

# 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 Lecture 01 Dec 15

### Keywords

*Mode expansion* of the electric field: mode functions  $\mathbf{f}_\kappa(\mathbf{x})$  with space dependence, solution to classical electrodynamics. Different sets of mode functions are possible: plane waves, spherical harmonics, Gauss-Laguerre modes for beams, optical fibre modes etc. For plane waves (used here), the label  $\kappa = (\mathbf{k}, \sigma)$  collects the  $k$ -vector and a polarization index (two directions transverse to  $\mathbf{k}$ )

Mode amplitudes  $q_\kappa(t)$  carry the time dependence (as in classical electrodynamics) and become *quadrature operators*. The magnetic field amplitude  $p_\kappa(t)$  provides the second quadrature (operator).

*Hilbert space* of modes: the modes span an infinite-dimensional space of field configurations which is a Hilbert space. This concept could have been introduced in classical electrodynamics, there is nothing specifically ‘quantum’ here. *But* the Hilbert space of the *quantized* electromagnetic field is much bigger (it is called the Fock space).

*Transverse vector fields*: have zero divergence  $\nabla \cdot \mathbf{E} = \nabla \cdot \mathbf{f}_\kappa = 0$  – because we start with the ‘free field’, no charges, no currents. In Fourier space (for plane waves), one has  $\mathbf{k} \cdot \mathbf{f}_\kappa = 0$ , hence the name ‘transverse’. (Longitudinal fields are related to the scalar potential and are created by charges.)

*Fock space*: is constructed by annihilation and creation operators. For each mode  $\kappa$ , one constructs from the quadratures the operators  $a_\kappa$  and  $a_\kappa^\dagger$ . They are the exact analog of the ladder operators  $a, a^\dagger$  of the quantized harmonic oscillator. Their commutation relations are

$$[a_\kappa, a_{\kappa'}^\dagger] = \delta(\kappa, \kappa') = \delta(\mathbf{k} - \mathbf{k}')\delta_{\sigma\sigma'} \quad (2.1)$$

(This reduces to an ordinary Kronecker  $\delta_{\mathbf{k}\mathbf{k}'}$  when the modes are computed in a finite ‘quantization volume’ where the allowed  $k$ -vectors are discrete.)

The Fock-Hilbert space contains ‘sectors’ which are labelled by their photon number. Photon number operator

$$N = \sum \int d\kappa a_{\kappa}^{\dagger} a_{\kappa} \quad (2.2)$$

where sum and integral mean:

$$\sum \int d\kappa = \int d^3k \sum_{\sigma} \quad (2.3)$$

and  $\sigma$  is the polarization index per  $k$ -vector.

*Vacuum state:* has zero photons, denoted  $|0\rangle$  or  $|\text{vac}\rangle$ . One must postulate that this state exists. By convention, one can also set its energy to zero. (But see the discussion of the vacuum energy density below.) The annihilation operators map the vacuum state to the zero vector:

$$a_{\kappa}|0\rangle = 0 \quad (2.4)$$

where  $0$  is *not* the vacuum state. It is *not* even a physical state because it has norm zero. It is easy to check that  $N|0\rangle = 0$ , too, consistent with the idea of a zero-photon state.

*One-photon states:* apply creation operators to the vacuum

$$a_{\kappa}^{\dagger}|0\rangle = |1_{\kappa}\rangle = |\kappa\rangle \quad (2.5)$$

Show that  $[N, a_{\kappa}] = -a_{\kappa}$ : this is the operator expression of the statement that the operator  $a_{\kappa}$  annihilates one photon. There is an infinite number of one-photon states (countable or not, depending on the choice of mode functions), and this sector is closely related to the classical Hilbert space of electrodynamics.

*Two-, three-, ... photon states:* apply more creation operators. For example two-photon states

$$a_{\kappa}^{\dagger} a_{\kappa'}^{\dagger}|0\rangle = a_{\kappa}^{\dagger}|1_{\kappa'}\rangle = |1_{\kappa}1_{\kappa'}\rangle, \quad \kappa \neq \kappa' \quad (2.6)$$

When the same operator is applied twice, one gets a different normalization factor

$$(a_{\kappa}^{\dagger})^2|0\rangle = \sqrt{2}|2_{\kappa}\rangle \quad (2.7)$$

The number 2 is called the ‘occupation number’ of this mode. This equation is somewhat tricky for a continuous set of modes, see mathematical details below.

Tensor product structure with infinitely many factors: take a countable set of modes  $1, \dots, \kappa, \dots$

$$a_\kappa \mapsto \mathbb{1}_1 \otimes \dots \otimes a_\kappa \otimes \dots \quad (2.8)$$

Similarly, a generic many-photon state can be characterized as a tensor product of one-mode-states with occupation numbers:

$$|\Psi\rangle = |n_1\rangle \otimes \dots |n_\kappa\rangle \otimes \dots \quad (2.9)$$

*Energy.* For each mode, the operator  $a_\kappa^\dagger a_\kappa$  in Eq.(2.2) above counts the number of photons (its eigenvalues are the positive integers  $0, 1, \dots$ , as in the harmonic oscillator). Hence the simple picture that ‘one photon carries one energy quantum  $h\nu$ ’ gives the following operator for the total field energy

$$\hat{H} = \int d\kappa \hbar \omega_\kappa a_\kappa^\dagger a_\kappa \quad (2.10)$$

where  $\omega_\kappa$  is the frequency of the mode. (Note that this is a classical quantity.)

*Span the Fock space.* The entire Fock space is taken as the ‘closure’ of all these states by linear combinations. One may combine different one-photon states: this gives states with specific spatial features like cavity modes. But also superpositions of different photon numbers are possible.<sup>1</sup>

## Scalar product

(mathematical complement, see also Wikipedia on ‘Fock space’ and the Chapter ‘Fock Spaces’ by Stéphane Attal, Université de Lyon 1, France <http://math.univ-lyon1.fr/%7Eattal/chapters.html>)

A Hilbert space is defined as a complete vector space with a scalar product. In the Hilbert space of classical fields, for example, we can define a scalar product in the form

$$(\mathbf{F}|\mathbf{G}) = \int dV \mathbf{F}^* \cdot \mathbf{G} \quad (2.11)$$

where the ordinary scalar product is integrated over space. The complex conjugation is not needed for classical fields which are real, but it is convenient for complex mode functions like plane waves or circular polarization.

In the Fock space of quantum field theory, we define the scalar product  $\langle \Psi|\Phi \rangle$  by the following properties:

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<sup>1</sup>And sometimes discarded by a ‘superselection rule’. This is problematic, however, if one takes the state generated by a classical source of photons like a radio antenna. See the discussion of coherent states later.

- (0) The vacuum state has norm unity  $\langle 0|0\rangle = 1$ .  
(1) States in different photon sectors are orthogonal, in particular  $\langle 0|1_\kappa\rangle = 0$ .  
(2) In the one-photon sector, we can identify a generic state with a set of plane-wave amplitudes  $\alpha(\kappa) = \alpha_\sigma(\mathbf{k})$ :

$$|\alpha\rangle = \int d\kappa \alpha_\sigma(\mathbf{k})|1_\kappa\rangle = \int d\kappa \alpha_\sigma(\mathbf{k})a_\kappa^\dagger|0\rangle \quad (2.12)$$

The scalar product in the one-photon sector is then

$$\langle\beta|\alpha\rangle = \int d\kappa \beta_\sigma^*(\mathbf{k})\alpha_\sigma(\mathbf{k}) = (\mathbf{B}|\mathbf{A}) \quad (2.13)$$

(Exercise: check that this is consistent with the commutation relation (2.1).) This is simply *the scalar product (2.11) in the classical Hilbert space*, using the Parseval-Plancherel formula for Fourier transforms and the definitions for the (complex) fields ( $\mathbf{e}_\sigma(\mathbf{k})$  is a normalized polarization vector)

$$\mathbf{A}(\mathbf{x}) = \int d\kappa \alpha_\sigma(\mathbf{k})\mathbf{f}_\kappa(\mathbf{x}) \quad (2.14)$$

$$\mathbf{f}_\kappa(\mathbf{x}) = \frac{\mathbf{e}_\sigma(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x})}{(2\pi)^{3/2}} \quad (2.15)$$

and similarly for  $\mathbf{B}(\mathbf{x})$ . – We note in particular that the one-photon states  $a_\kappa^\dagger|0\rangle$  are actually not normalizable, in the same way as plane waves are not. Only wave packets are physical states.

A generic many-photon state is represented by a function  $\alpha(\kappa_1 \dots \kappa_n)$  that is symmetric under any permutation of its arguments (superscript  $(n)$  for ‘state in  $n$ -photon sector’)

$$|\alpha\rangle^{(n)} = \int d\kappa_1 \dots d\kappa_n \alpha(\kappa_1 \dots \kappa_n)|1_{\kappa_1} \dots 1_{\kappa_n}\rangle = \int d\kappa_1 \dots d\kappa_n \alpha(\kappa_1 \dots \kappa_n)a_{\kappa_1}^\dagger \dots a_{\kappa_n}^\dagger|0\rangle \quad (2.16)$$

This is so because the creation operators commute among themselves. The scalar product between two such states is

$${}^{(n)}\langle\beta|\alpha\rangle^{(n)} = \int \frac{d\kappa_1 \dots d\kappa_n}{n!} \beta^*(\kappa_1 \dots \kappa_n)\alpha(\kappa_1 \dots \kappa_n) \quad (2.17)$$

With this formula, you can check how the norm of the two-photon state changes (continuously), as two modes become identical (the limit  $\kappa' \rightarrow \kappa$  in the previous section). In this discussion, one gets a reasonable answer only if one works with normalizable states. A simple example could be a one-dimensional model with spatially localized ‘pulses’ that are shifted one relative to the other, while keeping the same shape (gaussians are easiest to work with). But a polarization rotation would also do the job.

In this formalism, the Fock space is identified with a space of symmetric functions of several arguments, taken from the same ‘classical’ position space. In this way, one can connect one-photon states with ‘classical fields’ – although the corresponding states are complex fields. And for two-photon states, we may introduce a symmetric function

$$E_{ij}(\mathbf{x}, \mathbf{y}) = E_{ji}(\mathbf{y}, \mathbf{x}) \quad (2.18)$$

which is ‘doubly transverse’:  $\partial E_{ij}/\partial x_i = 0 = \partial E_{ij}/\partial y_j$  (summation over  $i$  or  $j$ ). Funnily enough, the literature contains a quite long discussion about the question: ‘What is the wave function of the photon?’, see Białynicki-Birula (1996).

## 2.2 Lecture 08 Dec 15

Remarks on scalar product in Fock-Hilbert space

Remark on energy (density) and operator Maxwell equations

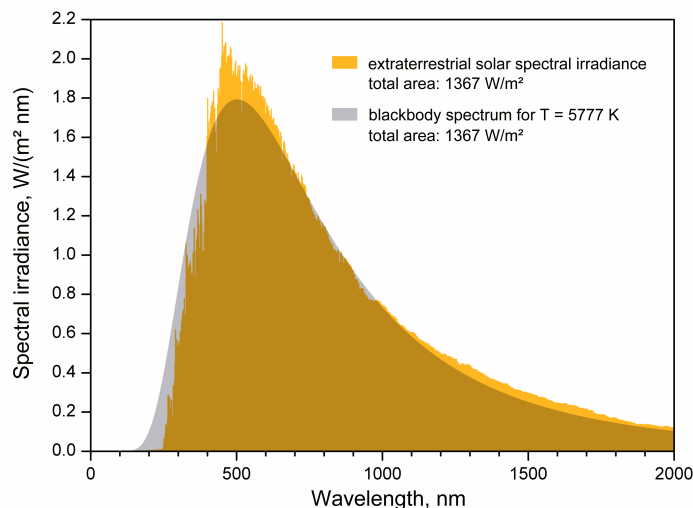
(Remark on Lagrangian, relevant variables, gauge condition)

Remark on interaction with matter: Jaynes-Cummings-Paul model

## 2.3 Lecture 15 Dec 15

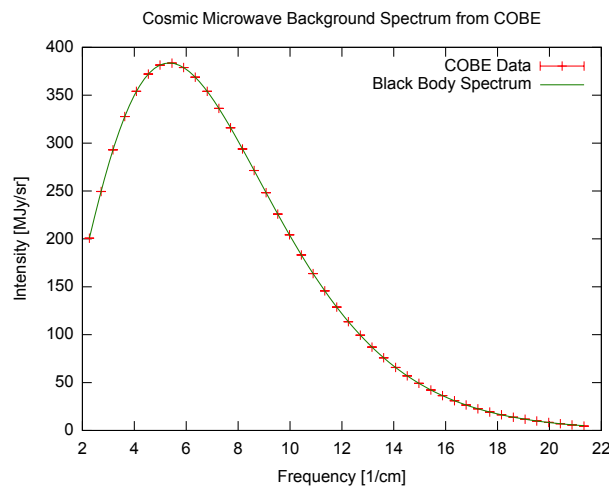
Blackbody radiation

Spectrum of Sun compared to 5777 K black body



[https://en.wikipedia.org/wiki/Planck%27s\\_law#/media/File:EffectiveTemperature\\_300dpi\\_e.png](https://en.wikipedia.org/wiki/Planck%27s_law#/media/File:EffectiveTemperature_300dpi_e.png)

The cosmic microwave background radiation observed today is the most perfect black-body radiation ever observed in nature, with a temperature of 2.72548(57) K. It is a “snapshot” of the radiation at the time of decoupling between matter and radiation in the early universe. Prior to this time, most matter in the universe was in the form of an ionized plasma in thermal, though not full thermodynamic, equilibrium with radiation.



[https://en.wikipedia.org/wiki/Cosmic\\_microwave\\_background#/media/File:Cmbr.svg](https://en.wikipedia.org/wiki/Cosmic_microwave_background#/media/File:Cmbr.svg)

Calculation of energy density in thermal state: density operator  $\hat{\rho}$  in discrete mode basis.

Different modes are not correlated, average occupation number per mode:

$$\langle a_{\kappa}^{\dagger} a_{\kappa'} \rangle_T = \bar{n}(\omega_{\kappa}) \delta(\kappa, \kappa') \quad (2.19)$$

with Bose-Einstein distribution: this is a result of combining ordinary (‘classical’) Boltzmann statistics with the discrete energy packets of the photons.

(Total) Energy density after summation over modes

$$\begin{aligned} u(T) &= \left\langle \frac{\epsilon_0}{2} \mathbf{E}^2 + \frac{\mu_0}{2} \mathbf{H}^2 \right\rangle_T \\ &= (\dots) \int_0^{\infty} d\omega \omega^2 \frac{\hbar\omega}{2} (2\bar{n}(\omega) + 1) \end{aligned} \quad (2.20)$$

identify the integrand as spectral density: temperature-dependent part = Planck spectrum

$$u(\omega, T) = \frac{\hbar\omega^3}{2 \dots c^3 (e^{\hbar\omega/k_B T} - 1)} \quad (2.21)$$

Remarks: vacuum energy, Lamb shift, Casimir energy

## 2.4 Lecture 05 Jan 16

Spontaneous decay (Dirac, 1927).

Sketch of composite system: “atom/molecule coupled to quantized radiation field”.

Electric dipole vs minimal coupling interaction

$$V = \begin{cases} -\mathbf{d} \cdot \mathbf{E}(\mathbf{x}_A) & \text{el. dipole (long wavelengths only)} \\ -\frac{e}{m}\mathbf{p} \cdot \mathbf{A}(\mathbf{r}) + \frac{e^2}{2m}\mathbf{A}^2(\mathbf{r}) & \text{minimal coupling (for one-electron atom)} \end{cases} \quad (2.22)$$

Minimal coupling involves electron momentum  $\mathbf{p}$  and position  $\mathbf{r}$  observables and the vector potential  $\mathbf{A}$ . Is an example of a ‘gauge symmetry’: a gauge transformation of the electromagnetic potential plus a local phase transformation of the quantum mechanical wave function leaves the ‘canonical momentum’  $\mathbf{p} - e\mathbf{A}$  invariant.

Fermi’s Golden Rule: inverse lifetime of excited state

$$\frac{1}{\tau_e} = \frac{2\pi}{\hbar} \sum_{\kappa} |\langle g | 1_{\kappa} | V | e 0 \rangle|^2 \delta(\hbar\omega_{\kappa} - (E_e - E_g)) \quad (2.23)$$

Discussion of quantum states: ‘one photon appears’.

Evaluate matrix element and perform summation (integral) over all photon energies, directions, and polarizations:

$$\frac{1}{\tau_e} = \dots = \frac{|\mathbf{d}_{ge}|^2}{3\pi\epsilon_0\hbar} \int_0^{\infty} d\omega \frac{\omega^2}{c^3} \delta(\omega - \omega_A) = \frac{|\mathbf{d}_{ge}|^2 \omega_A^3}{3\pi\epsilon_0\hbar c^3} \quad (2.24)$$

Discussion:

Typical number  $\tau_e \approx 10$  ns, much longer than period  $2\pi/\omega_A$  corresponding to transition frequency.

Dimensionless product  $\omega_A\tau_e \propto \alpha^{-3}$  (fine structure constant) very large: ‘atom is an oscillator with very high quality factor’, is weakly damped.

Energy  $\hbar\gamma_e = \hbar/\tau_e =$  uncertainty (width) of excited state(s), thick line in energy level diagrams.

Power  $\hbar\omega_A\gamma_e$  of spontaneously radiated photons, (semi)classical picture with radiation from oscillating dipole.

## 2.5 Canonical quantization

The following sections were not treated in WS 15/16.



## 2.5.1 Fields

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

$$\begin{aligned}\mu_0 \nabla \cdot \mathbf{H} &= 0 & \varepsilon_0 \nabla \cdot \mathbf{E} &= \rho \\ \mu_0 \partial_t \mathbf{H} &= -\nabla \times \mathbf{E} & \varepsilon_0 \partial_t \mathbf{E} &= \nabla \times \mathbf{H} - \mathbf{j}\end{aligned}\quad (2.25)$$

Introducing the scalar and vector potentials via

$$\mu_0 \mathbf{H} = \nabla \times \mathbf{A} \quad (2.26)$$

$$\mathbf{E} = -\nabla \phi - \partial_t \mathbf{A}, \quad (2.27)$$

the left column of (2.25) is identically fulfilled. The Coulomb law then becomes

$$-\varepsilon_0 \nabla^2 \phi - \varepsilon_0 \nabla \partial_t \mathbf{A} = \rho \quad (2.28)$$

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:

$$-\varepsilon_0 \nabla^2 \phi = \rho \quad (2.29)$$

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

$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int d^3x' \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \quad (2.30)$$

which is a superposition of well-known Coulomb potentials.

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

$$\nabla \times (\nabla \times \mathbf{A}) + \varepsilon_0 \mu_0 \partial_t^2 \mathbf{A} = \mu_0 (\mathbf{j} - \varepsilon_0 \partial_t \nabla \phi) \equiv \mu_0 \mathbf{j}_\perp. \quad (2.31)$$

On the right hand side, we have introduced the ‘transverse current’. Its divergence is zero because of Eq.(2.29) and charge conservation:

$$\nabla \cdot \mathbf{j}_\perp = \nabla \cdot \mathbf{j} + \partial_t \rho = 0. \quad (2.32)$$

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 (2.31) 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):

$$\partial_t u + \nabla \cdot \mathbf{S} = -\mathbf{j} \cdot \mathbf{E} \quad (2.33)$$

$$u = \frac{\varepsilon_0}{2} \mathbf{E}^2 + \frac{\mu_0}{2} \mathbf{H}^2 \quad \text{energy density} \quad (2.34)$$

$$\mathbf{S} = \mathbf{E} \times \mathbf{H} \quad \text{Poynting vector} \quad (2.35)$$

Field momentum and angular momentum: see textbooks, for example Cohen-Tannoudji & al. (1987).

## 2.5.2 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)

$$\mathbf{\Pi} = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{A}}} = -\varepsilon_0 \mathbf{E} \quad (2.36)$$

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

$$H = \int dV \left( \frac{1}{2\varepsilon_0} \mathbf{\Pi}^2 + \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 \right) \quad (2.37)$$

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

$$\{A_i(\mathbf{x}), \Pi_j(\mathbf{x}')\} = -\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') \quad (2.38)$$

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

$$F_i(\mathbf{x}) = \sum_j \int d^3x' \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') F_j(\mathbf{x}') \quad (2.39)$$

while vector fields that are not transverse are projected into the subspace of transverse fields. The Poisson bracket in Eq.(2.38) is an integral over (functional derivatives) with respect to the vector potential and the conjugate momentum field. More details follow in Section 2.8.

**Diagonalize the field energy.** In the field Hamiltonian (2.37), 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  $\mathbf{\Pi}$ )

$$\mathbf{A}(\mathbf{x}) = \sum_{\mathbf{k}} \mathbf{A}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \quad (2.40)$$

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

$$H = V \sum_{\mathbf{k}} \left( \frac{1}{2\varepsilon_0} \mathbf{\Pi}_{\mathbf{k}} \cdot \mathbf{\Pi}_{-\mathbf{k}} + \frac{\varepsilon_0 c^2 k^2}{2} \mathbf{A}_{\mathbf{k}} \cdot \mathbf{A}_{-\mathbf{k}} \right). \quad (2.41)$$

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  $\omega_{\mathbf{k}}^2 = k^2 / \varepsilon_0 \mu_0 = c^2 k^2$ .

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.(2.38), we introduce the plane wave expansion of the transverse  $\delta$ -function:

$$\delta_{ij}^{\perp}(\mathbf{x} - \mathbf{x}') = \sum_{\mathbf{k}\mu} \frac{e_{\mathbf{k}\mu i} e_{\mathbf{k}\mu j}^*}{V} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \quad (2.42)$$

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.

### 2.5.3 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

$$i [\hat{A}_i(\mathbf{x}), \hat{\Pi}_j(\mathbf{x}')] = -\hbar \delta_{ij}^{\perp}(\mathbf{x} - \mathbf{x}') \quad (2.43)$$

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  $\delta$ -function is not local in space (see the exercises).

When we insert the mode expansions for  $\mathbf{A}$  and  $\mathbf{\Pi}$  in the commutator (2.43), we get a (double) sum over  $\mathbf{k}, \mu$ . Comparing each term in the sum to the plane-wave expansion of the transverse  $\delta$ -function [Eq.(2.42)], we get

$$i [\hat{A}_{\mathbf{k}i}, \hat{\Pi}_{\mathbf{k}'j}] = -\frac{\hbar}{V} \delta_{\mathbf{k}+\mathbf{k}',0} \sum_{\mu} e_{\mathbf{k}\mu i} e_{\mathbf{k}\mu j}^* \quad (2.44)$$

We implement this commutator by introducing annihilation and creation operators  $a_{\mathbf{k}\mu}, a_{\mathbf{k}\mu}^{\dagger}$ , see Eqs.(2.52, 2.53) 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 (2.41))

$$\hat{H} = \frac{V}{2\varepsilon_0} \hat{p}^2 + \frac{V\varepsilon_0\omega_k^2}{2} \hat{x}^2 \quad (2.45)$$

We also simplify the commutation relation (2.43) into

$$i [\hat{x}, \hat{p}] = -\frac{\hbar}{V} \quad (2.46)$$

To implement this, we try the definitions

$$\hat{x} = \sqrt{\frac{\hbar}{2V}} \lambda (a + a^{\dagger}) \quad (2.47)$$

$$\hat{p} = \sqrt{\frac{\hbar}{2V}} \frac{1}{i\lambda} (a - a^{\dagger}) \quad (2.48)$$

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

$$-\frac{\hbar}{V} \stackrel{!}{=} i[\hat{x}, \hat{p}] = \frac{\hbar}{2V} [\hat{a} + \hat{a}^\dagger, \hat{a} - \hat{a}^\dagger] = -\frac{\hbar}{V} [\hat{a}, \hat{a}^\dagger] \implies [\hat{a}, \hat{a}^\dagger] = 1 \quad (2.49)$$

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  $\lambda$  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 (2.45). Inserting Eqs.(2.47, 2.48), we get

$$\hat{H} = \frac{\hbar}{4} \left( -\frac{1}{\varepsilon_0 \lambda^2} (\hat{a} - \hat{a}^\dagger)^2 + \varepsilon_0 \omega_k^2 \lambda^2 (\hat{a} + \hat{a}^\dagger)^2 \right) \quad (2.50)$$

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  $\{\cdot, \cdot\}_+$ )

$$\hat{H} = \frac{\hbar \omega_k}{2} \{\hat{a}, \hat{a}^\dagger\}_+ = \frac{\hbar \omega_k}{2} (2\hat{a}^\dagger \hat{a} + 1) \quad (2.51)$$

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  $a^\dagger a b$  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 (2.47, 2.48) for the canonical operators to include the polarization label

$$\hat{\mathbf{A}}_{\mathbf{k}} = \sqrt{\frac{\hbar}{2\varepsilon_0\omega_k V}} \sum_{\mu} \left( \hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} + \hat{a}_{-\mathbf{k}\mu}^{\dagger} \mathbf{e}_{-\mathbf{k}\mu}^* \right) \quad (2.52)$$

$$\hat{\mathbf{\Pi}}_{\mathbf{k}} = \sqrt{\frac{\hbar\varepsilon_0\omega_k}{2V}} (-i) \sum_{\mu} \left( \hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} - \hat{a}_{-\mathbf{k}\mu}^{\dagger} \mathbf{e}_{-\mathbf{k}\mu}^* \right) \quad (2.53)$$

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 (2.49)):

$$[\hat{a}_{\mathbf{k}\mu}, \hat{a}_{\mathbf{k}'\mu'}] = 0, \quad [\hat{a}_{\mathbf{k}\mu}, \hat{a}_{\mathbf{k}'\mu'}^{\dagger}] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\mu\mu'} \quad (2.54)$$

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

$$i [\hat{A}_{\mathbf{k}i}, \hat{\Pi}_{\mathbf{k}'j}] = -\frac{\hbar}{2V} \delta_{\mathbf{k}, -\mathbf{k}'} \sum_{\mu} \left\{ e_{\mathbf{k}\mu i} e_{\mathbf{k}\mu j}^* + e_{-\mathbf{k}\mu i}^* e_{-\mathbf{k}\mu j} \right\} \quad (2.55)$$

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.(2.44).

## 2.5.4 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.(2.52) shows.) The operator ordering has fundamental consequences for the vacuum energy, as we shall see. There are two conventional choices

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

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

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

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

$$: a_{k\mu} a_{k'\mu'}^\dagger : = a_{k'\mu'}^\dagger a_{k\mu}. \quad (2.56)$$

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 (2.41), one gets

$$\begin{aligned} \hat{H} &= \sum_{\mathbf{k}} \frac{\hbar\omega_k}{8} (-) \sum_{\mu\mu'} \left\{ \hat{a}_{k\mu} \mathbf{e}_{k\mu} - \hat{a}_{-k\mu}^\dagger \mathbf{e}_{-k\mu}^*, \hat{a}_{-k\mu'} \mathbf{e}_{-k\mu'} - \hat{a}_{k\mu'}^\dagger \mathbf{e}_{k\mu'}^* \right\}_+ \\ &+ \sum_{\mathbf{k}} \frac{\hbar\omega_k}{8} \sum_{\mu\mu'} \left\{ \hat{a}_{k\mu} \mathbf{e}_{k\mu} + \hat{a}_{-k\mu}^\dagger \mathbf{e}_{-k\mu}^*, \hat{a}_{-k\mu'} \mathbf{e}_{-k\mu'} + \hat{a}_{k\mu'}^\dagger \mathbf{e}_{k\mu'}^* \right\}_+ \end{aligned} \quad (2.57)$$

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

$$\mathbf{e}_{k\mu} \cdot \mathbf{e}_{k\mu'}^* = \mathbf{e}_{-k\mu}^* \cdot \mathbf{e}_{-k\mu'} = \delta_{\mu\mu'} \quad (2.58)$$

which brings us to a single sum over polarizations:

$$\hat{H} = \sum_{k\mu} \frac{\hbar\omega_k}{4} \left( \left\{ \hat{a}_{k\mu}, \hat{a}_{k\mu}^\dagger \right\}_+ + \left\{ \hat{a}_{-k\mu}^\dagger, \hat{a}_{-k\mu} \right\}_+ \right) \quad (2.59)$$

The second term gives, after the summation, the same result as the first term because the mode frequency  $\omega_k$  does not depend on the sign of  $\mathbf{k}$ . Hence, we get

a sum over modes as a simple generalization of Eq.(2.51):

$$\hat{H} = \sum_{\mathbf{k}\mu} \frac{\hbar\omega_k}{2} (2\hat{a}_{\mathbf{k}\mu}^\dagger \hat{a}_{\mathbf{k}\mu} + 1) \quad (2.60)$$

We discuss the structure of the Hilbert space (the eigenstates of  $\hat{H}$ ) in Sec.2.7.2. 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,

$$\hat{a}_{\mathbf{k}\mu}|\text{vac}\rangle = 0, \quad \text{for all } \mathbf{k}, \mu \quad (2.61)$$

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 (2.60) with an energy

$$\hat{H}|\text{vac}\rangle = E_{\text{vac}}|\text{vac}\rangle, \quad E_{\text{vac}} = \sum_{\mathbf{k}\mu} \frac{\hbar\omega_k}{2} \quad (2.62)$$

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.2.7.3, ??.

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

$$a_{\mathbf{k}\mu}(t) = a_{\mathbf{k}\mu} e^{-i\omega_k t} \quad (2.63)$$

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.(2.52) with the mode expansion to get

$$\hat{\mathbf{A}}(\mathbf{x}, t) = \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar}{2\varepsilon_0\omega_k V}} \left( \hat{a}_{\mathbf{k}\mu}(t) \mathbf{e}_{\mathbf{k}\mu} + \hat{a}_{-\mathbf{k}\mu}^\dagger(t) \mathbf{e}_{-\mathbf{k}\mu}^* \right) e^{i\mathbf{k}\cdot\mathbf{x}} \quad (2.64)$$



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:

$$\hat{\mathbf{A}}(\mathbf{x}, t) = \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar}{2\varepsilon_0\omega_k V}} \left( \hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_k t} + \text{h.c.} \right) \quad (2.65)$$

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

$$\hat{\mathbf{E}}(\mathbf{x}, t) = \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}} i \left( \hat{a}_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_k t} - \text{h.c.} \right) \quad (2.66)$$

$$\hat{\mathbf{B}}(\mathbf{x}, t) = \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar\omega_k \mu_0}{2V}} i \left( \hat{a}_{\mathbf{k}\mu} \mathbf{b}_{\mathbf{k}\mu} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_k t} - \text{h.c.} \right) \quad (2.67)$$

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,  $\frac{1}{2}\varepsilon_0 |\mathbf{E}|^2$ , 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 (2.65, 2.66, 2.67) yield the following commutation relations between the field operators (all of them follow from the basic commutator (2.43)):

$$i \left[ \hat{A}_i(\mathbf{x}), \hat{E}_j(\mathbf{x}') \right] = \frac{\hbar}{\varepsilon_0} \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') \quad (2.68)$$

$$i [\hat{B}_i(\mathbf{x}), \hat{E}_j(\mathbf{x}')] = -\frac{\hbar}{\varepsilon_0} \epsilon_{ijk} \partial_k \delta(\mathbf{x} - \mathbf{x}') \quad (2.69)$$

where 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  $\delta$ -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:

$$H_{\text{int}} = - \int d^3x \mathbf{j}^\perp(\mathbf{x}) \cdot \mathbf{A}(\mathbf{x}) \quad (2.70)$$

$$= - \sum_{\mathbf{k}\mu} \sqrt{\frac{\hbar}{2\varepsilon_0\omega_k V}} \{ a_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{k}\mu} \cdot \mathbf{j}_{\mathbf{k}}^{\perp*} + \text{h.c.} \}, \quad (2.71)$$

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).

## 2.6 Alternative formulations

- with continuous momentum (Fourier integrals).
- with general mode functions (Sec.2.8.4)
- 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

$$\mathbf{E}(\mathbf{x}, t) = \int d^3k \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0(2\pi)^3}} \sum_{\mu} \left( \mathbf{e}_{\mathbf{k}\mu} a_{\mathbf{k}\mu} e^{i\mathbf{k}\cdot\mathbf{x}} + \text{h.c.} \right) \quad (2.72)$$

We read off the replacement rule by comparison to (2.66): 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 (2.54) becomes

$$[\hat{a}_{\mathbf{k}\mu}, \hat{a}_{\mathbf{k}'\mu'}^\dagger] = \delta(\mathbf{k} - \mathbf{k}')\delta_{\mu\mu'} \quad (2.73)$$

The interpretation is now that the operator

$$d\hat{N} = \hat{a}_{\mathbf{k}\mu}^\dagger \hat{a}_{\mathbf{k}\mu} d^3k \quad (2.74)$$

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

$$\hat{N} = \int d^3k \sum_{\mu} \hat{a}_{\mathbf{k}\mu}^\dagger \hat{a}_{\mathbf{k}\mu}, \quad \hat{H} = \int d^3k \sum_{\mu} \hbar\omega_{\mathbf{k}} \hat{a}_{\mathbf{k}\mu}^\dagger \hat{a}_{\mathbf{k}\mu} \quad (2.75)$$

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

$$\begin{aligned} \hat{a} &= \int d^3k \sum_{\mu} \mathbf{f}(\mathbf{k}) \cdot \mathbf{e}_{\mathbf{k}\mu} a_{\mathbf{k}\mu} \\ \hat{b} &= \int d^3k \sum_{\mu} \mathbf{g}(\mathbf{k}) \cdot \mathbf{e}_{\mathbf{k}\mu} a_{\mathbf{k}\mu} \end{aligned} \quad (2.76)$$

Then the commutator is

$$\begin{aligned} [\hat{a}, \hat{b}^\dagger] &= \int d^3k d^3k' \sum_{\mu\mu'} \mathbf{f}(\mathbf{k}) \cdot \mathbf{e}_{\mathbf{k}\mu} \mathbf{g}^*(\mathbf{k}') \cdot \mathbf{e}_{\mathbf{k}'\mu'}^* [a_{\mathbf{k}\mu}, a_{\mathbf{k}'\mu'}^\dagger] \\ &= \int d^3k \sum_{\mu} \mathbf{f}(\mathbf{k}) \cdot \mathbf{g}^*(\mathbf{k}) = 0 \end{aligned} \quad (2.77)$$

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.

## 2.7 Photons and the quantum vacuum

### 2.7.1 ‘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

$$\int_{L^3} d^3x \mathbf{f}^*(\mathbf{x}) \cdot \mathbf{g}(\mathbf{x}). \quad (2.78)$$

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.

## 2.7.2 The Fock-Hilbert space

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

$$a_\kappa|\text{vac}\rangle = 0 \quad (2.79)$$

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

$$|1_\kappa\rangle = a_\kappa^\dagger|\text{vac}\rangle \quad (2.80)$$

...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  $n_\kappa$  photons in the mode  $\kappa$ . 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 infinitely many modes, even labelled by 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  $a_\kappa$  and  $a_\kappa^\dagger$  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).

### 2.7.3 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  $a_\kappa$  annihilates the vacuum state and  $a_\kappa^\dagger$  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. 2.7.2.

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

$$\frac{\hbar\omega_\kappa}{2\varepsilon_0} \langle (\mathbf{f}_\kappa(\mathbf{x})a(t) + \text{h.c.})^2 \rangle = \frac{\hbar\omega_\kappa}{2\varepsilon_0} |\mathbf{f}_\kappa(\mathbf{x})|^2 \langle a_\kappa(t)a_\kappa^\dagger(t) \rangle = \frac{\hbar\omega_\kappa}{2\varepsilon_0} |\mathbf{f}_\kappa(\mathbf{x})|^2 \quad (2.81)$$

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  $\lambda$  can be written in the form

$$\langle \mathbf{E}^2(\mathbf{x}, t) \rangle = \int_0^\infty \frac{d\omega}{2\pi} \frac{\hbar\omega}{2\varepsilon_0} \rho(\omega) \quad (2.82)$$

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

$$\rho(\mathbf{x}; \omega) = 2\pi \sum_\kappa |\mathbf{f}_\kappa(\mathbf{x})|^2 \delta(\omega - \omega_\kappa) = \frac{2\pi}{V} \sum_\kappa \delta(\omega - \omega_\kappa) \quad (2.83)$$

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

$$\sum_{\mathbf{k}} = V \int \frac{d^3k}{(2\pi)^3} \quad (2.84)$$

we get after a simple integration

$$\rho(\omega) = \frac{2}{\pi} \frac{\omega^2}{c^3} \quad (2.85)$$

The full vacuum fluctuation of the electric field is then infinite

$$\langle \mathbf{E}^2(\mathbf{x}, t) \rangle = \frac{\hbar}{\pi\varepsilon_0 c^3} \int_0^\infty \frac{d\omega}{2\pi} \omega^3 \quad (2.86)$$

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/cm<sup>3</sup>, 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

$$\langle \mathbf{E}(\mathbf{x}, t) \cdot \mathbf{E}(\mathbf{x}, t') \rangle = \int_0^\infty \frac{d\omega}{2\pi} \frac{\hbar\omega_\kappa}{2\varepsilon_0 c^3} \rho(\omega) e^{-i\omega(t-t')} \quad (2.87)$$

This leads to the integral representation of the  $\Gamma$ -function in the complex plane and finally to

$$\langle \mathbf{E}(\mathbf{x}, t) \cdot \mathbf{E}(\mathbf{x}, t') \rangle = \frac{3\hbar}{\pi^2 \varepsilon_0 c^3 \tau^4} \quad (2.88)$$

which is finite for all  $\tau = t - t' \neq 0$ . For any finite value of  $\tau$ , 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  $\lambda_\tau = c\tau$ .

## 2.8 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.

### 2.8.1 Transverse $\delta$ -function

We have encountered the ‘transverse  $\delta$ -function’  $\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}')$  in the commutator (2.43) between the vector potential and its canonically conjugate momentum. This is a distribution that acts like a  $\delta$ -function on fields with zero divergence, and projects an arbitrary vector field  $\mathbf{F}$  on its transverse part  $\mathbf{F}^\perp$

$$F_i^\perp(\mathbf{x}) = \int d^3x' \delta_{im}^\perp(\mathbf{x} - \mathbf{x}') F_m(\mathbf{x}') \quad (2.89)$$

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

$$F_j^\perp(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \frac{k^2 \delta_{jl} - k_j k_l}{k^2} \tilde{F}_l(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} \quad (2.90)$$

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  $\delta$ -function.

Note that in the wave equation (2.31) 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.

### 2.8.2 Matter

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

$$\rho(\mathbf{x}, t) = \sum_\alpha e_\alpha \delta(\mathbf{x} - \mathbf{r}_\alpha(t)), \quad \mathbf{j}(\mathbf{x}, t) = \sum_\alpha e_\alpha \mathbf{v}_\alpha(t) \delta(\mathbf{x} - \mathbf{r}_\alpha(t)) \quad (2.91)$$

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:

$$\frac{d}{dt} \frac{m_\alpha \mathbf{v}_\alpha}{\sqrt{1 - v_\alpha^2/c^2}} = e_\alpha (\mathbf{E}(\mathbf{r}_\alpha) + \mathbf{v}_\alpha \times \mathbf{B}(\mathbf{r}_\alpha)) \quad (2.92)$$

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  $\mathbf{r}_\alpha$  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.(2.30).) 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

$$E_n = -\frac{\text{Ryd}}{n^2} = -\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2} \frac{1}{n^2} \quad (2.93)$$

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

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \quad (2.94)$$

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

$$\lambda = \frac{\hbar c}{\text{Ryd}} = \frac{2}{\alpha_{\text{fs}}} a_0 \quad (2.95)$$

$$\frac{1}{\alpha_{\text{fs}}} = \frac{4\pi\epsilon_0 \hbar c}{e^2} \approx 137 \quad (2.96)$$

Here,  $\alpha_{\text{fs}}$  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 (2.92) has therefore only a weak dependence on  $\mathbf{r}_\alpha$ ;
- 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.



### 2.8.3 Lagrange-Hamilton formulation

**Lagrangian.** We now proceed to quantize the wave equation (2.31) in the ‘canonical way’. The first step is to guess the corresponding Lagrangian. A good guess is the Lagrangian

$$L = - \sum_{\alpha} m_{\alpha} c^2 \sqrt{1 - \dot{\mathbf{r}}_{\alpha}^2 / c^2} + \int d^3x \mathcal{L}_{F+I} \quad (2.97)$$

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

$$\mathcal{L}_{F+I} = \frac{\varepsilon_0}{2} \left( \dot{\mathbf{A}} + \nabla\phi \right)^2 - \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 - \phi\rho + \mathbf{A} \cdot \mathbf{j}. \quad (2.98)$$

Via the Euler-Lagrange equations, one gets the Maxwell equations (2.29,2.31) for the fields and the Newton-Lorentz equation (2.92) for the particles. Note that the Lagrangian (2.97,2.98) is invariant under gauge transformations

$$\phi \mapsto \phi - \partial_t \chi, \quad \mathbf{A} \mapsto \mathbf{A} + \nabla \chi \quad (2.99)$$

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 (2.98). The mixed term is

$$\dot{\mathbf{A}} \cdot \nabla\phi = \nabla \cdot (\dot{\mathbf{A}}\phi) - \phi \nabla \cdot \dot{\mathbf{A}} \quad (2.100)$$

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

$$(\nabla\phi)^2 = \nabla \cdot (\phi \nabla\phi) - \phi \nabla^2 \phi = \nabla \cdot (\phi \nabla\phi) + \phi\rho/\varepsilon_0 \quad (2.101)$$

using the Laplace equation (2.29). 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:

$$V_{\text{Coul}} = \frac{1}{2} \int d^3x \phi\rho = \frac{1}{2} \int d^3x d^3x' \frac{\rho(\mathbf{x})\rho(\mathbf{x}')}{4\pi\varepsilon_0 |\mathbf{x} - \mathbf{x}'|} \quad (2.102)$$

$$= \frac{1}{2} \sum_{\alpha\beta} \frac{e_{\alpha}e_{\beta}}{4\pi\varepsilon_0 |\mathbf{r}_{\alpha} - \mathbf{r}_{\beta}|} \quad (2.103)$$

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:

$$L = - \sum_{\alpha} m_{\alpha} c^2 \sqrt{1 - v_{\alpha}^2/c^2} - V_{\text{Coul}}(\{\mathbf{r}_{\alpha}\}) + \int d^3x \mathcal{L}_{\text{F+I}}^{\perp} \quad (2.104)$$

with

$$\mathcal{L}_{\text{F+I}}^{\perp} = \frac{\varepsilon_0}{2} \dot{\mathbf{A}}^2 - \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 + \mathbf{A} \cdot \mathbf{j}. \quad (2.105)$$

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  $\mathbf{r}_{\alpha}$  and  $\mathbf{A}$ :

$$\mathbf{p}_{\alpha} = \frac{\partial L}{\partial \dot{\mathbf{r}}_{\alpha}} = \frac{m \dot{\mathbf{r}}_{\alpha}}{\sqrt{1 - \dot{\mathbf{r}}_{\alpha}^2/c^2}} + e_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha}) \quad (2.106)$$

$$\mathbf{\Pi}(\mathbf{x}) = \frac{\delta L}{\delta \dot{\mathbf{A}}(\mathbf{x})} = \varepsilon_0 \dot{\mathbf{A}}(\mathbf{x}) \quad (2.107)$$

The particle momentum contains the relativistic kinetic momentum and an electromagnetic contribution. For the field momentum, it looks as if  $\varepsilon_0$  where 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:

$$L[\mathbf{A}(\mathbf{x}) + \delta \mathbf{A}(\mathbf{x})] \approx L[\mathbf{A}(\mathbf{x})] + \int d^3x \left. \frac{\delta L}{\delta \mathbf{A}(\mathbf{x})} \right|_{\mathbf{A}(\mathbf{x})} \delta \mathbf{A}(\mathbf{x}) + \mathcal{O}(\delta \mathbf{A}^2) \quad (2.108)$$

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 (2.108) expression (2.107) for the field momentum  $\mathbf{\Pi}$ . We shall return to a less trivial example below.

The Hamiltonian is given by

$$H = \sum_{\alpha} \mathbf{p}_{\alpha} \cdot \dot{\mathbf{r}}_{\alpha} + \int d^3x \mathbf{\Pi} \cdot \dot{\mathbf{A}} - L \quad (2.109)$$

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

$$H = \sqrt{[\mathbf{p}_{\alpha} - e_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha})]^2 c^2 + m^2 c^4} + V_{\text{Coul}}(\{\mathbf{r}_{\alpha}\}) + \int d^3x \left[ \frac{\mathbf{\Pi}^2}{2\varepsilon_0} + \frac{(\nabla \times \mathbf{A})^2}{2\mu_0} \right] \quad (2.110)$$

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 (2.109).)

**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 (2.31).

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

$$\dot{Q} = \{H, Q\} \quad (2.111)$$

where we define

$$\begin{aligned} \{A, B\} = & \sum_{\alpha} \frac{\partial A}{\partial \mathbf{p}_{\alpha}} \cdot \frac{\partial B}{\partial \mathbf{r}_{\alpha}} - \frac{\partial A}{\partial \mathbf{r}_{\alpha}} \cdot \frac{\partial B}{\partial \mathbf{p}_{\alpha}} \\ & + \int d^3x \left[ \frac{\delta A}{\delta \mathbf{\Pi}(\mathbf{x})} \cdot \frac{\delta B}{\delta \mathbf{A}(\mathbf{x})} - \frac{\delta A}{\delta \mathbf{A}(\mathbf{x})} \cdot \frac{\delta B}{\delta \mathbf{\Pi}(\mathbf{x})} \right] \end{aligned} \quad (2.112)$$

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 (2.112) contributes, and we get (after some calculations) the relativistic relation between velocity and momentum, Eq.(2.106). 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

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})} \sqrt{[\mathbf{p}_{\alpha} - e_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha})]^2 c^2 + m^2 c^4} \quad (2.113)$$

We note first that

$$\frac{\delta \mathbf{A}(\mathbf{r}_{\alpha})}{\delta \mathbf{A}(\mathbf{x})} = \delta(\mathbf{r}_{\alpha} - \mathbf{x}) \quad (2.114)$$

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

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})} \sqrt{[\mathbf{p}_{\alpha} - e_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha})]^2 c^2 + m^2 c^4} = \delta(\mathbf{r}_{\alpha} - \mathbf{x}) \frac{e_{\alpha} (\mathbf{p}_{\alpha} - e_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha})) c^2}{\sqrt{[\mathbf{p}_{\alpha} - e_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha})]^2 c^2 + m^2 c^4}} \quad (2.115)$$

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

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})} \frac{1}{2\mu_0} \int d^3x (\nabla \times \mathbf{A})^2 \quad (2.116)$$

that we handle with the mathematical definition (2.108). Consider a small change  $\mathbf{a}(\mathbf{x})$  of the vector potential. To linear order, this gives a change

$$\begin{aligned} (\nabla \times (\mathbf{A} + \mathbf{a}))^2 - (\nabla \times \mathbf{A})^2 &\approx 2(\nabla \times \mathbf{a}) \cdot (\nabla \times \mathbf{A}) \\ &= 2\nabla \cdot [\mathbf{a} \times (\nabla \times \mathbf{A})] + 2\mathbf{a} \cdot [\nabla \times (\nabla \times \mathbf{A})] \end{aligned} \quad (2.117)$$

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

$$-\frac{1}{2\mu_0} \frac{\delta}{\delta \mathbf{A}(\mathbf{x})} \int d^3x (\nabla \times \mathbf{A})^2 = -\frac{1}{\mu_0} \nabla \times (\nabla \times \mathbf{A}) \quad (2.118)$$

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

$$\dot{\mathbf{H}} = \varepsilon_0 \ddot{\mathbf{A}} = \mathbf{j}(\mathbf{x}) - \frac{1}{\mu_0} \nabla \times (\nabla \times \mathbf{A}) \quad \dots \text{wrong} \quad (2.119)$$

which is nearly equivalent to the wave equation (2.31). 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 (2.104) and the Hamiltonian (2.110). 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 (2.99) to remove the nonzero divergence. This fixes the ‘gauge function’ to satisfy

$$\nabla^2 \chi = -\nabla \cdot \mathbf{A} \quad (2.120)$$

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

$$\chi(\mathbf{x}) = \frac{1}{4\pi} \int d^3x' \frac{\nabla' \cdot \mathbf{A}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \quad (2.121)$$

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

$$\mathbf{A}_\perp(\mathbf{x}) = \mathbf{A}(\mathbf{x}) + \frac{1}{4\pi} \int d^3x' [\nabla' \cdot \mathbf{A}(\mathbf{x}')] \nabla \frac{1}{|\mathbf{x} - \mathbf{x}'|} \quad (2.122)$$

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

$$A_{\perp i}(\mathbf{x}) = \int d^3x' \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') A_j(\mathbf{x}') \quad (2.123)$$

where the transverse  $\delta$ -function appears for which we have just derived the following representation

$$\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') = \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') + \frac{1}{4\pi} \frac{\partial'_j \partial'_i}{|\mathbf{x} - \mathbf{x}'|} \quad (2.124)$$

A careful evaluation of the second derivatives yields the explicit result

$$\delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') = \frac{2}{3} \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') - \frac{1}{4\pi} \left( \frac{\delta_{ij}}{r^3} - 3 \frac{r_i r_j}{r^5} \right), \quad \mathbf{r} = \mathbf{x} - \mathbf{x}' \quad (2.125)$$

By construction, the transverse  $\delta$ -function acts like a usual  $\delta$ -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

$$\int d^3x' \frac{\delta H}{\delta \Pi_j(\mathbf{x}')} \frac{\delta A_{\perp i}(\mathbf{x})}{\delta A_j(\mathbf{x}')} = \int d^3x' \frac{\delta H}{\delta \Pi_j(\mathbf{x}')} \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') = \left( \frac{\delta H}{\delta \Pi(\mathbf{x}')} \right)_{\perp i} \quad (2.126)$$

The functional derivative with respect to  $\mathbf{A}$  makes the transverse  $\delta$ -function appear. The integral over  $\mathbf{x}'$  then projects the functional derivative with respect to  $\Pi$  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 (2.31).

## 2.8.4 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. 2.5.2. Note that we ignore for the moment the matter-field coupling: we focus on the field Hamiltonian only.

We adopt the expansion

$$\begin{pmatrix} \mathbf{A}(\mathbf{x}, t) \\ \Pi(\mathbf{x}, t) \end{pmatrix} = \sum_{\kappa} \mathbf{f}_{\kappa}(\mathbf{x}) \begin{pmatrix} q_{\kappa}(t) \\ p_{\kappa}(t) \end{pmatrix} \quad (2.127)$$

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  $\Pi^2$  becomes simple if we impose the modes to be orthogonal:

$$\int d^3x \mathbf{f}_{\kappa}(\mathbf{x}) \cdot \mathbf{f}_{\kappa'}(\mathbf{x}) = N_{\kappa} \delta_{\kappa\kappa'} \quad (2.128)$$

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

$$\frac{1}{2\varepsilon_0} \int d^3x \Pi^2 = \sum_{\kappa} N_{\kappa} \frac{p_{\kappa}^2}{2\varepsilon_0} \quad (2.129)$$

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

$$\begin{aligned} & \int d^3x (\nabla \times \mathbf{f}_{\kappa}) \cdot (\nabla \times \mathbf{f}_{\kappa'}) \\ &= \int d\mathbf{A} \cdot [\mathbf{f}_{\kappa} \times (\nabla \times \mathbf{f}_{\kappa'})] + \int d^3x \mathbf{f}_{\kappa} \cdot [\nabla \times (\nabla \times \mathbf{f}_{\kappa'})] \end{aligned} \quad (2.130)$$

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  $\kappa$ . The boundary term can nevertheless be

made to vanish if either (i) the mode function  $\mathbf{f}_\kappa$  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,  $\mathbf{f}_\kappa$  is proportional to the electric field, and the integrand in Eq.(2.130) 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 (2.130) is reduced to the orthogonality relation if we require the mode functions to be eigenfunctions of the (vector) Helmholtz equation:

$$\nabla \times (\nabla \times \mathbf{f}_\kappa) = \varepsilon_0 \mu_0 \omega_\kappa^2 \mathbf{f}_\kappa \quad (2.131)$$

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

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

$$H_F = \sum_\kappa \left[ \frac{N_\kappa}{2\varepsilon_0} p_\kappa^2 + \frac{\varepsilon_0}{2} N_\kappa \omega_\kappa^2 q_\kappa^2 \right] \quad (2.132)$$

We now fix the normalization to be  $N_\kappa = 1$  and get a sum of harmonic oscillator Hamiltonians, one for each mode  $\kappa$  with ‘mass’  $\varepsilon_0$  and frequency  $\omega_\kappa$ .

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  $\kappa$  is discrete) is therefore misleading. Quantization is something different, as we shall see now.

**Mode operators.** Quantization proceeds by promoting the  $p_\kappa$  and  $q_\kappa$  to operators with the commutation relations

$$\frac{i}{\hbar} [p_\kappa, q_{\kappa'}] = \delta_{\kappa\kappa'} \quad (2.133)$$

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

$$\frac{i}{\hbar} [\Pi_i(\mathbf{x}), A_j(\mathbf{x}')] = \sum_\kappa f_{\kappa i}(\mathbf{x}) f_{\kappa j}(\mathbf{x}') \stackrel{!}{=} \delta_{ij}^\perp(\mathbf{x} - \mathbf{x}') \quad (2.134)$$

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  $\delta$ -function—the one that comes by applying the finite volume boundary conditions to the equation (2.120).

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,  $a_\kappa^\dagger$  and  $a_\kappa$ , correspond to the ‘creation’ and ‘destruction’ of one ‘photon’. The mode coordinate and momentum operators are given by

$$q_\kappa = \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa}} (a_\kappa + a_\kappa^\dagger) \quad (2.135)$$

$$p_\kappa = \sqrt{\frac{\hbar\varepsilon_0\omega_\kappa}{2}} i (a_\kappa^\dagger - a_\kappa) \quad (2.136)$$

where we continue to write  $\varepsilon_0$  for the oscillator mass and where the commutation relation is

$$[a_\kappa, a_{\kappa'}^\dagger] = \delta_{\kappa\kappa'} \quad (2.137)$$

The field Hamiltonian then takes the form

$$H_F = \sum_\kappa \frac{\hbar\omega_\kappa}{2} (a_\kappa a_\kappa^\dagger + a_\kappa^\dagger a_\kappa) = \sum_\kappa \hbar\omega_\kappa (a_\kappa^\dagger a_\kappa + \frac{1}{2}) \quad (2.138)$$

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  $\kappa$ . 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

$$\mathbf{A}(\mathbf{x}, t) = \sum_\kappa \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa}} \mathbf{f}_\kappa(\mathbf{x}) (a_\kappa e^{-i\omega_\kappa t} + a_\kappa^\dagger e^{i\omega_\kappa t}). \quad (2.139)$$

We have used here the Heisenberg picture for the vector potential operator. From the Hamiltonian (2.138), 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

$$\int d^3x \mathbf{f}_\kappa^*(\mathbf{x}) \cdot \mathbf{f}_{\kappa'}(\mathbf{x}) = \delta_{\kappa\kappa'} \quad (2.140)$$

instead of Eq.(2.128). This can be ensured with the choice

$$\mathbf{f}_\kappa(\mathbf{x}) = \frac{1}{\sqrt{V}} \mathbf{e}_\kappa e^{i\mathbf{k}\cdot\mathbf{x}} \quad (2.141)$$

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  $\mathbf{e}_\kappa$  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 (2.131). 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

$$\mathbf{A}_\perp(\mathbf{x}, t) = \sum_\kappa \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa V}} \left( \mathbf{e}_\kappa e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_\kappa t)} a_\kappa + \text{h.c.} \right). \quad (2.142)$$

$$\mathbf{E}_\perp(\mathbf{x}, t) = \sum_\kappa \sqrt{\frac{\hbar\omega_\kappa}{2\varepsilon_0 V}} \left( i\mathbf{e}_\kappa e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_\kappa t)} a_\kappa + \text{h.c.} \right). \quad (2.143)$$

$$\mathbf{B}(\mathbf{x}, t) = \sum_\kappa \sqrt{\frac{\hbar\omega_\kappa\mu_0}{2V}} \left( i\mathbf{b}_\kappa e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_\kappa t)} a_\kappa + \text{h.c.} \right). \quad (2.144)$$

Sometimes, you may encounter these formulas without the factor  $i$ . Then the operators  $a_{\mathbf{k}\lambda}$  are being used instead, but they have the same commutation relations. Note that Eq.(2.143) gives only the ‘transverse’ part of the electric field. The ‘longitudinal’ part,  $-\nabla\phi$ , is determined according to (2.29) by the charge density.

Note: A useful shortcut to derive the prefactors is the following: for each mode, match the energy density  $\frac{1}{2}\varepsilon_0\mathbf{E}^2 + (1/2\mu_0)\mathbf{B}^2$  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  $a_\kappa$  and include the source current. Solve it for known time-dependence of current.

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