (\langle n_1| \otimes \langle n_2|).$$

The trace of the two-mode density matrix (3.107) also factorizes because the matrix elements of a tensor product operator are, by definition, the products of the individual matrix elements

$$\begin{aligned}
\text{tr}(\hat{\rho}) &= Z^{-1} \sum_{n_1, n_2} \langle n_1; n_2 | \tilde{\rho}_1 \otimes \tilde{\rho}_2 | n_1; n_2 \rangle \\
&= Z^{-1} \sum_{n_1, n_2} \langle n_1 | \tilde{\rho}_1 | n_1 \rangle \langle n_2 | \tilde{\rho}_2 | n_2 \rangle \\
&= Z^{-1} (\text{tr} \tilde{\rho}_1) (\text{tr} \tilde{\rho}_2)
\end{aligned} \tag{3.108}$$

and therefore $Z = Z_1 Z_2 = (1 - e^{-\beta})^{-2}$.

Since the density matrix of this thermal two-mode state factorizes, this state is not entangled (averages of products of single-mode operators factorize). This is no longer true, however, if we allow for an interaction between the modes. Then the energy is no longer a sum of single-mode energies, and the previous factorization does no longer work. This is by the way a general rule: interactions between quantum systems lead to entangled states. For this reason, entangled states are much more frequent in Nature than are factorized states. It is a nontrivial task, however, to decide whether a given density matrix describes an entangled state or not.

Digression (*Einschub*): tensor product states and operators

It is somewhat tricky to guess the right formulas for multimode field states and operators. The general rule is the following:

$$\begin{array}{ll}
\text{Field operator} & \leftrightarrow \text{sum of modes} \\
\text{Field state} & \leftrightarrow \text{product of modes}
\end{array}$$

For example, the electric field operator for a two-mode field is given by

$$\mathbf{E}(\mathbf{x}, t) = E_1 \boldsymbol{\varepsilon}_1 a_1(t) e^{i\mathbf{k}_1 \cdot \mathbf{x}} + E_2 \boldsymbol{\varepsilon}_2 a_2(t) e^{i\mathbf{k}_2 \cdot \mathbf{x}} + \text{h.c.}$$

while a typical state is for example the product state $|n_1; n_2\rangle = |n_1\rangle \otimes |n_2\rangle$. The general rule gets complicated (1) when we allow for superpositions (sums) of product states and (2) when we consider measurements that involve products of different mode operators.

In calculations, one often needs products of operators, like $\mathbf{E}^2(\mathbf{x}, t)$. These are computed in the usual way, one has just to take care that operators sometimes do not commute. But this is only relevant for operators acting on the same mode, $[a_1, a_1^\dagger] = 1$, while for different modes

$$[a_1, a_2^\dagger] = 0$$

because they correspond to independent degrees of freedom.

Operator averages in product states. Let us consider the average electric field for the two-mode case written above. Using the mode expansion, we find terms like $\langle a_i(t) \rangle$ ($i = 1, 2$) and their adjoints. Now the operator $a_1|\psi\rangle$ is evaluated by letting a_1 act on the first factor of a product state:

$$a_1|n_1; n_2\rangle = (a_1|n_1\rangle) \otimes |n_2\rangle$$

If $|\psi\rangle$ is a sum of product states (entangled state), then this procedure is done for every term in this sum. Sometimes this is formalized by writing the operator as $a_1 \otimes \mathbb{1}$, thus indicating that for the second mode nothing happens. The action of such operator tensor products is apparently defined as

$$A_1 \otimes B_2|n_1; n_2\rangle = A_1|n_1\rangle \otimes B_2|n_2\rangle \quad (3.109)$$

by letting each operator factor act on the respective state factor. This notation allows to avoid the subscripts 1 and 2 as the relevant mode is indicated by the position in the operator product.

Similarly, the scalar product of tensor products of states is defined by

$$\langle n_1; n_2 | m_1; m_2 \rangle = \langle n_1 | \otimes \langle n_2 | m_1 \rangle \otimes | m_2 \rangle = \langle n_1 | m_1 \rangle \langle n_2 | m_2 \rangle$$

by taking the scalar product of the corresponding factors.

The average of the electric field for a product of number states is thus zero, as for a single-mode field, because $\langle n | a | n \rangle = 0$, and this is true for both modes. What about a product state of two coherent states, $|\psi\rangle = |\alpha; \beta\rangle$? It is simple to see that we get the classical result (we assume that both modes have the same frequency ω)

$$\langle \mathbf{E}(\mathbf{x}, t) \rangle = E_1 \boldsymbol{\varepsilon}_1 \alpha e^{-i\omega t + i\mathbf{k}_1 \cdot \mathbf{x}} + E_2 \boldsymbol{\varepsilon}_2 \beta e^{-i\omega t + i\mathbf{k}_2 \cdot \mathbf{x}} + \text{c.c.} \quad (3.110)$$

(Note that ‘c.c.’ and not ‘h.c.’ occurs.) As a general rule, classical fields can be described by tensor products of coherent states.

Last example where we go quantum: a superposition of coherent product states,

$$|\psi\rangle = c|\alpha; \beta\rangle + d|\beta; \alpha\rangle$$

with some complex amplitudes c, d . Then we find

$$\langle a_1 \rangle = |c|^2 \alpha + |d|^2 \beta$$

if $\langle \alpha | \beta \rangle = 0$. (This is actually never exactly the case, but can be achieved to a very good precision if $|\alpha - \beta| \gg 1$.) This result is an average over the two possible coherent amplitude, weighted with the corresponding probabilities. The average field thus becomes:

$$\langle \mathbf{E}(\mathbf{x}, t) \rangle = E_1 \boldsymbol{\varepsilon}_1 \left(|c|^2 \alpha + |d|^2 \beta \right) e^{-i\omega t + i\mathbf{k}_1 \cdot \mathbf{x}} + E_2 \boldsymbol{\varepsilon}_2 \left(|c|^2 \beta + |d|^2 \alpha \right) e^{-i\omega t + i\mathbf{k}_2 \cdot \mathbf{x}} + \text{c.c.}$$

Question: this result does not allow to distinguish this state from an ‘incoherent mixture’ of coherent product states like in (3.110), each state occurring with a probability $|c|^2, |d|^2$. This mixture would be described by the density operator

$$\hat{\rho}_{\text{mix}} = |c|^2 |\alpha; \beta\rangle \langle \alpha; \beta| + |d|^2 |\beta; \alpha\rangle \langle \beta; \alpha|$$

and gives the same average electric field (exercise). If the coherent amplitudes α, β are closer together, then due to the nonzero overlap $\langle \alpha | \beta \rangle$, one can distinguish superposition and mixture (exercise). Are there observables that can make the difference in the case $\langle \alpha | \beta \rangle = 0$?

Average of single-mode operator. Let us calculate as another example the average photon number in mode 1 for a two-mode field in the entangled state (3.105). The relevant photon number operator is given by $a_1^\dagger a_1$ or, to be more precise, $a_1^\dagger a_1 \otimes \mathbb{1}$. Its action on the entangled state is worked out using linearity and the operator product rule (3.109)

$$\begin{aligned} & \frac{1}{\sqrt{2}} a_1^\dagger a_1 \otimes \mathbb{1} (|0; 1\rangle + |1; 0\rangle) \\ &= \frac{1}{\sqrt{2}} \left(a_1^\dagger a_1 |0\rangle \otimes |1\rangle + a_1^\dagger a_1 |1\rangle \otimes |0\rangle \right) \\ &= \frac{1}{\sqrt{2}} |1\rangle \otimes |0\rangle = \frac{1}{\sqrt{2}} |1; 0\rangle \end{aligned}$$

Taking the scalar product with the original state, we find

$$\langle \hat{n}_1 \rangle = \frac{1}{2} (\langle 0; 1| + \langle 1; 0|) |1; 0\rangle = \frac{1}{2}.$$

Once you have done this calculation, you can use the shorter rule: all we need are the probabilities of having $n_1 = 0, 1, \dots$ photons in mode 1. For this, collect all product states in the state with the same number of photons n_1 and compute the squared norm of these states. From the probabilities for n_1 photons, you get the average photon number.

Product operators. As a second example, let us compute the average value of the product $a_i^\dagger a_j$ ($i, j = 1, 2$) in a thermal two-mode state. This object occurs when you measure the two-mode field with a photodetector (see paragraph ?? below). The tensor product notation is more cumbersome here and gives

$$a_1^\dagger a_1 \otimes \mathbb{1} \quad \text{or} \quad \mathbb{1} \otimes a_2^\dagger a_2 \quad \text{or} \quad a_1^\dagger \otimes a_2 \quad \text{or} \quad a_1 \otimes a_2^\dagger.$$

The density matrix is a tensor product of thermal single-mode density matrices. We shall see that the result is:

$$\langle a_i^\dagger a_j \rangle_T = \delta_{ij} \bar{n}(T) \quad (3.111)$$

where $\bar{n}(T)$ is the average photon number in a single mode. How does this come about?

When $i = j$, we are left with the calculation of the average photon number for a single mode:

$$\langle a_i^\dagger a_i \rangle = \sum_{n_1, n_2} \langle n_1; n_2 | a_i^\dagger a_i \hat{\rho}_1 \otimes \hat{\rho}_2 | n_1; n_2 \rangle$$

The action of the product density operators factorizes:

$$\hat{\rho}_1 \otimes \hat{\rho}_2 | n_1; n_2 \rangle = \hat{\rho}_1 | n_1 \rangle \otimes \hat{\rho}_2 | n_2 \rangle$$

Each single-mode density operator, acting on a number state, gives the corresponding occupation probability:

$$\hat{\rho}_1 | n_1 \rangle = \sum_{m_1} p_{m_1}(T) | m_1 \rangle \langle m_1 | n_1 \rangle = p_{n_1}(T) | n_1 \rangle,$$

so that we have, using the result for the photon number of one mode

$$\begin{aligned} \langle a_i^\dagger a_i \rangle &= \sum_{n_1, n_2} p_{n_1}(T) p_{n_2}(T) \langle n_1; n_2 | a_i^\dagger a_i | n_1; n_2 \rangle \\ &= \sum_{n_1, n_2} p_{n_1}(T) p_{n_2}(T) n_i \\ &= \sum_{n_i} p_{n_i}(T) n_i \sum_{n_j} p_{n_j}(T) \end{aligned}$$

In the last step, we have noted that the double sum can be factorized ($j \neq i$ is the other index). The second sum gives unity because the probabilities are normalized, the first sum gives the average photon number $\bar{n}(T)$ at temperature T and does no longer depend

on the mode label (this is because we assumed equal frequencies for both modes). This completes the proof in the case $i = j$.

A similar calculation shows that the average of $a_1^\dagger a_2$ vanishes: indeed, we have

$$\langle n_1; n_2 | a_1^\dagger a_2 | n_1; n_2 \rangle = \langle n_1 | a_1^\dagger | n_1 \rangle \langle n_2 | a_2 | n_2 \rangle = 0.$$

Bibliography

- R. J. Adler, B. Casey & O. C. Jacob (1995). Vacuum catastrophe: An elementary exposition of the cosmological constant problem, *Am. J. Phys.* **63** (7), 620–26. Comment by S. R. Ovshinsky and H. Fritzsche, *Am. J. Phys.* 65 (1997) 927 and reply p. 928.
- J. S. Bell (1987). On the Einstein–Podolsky–Rosen paradox. in *Speakable and unspeakable in quantum mechanics: collected papers in quantum mechanics*, pages 14–21. Cambridge University Press, Cambridge. [*Physics* **1** (1964) 195–200].
- P. R. Berman & V. S. Malinovsky (2011). *Principles of Laser Spectroscopy and Quantum Optics*. Princeton University Press, Princeton Oxford.
- J. F. Clauser, M. A. Horne, A. Shimony & R. A. Holt (1969). Proposed experiment to test local hidden-variable theories, *Phys. Rev. Lett.* **23**, 880–84. Erratum: **24** (1970) 549.
- C. Cohen-Tannoudji, J. Dupont-Roc & G. Grynberg (1987). *Photons et atomes — Introduction à l'électrodynamique quantique*. InterEditions, Paris. English translation: *Photons and Atoms — Introduction to Quantum Electrodynamics* (Wiley, New York 1989).
- D. P. Craig & T. Thirunamachandran (1984). *Molecular Quantum Electrodynamics*. Academic Press, London.
- J. Dalibard, Y. Castin & K. Mølmer (1992). Wave-Function Approach to Dissipative Processes in Quantum Optics, *Phys. Rev. Lett.* **68**, 580–83.
- A. Einstein, B. Podolsky & N. Rosen (1935). Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?, *Phys. Rev.* **47**, 777–80.
- J. Eisert & M. B. Plenio (2003). Introduction to the basics of entanglement theory in continuous-variable systems, *Int. J. Quant. Inf.* **1** (4), 479–506.
- R. J. Glauber (1963). Coherent and Incoherent States of the Radiation Field, *Phys. Rev.* **131**, 2766–88.

- H. Haken & H. C. Wolf (2000). *The Physics of Atoms and Quanta*. Advanced Texts in Physics. Springer, Heidelberg Berlin, 6th edition.
- C. Henkel (2007). Laser theory in manifest Lindblad form, *J. Phys. B* **40**, 2359–71.
- C. Itzykson & J. B. Zuber (2006). *Quantum field theory*. Dover, New York.
- R. Loudon (2000). *The Quantum Theory of Light*. Oxford University Press, Oxford, 3rd edition.
- L. Mandel & E. Wolf (1995). *Optical coherence and quantum optics*. Cambridge University Press, Cambridge.
- P. Meystre & M. Sargent III (1999). *Elements of Quantum Optics*. Springer, Berlin, 3rd edition.
- K. Mølmer (1997a). Optical coherence, a convenient fiction, *Phys. Rev. A* **55**, 3195–3203.
- K. Mølmer (1997b). Quantum entanglement and classical behaviour, *J. Mod. Opt.* **44**, 1937–56.
- M. A. Nielsen & I. L. Chuang (2000). *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge.
- M. B. Plenio & S. Virmani (2007). An introduction to entanglement measures, *Quant. Inf. Comp.* **7** (1–2), 1–51.
- M. D. Reid, P. D. Drummond, W. P. Bowen, E. G. Cavalcanti, P. K. Lam, H. A. Bachor, U. L. Andersen & G. Leuchs (2009). Colloquium: The Einstein-Podolsky-Rosen paradox: From concepts to applications, *Rev. Mod. Phys.* **81**, 1727–51.
- E. C. G. Sudarshan (1963). Equivalence of Semiclassical and Quantum Mechanical Descriptions of Statistical Light Beams, *Phys. Rev. Lett.* **10** (7), 277–79.
- W. Vogel, D.-G. Welsch & S. Wallentowitz (2001). *Quantum Optics – An Introduction*. Wiley-VCH, Berlin Weinheim.
- W. H. Zurek (1991). Decoherence and the transition from quantum to classical, *Physics Today* **44** (10), 36–44. Update: quant-ph/0306072.