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Introduction to Quantum Optics

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The preliminary programme for this lecture:

1. Field quantization: QED

   — canonical scheme in the Coulomb gauge

   — field states (photon number states, thermal, coherent, squeezed states)

   — quantum (or vacuum) fluctuations

2. Atom-field dynamics

   — atom-light coupling

   — the model of a two-level atom

   — spontaneous emission and Bloch equations

   — elementary photodetector theory

3. Applications in photonics

   — quantum laser theory

   — quantum state manipulation with optical elements

Chapter 1

The quantized field

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

1.1 Canonical quantization

1.1.1 Fields

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

$$\begin{aligned} \nabla \cdot \mathbf{B} = 0 \qquad & \varepsilon_0 \nabla \cdot \mathbf{E} = \rho \\ \nabla \times \mathbf{E} + \partial_t \mathbf{B} = 0 \qquad & \nabla \times \mathbf{B} - \frac{1}{c^2} \partial_t \mathbf{E} = \mu_0 \mathbf{j} \end{aligned} \tag{1.1}$$

Introducing the scalar and vector potentials via

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{1.2}$$

$$\mathbf{E} = -\nabla \phi - \partial_t \mathbf{A}, \tag{1.3}$$

the left column of (1.1) is identically fulfilled. The Coulomb law then becomes

$$-\varepsilon_0 \triangle \phi - \varepsilon_0 \nabla \partial_t \mathbf{A} = \rho \tag{1.4}$$

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:

$$-\varepsilon_0 \triangle \phi = \rho \tag{1.5}$$

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 $\triangle \phi = 0$ has no nontrivial solutions. In free space, with $\phi(\mathbf{x} \to \infty) \to 0$, we get

$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int \mathrm{d}^3 x' \, \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \tag{1.6}$$

which is a superposition of well-known Coulomb potentials.

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

$$\nabla \times (\nabla \times \mathbf{A}) + \frac{1}{c^2} \partial_t^2 \mathbf{A} = \mu_0 \left(\mathbf{j} - \varepsilon_0 \partial_t \nabla \phi \right) \equiv \mu_0 \mathbf{j}_\perp . \tag{1.7}$$

On the right hand side, we have introduced the 'transverse current'. Its divergence is zero because of Eq.(1.5) and charge conservation:

$$\nabla \cdot \mathbf{j}_\perp = \nabla \cdot \mathbf{j} + \partial_t \rho = 0. \tag{1.8}$$

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 (1.7) ensures that if $\mathbf{A}$ is transverse at one time, it is also transverse at all later times.

Conservation laws. Energy (Poynting theorem):

$$\partial_t u + \nabla \cdot \mathbf{S} = -\mathbf{j} \cdot \mathbf{E} \tag{1.9}$$

$$u = \frac{\varepsilon_0}{2} \mathbf{E}^2 + \frac{1}{2\mu_0} \mathbf{B}^2 \qquad \text{energy density} \tag{1.10}$$

$$\mathbf{S} = \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B} \qquad \text{Poynting vector} \tag{1.11}$$

Momentum (see exercise). Charge: $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$.

1.1.2 Matter

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

$$\rho(\mathbf{x},t) = \sum_\alpha e_\alpha \delta(\mathbf{x} - \mathbf{r}_\alpha(t)), \qquad \mathbf{j}(\mathbf{x},t) = \sum_\alpha e_\alpha \mathbf{v}_\alpha(t) \delta(\mathbf{x} - \mathbf{r}_\alpha(t)) \tag{1.12}$$

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:

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{m_\alpha \mathbf{v}_\alpha}{\sqrt{1 - v_\alpha^2/c^2}} = e_\alpha \left(\mathbf{E}(\mathbf{r}_\alpha) + \mathbf{v}_\alpha \times \mathbf{B}(\mathbf{r}_\alpha) \right) \tag{1.13}$$

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.(1.6).) 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

$$E_n = -\frac{\mathrm{Ryd}}{n^2} = -\frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2}\frac{1}{n^2} \tag{1.14}$$

where the Rydberg constant is $1\,\mathrm{Ryd} \approx 13.6\,\mathrm{eV}$. (In cgs units, drop the factor $(4\pi\varepsilon_0)^2$.) The size of the Hydrogen atom is of the order of the Bohr

radius

$$a_0 = \frac{4\pi\varepsilon_0\,\hbar^2}{me^2} \tag{1.15}$$

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

$$\lambda = \frac{\hbar c}{\mathrm{Ryd}} = \frac{2}{\alpha_{\mathrm{fs}}} a_0 \tag{1.16}$$

$$\frac{1}{\alpha_{\mathrm{fs}}} = \frac{4\pi\varepsilon_0\,\hbar c}{e^2} \approx 137 \tag{1.17}$$

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 $1/\alpha_{\mathrm{fs}} \approx 137$ 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 (1.13) 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.

1.1.3 Lagrange-Hamilton formulation

Lagrangian. We now proceed to quantize the wave equation (1.7) in the 'canonical way'. The first step is to guess the corresponding Lagrangian. A good guess is the Lagrangian

$$L = -\sum_\alpha m_\alpha c^2 \sqrt{1 - \dot{\mathbf{r}}_\alpha^2/c^2} + \int \mathrm{d}^3x\, \mathcal{L}_{F+I} \tag{1.18}$$

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

$$\mathcal{L}_{F+I} = \frac{\varepsilon_0}{2}\left(\dot{\mathbf{A}} + \nabla\phi\right)^2 - \frac{1}{2\mu_0}(\nabla\times\mathbf{A})^2 - \phi\rho + \mathbf{A}\cdot\mathbf{j}. \tag{1.19}$$

Via the Euler-Lagrange equations, one gets the Maxwell equations (1.5,1.7) for the fields and the Newton-Lorentz equation (1.13) for the particles. Note that the Lagrangian (1.18,1.19) is invariant under gauge transformations

$$\phi \mapsto \phi - \partial_t \chi, \qquad \mathbf{A} \mapsto \mathbf{A} + \nabla\chi \tag{1.20}$$

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 (1.19). The mixed term is

$$\dot{\mathbf{A}} \cdot \nabla\phi = \nabla \cdot (\dot{\mathbf{A}}\phi) - \phi \nabla \cdot \dot{\mathbf{A}} \tag{1.21}$$

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

$$(\nabla\phi)^2 = \nabla \cdot (\phi\nabla\phi) - \phi\triangle\phi = \nabla \cdot (\phi\nabla\phi) + \phi\rho/\varepsilon_0 \tag{1.22}$$

using the Laplace equation (1.5). 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:

$$V_{\text{Coul}} = \frac{1}{2}\int \mathrm{d}^x\, \phi\rho = \frac{1}{2}\int \mathrm{d}^3x\, \mathrm{d}^3x'\, \frac{\rho(\mathbf{x})\rho(\mathbf{x}')}{4\pi\varepsilon_0\,|\mathbf{x}-\mathbf{x}'|} \tag{1.23}$$

$$= \frac{1}{2}\sum_{\alpha\beta} \frac{e_\alpha e_\beta}{4\pi\varepsilon_0\,|\mathbf{r}_\alpha - \mathbf{r}_\beta|} \tag{1.24}$$

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:

$$L = -\sum_\alpha m_\alpha c^2 \sqrt{1 - v_\alpha^2/c^2} - V_{\mathrm{Coul}}(\{\mathbf{r}_\alpha\}) + \int \mathrm{d}^3x\, \mathcal{L}^\perp_{\mathrm{F+I}} \tag{1.25}$$

with

$$\mathcal{L}^\perp_{\mathrm{F+I}} = \frac{\varepsilon_0}{2}\dot{\mathbf{A}}^2 - \frac{1}{2\mu_0}(\nabla \times \mathbf{A})^2 + \mathbf{A}\cdot\mathbf{j}. \tag{1.26}$$

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 $\mathbf{A}$:

$$\mathbf{p}_\alpha = \frac{\partial L}{\partial \dot{\mathbf{r}}_\alpha} = \frac{m\dot{\mathbf{r}}_\alpha}{\sqrt{1 - \dot{\mathbf{r}}_\alpha^2/c^2}} + e_\alpha \mathbf{A}(\mathbf{r}_\alpha) \tag{1.27}$$

$$\mathbf{\Pi}(\mathbf{x}) = \frac{\delta L}{\delta \dot{\mathbf{A}}(\mathbf{x})} = \varepsilon_0 \dot{\mathbf{A}}(\mathbf{x}) \tag{1.28}$$

The particle momentum contains the relativistic kinetic momentum and an electromagnetic contribution. For the field momentum, it looks as if ε_0 where the 'mass' and $\dot{\mathbf{A}}$ the velocity.

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:

$$\begin{aligned} &L[\mathbf{A}(\mathbf{x}) + \delta\mathbf{A}(\mathbf{x})] \approx L[\mathbf{A}(\mathbf{x})] \\ &+ \int \mathrm{d}^3x\, \left.\frac{\delta L}{\delta \mathbf{A}(\mathbf{x})}\right|_{\mathbf{A}(\mathbf{x})} \delta\mathbf{A}(\mathbf{x}) + \mathcal{O}(\delta\mathbf{A}^2) \end{aligned} \tag{1.29}$$

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 (1.29) expression (1.28) for the field momentum $\mathbf{\Pi}$. We shall return to a less trivial example below.

The Hamiltonian is given by

$$H = \sum_\alpha \mathbf{p}_\alpha \cdot \dot{\mathbf{r}}_\alpha + \int \mathrm{d}^3x\, \mathbf{\Pi} \cdot \dot{\mathbf{A}} - L \tag{1.30}$$

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

$$\begin{aligned} H &= \sqrt{[\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha)]^2 c^2 + m^2 c^4} + V_{\mathrm{Coul}}(\{\mathbf{r}_\alpha\}) \\ &\quad + \int \mathrm{d}^3x \left[\frac{\mathbf{\Pi}^2}{2\varepsilon_0} + \frac{(\nabla \times \mathbf{A})^2}{2\mu_0} \right] \end{aligned} \tag{1.31}$$

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 (1.30).)

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 (1.7).

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

$$\dot{Q} = \{H,\, Q\} \tag{1.32}$$

where we define

$$\begin{aligned} \{A,\, B\} &= \sum_\alpha \frac{\partial A}{\partial \mathbf{p}_\alpha} \cdot \frac{\partial B}{\partial \mathbf{r}_\alpha} - \frac{\partial A}{\partial \mathbf{r}_\alpha} \cdot \frac{\partial B}{\partial \mathbf{p}_\alpha} \\ &\quad + \int \mathrm{d}^3x \left[\frac{\delta A}{\delta \mathbf{\Pi}(\mathbf{x})} \cdot \frac{\delta B}{\delta \mathbf{A}(\mathbf{x})} - \frac{\delta A}{\delta \mathbf{A}(\mathbf{x})} \cdot \frac{\delta B}{\delta \mathbf{\Pi}(\mathbf{x})} \right] \end{aligned} \tag{1.33}$$

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 $\{H, \mathbf{r}\}$, only the second term of the first line in (1.33) contributes, and we get (after some calculations) the relativistic relation between velocity and momentum, Eq.(1.27). 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

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})}\sqrt{[\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha)]^2 c^2 + m^2 c^4} \tag{1.34}$$

We note first that

$$\frac{\delta \mathbf{A}(\mathbf{r}_\alpha)}{\delta \mathbf{A}(\mathbf{x})} = \delta(\mathbf{r}_\alpha - \mathbf{x}) \tag{1.35}$$

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

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})}\sqrt{[\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha)]^2 c^2 + m^2 c^4} = \delta(\mathbf{r}_\alpha - \mathbf{x})\frac{e_\alpha(\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha))c^2}{\sqrt{[\mathbf{p}_\alpha - e_\alpha \mathbf{A}(\mathbf{r}_\alpha)]^2 c^2 + m^2 c^4}} \tag{1.36}$$

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

$$-\frac{\delta}{\delta \mathbf{A}(\mathbf{x})}\frac{1}{2\mu_0}\int \mathrm{d}^3x (\nabla \times \mathbf{A})^2 \tag{1.37}$$

that we handle with the mathematical definition (1.29). Consider a small change $\mathbf{a}(\mathbf{x})$ of the vector potential. To linear order, this gives a change

$$\begin{aligned}&(\nabla \times (\mathbf{A} + \mathbf{a}))^2 - (\nabla \times \mathbf{A})^2 \approx 2(\nabla \times \mathbf{a}) \cdot (\nabla \times \mathbf{A}) \\ &= 2\nabla \cdot [\mathbf{a} \times (\nabla \times \mathbf{A})] + 2\mathbf{a} \cdot [\nabla \times (\nabla \times \mathbf{A})]\end{aligned} \tag{1.38}$$

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

$$-\frac{1}{2\mu_0}\frac{\delta}{\delta \mathbf{A}(\mathbf{x})}\int \mathrm{d}^3x (\nabla \times \mathbf{A})^2 = -\frac{1}{\mu_0}\nabla \times (\nabla \times \mathbf{A}) \tag{1.39}$$

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

$$\dot{\mathbf{\Pi}} = \varepsilon_0 \ddot{\mathbf{A}} = \mathbf{j}(\mathbf{x}) - \frac{1}{\mu_0} \nabla \times (\nabla \times \mathbf{A}) \qquad \ldots \text{wrong} \tag{1.40}$$

which is nearly equivalent to the wave equation (1.7). 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 (1.25) and the Hamiltonian (1.31). 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 (1.20) to remove the nonzero divergence. This fixes the 'gauge function' to satisfy

$$\triangle \chi = -\nabla \cdot \mathbf{A} \tag{1.41}$$

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

$$\chi(\mathbf{x}) = \frac{1}{4\pi} \int \mathrm{d}^3 x' \, \frac{\nabla' \cdot \mathbf{A}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \tag{1.42}$$

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

$$\mathbf{A}_\perp(\mathbf{x}) = \mathbf{A}(\mathbf{x}) + \frac{1}{4\pi} \int \mathrm{d}^3 x' \, [\nabla' \cdot \mathbf{A}(\mathbf{x}')] \nabla \frac{1}{|\mathbf{x} - \mathbf{x}'|} \tag{1.43}$$

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

$$A_{\perp i}(\mathbf{x}) = \int \mathrm{d}^3 x' \, \delta^\perp_{ij}(\mathbf{x} - \mathbf{x}') A_j(\mathbf{x}) \tag{1.44}$$

where the so-called 'transverse δ-function' is given by

$$\delta^\perp_{ij}(\mathbf{x} - \mathbf{x}') = \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') + \frac{1}{4\pi} \partial'_j \partial'_i \frac{1}{|\mathbf{x} - \mathbf{x}'|} \tag{1.45}$$

A careful evaluation of the second derivatives yields the explicit result

$$\delta^\perp_{ij}(\mathbf{x} - \mathbf{x}') = \frac{2}{3} \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') - \frac{1}{4\pi} \left(\frac{\delta_{ij}}{r^3} - 3 \frac{r_i r_j}{r^5} \right), \qquad \mathbf{r} = \mathbf{x} - \mathbf{x}' \tag{1.46}$$

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

$$\int \mathrm{d}^3x' \frac{\delta H}{\delta \Pi_j(\mathbf{x}')} \frac{\delta A_{\perp i}(\mathbf{x})}{\delta A_j(\mathbf{x}')} = \int \mathrm{d}^3x' \frac{\delta H}{\delta \Pi_j(\mathbf{x}')} \delta^\perp_{ij}(\mathbf{x}-\mathbf{x}') = \left(\frac{\delta H}{\delta \mathbf{\Pi}(\mathbf{x}')} \right)_{\perp i} \tag{1.47}$$

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 $\mathbf{\Pi}$ into the transverse subspace. In this way, the time derivative of $\mathbf{A}_\perp$ is transverse, as it should do in order to maintain the Coulomb gauge at all times.

The same procedure applies to the equation of motion for the field momentum: the bottomline is that the source current $\mathbf{j}$ is 'transversalized', leading to the correct wave equation (1.7).

1.1.4 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 the exercises. Note that we ignore for the moment the matter-field coupling: wo focus on the field Hamiltonian only.

We adopt the expansion

$$\begin{pmatrix} \mathbf{A}(\mathbf{x},t) \\ \mathbf{\Pi}(\mathbf{x},t) \end{pmatrix} = \sum_\kappa \mathbf{f}_\kappa(\mathbf{x}) \begin{pmatrix} q_\kappa(t) \\ p_\kappa(t) \end{pmatrix} \tag{1.48}$$

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:

$$\int \mathrm{d}^3x\, \mathbf{f}_\kappa(\mathbf{x}) \cdot \mathbf{f}_{\kappa'}(\mathbf{x}) = N_\kappa \delta_{\kappa\kappa'} \tag{1.49}$$

where N_κ is a normalization constant that we fix later. The momentum-part of the Hamiltonian then becomes

$$\frac{1}{2\varepsilon_0}\int \mathrm{d}^3x\, \mathbf{\Pi}^2 = \sum_\kappa N_\kappa \frac{p_\kappa^2}{2\varepsilon_0} \tag{1.50}$$

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

$$\begin{aligned}&\int \mathrm{d}^3x\, (\nabla\times\mathbf{f}_\kappa)\cdot(\nabla\times\mathbf{f}_{\kappa'})\\ &= \int \mathbf{dA}\cdot[\mathbf{f}_\kappa\times(\nabla\times\mathbf{f}_{\kappa'})] + \int \mathrm{d}^3x\, \mathbf{f}_\kappa\cdot[\nabla\times(\nabla\times\mathbf{f}_{\kappa'})]\end{aligned} \tag{1.51}$$

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 $\mathbf{f}_\kappa$ 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.(1.51) 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 (1.51) is reduced to the orthogonality relation if we require the mode functions to be eigenfunctions of the (vector) Helmholtz equation:

$$\nabla\times(\nabla\times\mathbf{f}_\kappa) = \varepsilon_0\mu_0\omega_\kappa^2\mathbf{f}_\kappa \tag{1.52}$$

(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

$$H_\mathrm{F} = \sum_\kappa \left[\frac{N_\kappa}{2\varepsilon_0}p_\kappa^2 + \frac{\varepsilon_0}{2}N_\kappa\omega_\kappa^2 q_\kappa^2\right] \tag{1.53}$$

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

$$\frac{\mathrm{i}}{\hbar}\,[p_\kappa,\, q_{\kappa'}] = \delta_{\kappa\kappa'} \tag{1.54}$$

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

$$\frac{\mathrm{i}}{\hbar}\,[\Pi_i(\mathbf{x}),\, A_j(\mathbf{x}')] = \sum_\kappa f_{\kappa i}(\mathbf{x}) f_{\kappa j}(\mathbf{x}') \stackrel{!}{=} \delta^\perp_{ij}(\mathbf{x}-\mathbf{x}') \tag{1.55}$$

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 (1.41).

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, $a^\dagger_\kappa$ and a_κ, correspond to the 'creation' and 'destruction' of one 'photon'. The mode coordinate and momentum operators are given by

$$q_\kappa \;=\; \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa}}\left(a_\kappa + a^\dagger_\kappa\right) \tag{1.56}$$

$$p_\kappa \;=\; \sqrt{\frac{\hbar\varepsilon_0\omega_\kappa}{2}}\mathrm{i}\left(a_\kappa - a_\kappa^\dagger\right) \tag{1.57}$$

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

$$\left[a_\kappa,\, a_{\kappa'}^\dagger\right] = \delta_{\kappa\kappa'} \tag{1.58}$$

The field Hamiltonian then takes the form

$$H_\mathrm{F} = \sum_\kappa \frac{\hbar\omega_\kappa}{2}\left(a_\kappa a_\kappa^\dagger + a_\kappa^\dagger a_\kappa\right) = \sum_\kappa \hbar\omega_\kappa\left(a_\kappa^\dagger a_\kappa + \tfrac{1}{2}\right) \tag{1.59}$$

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 $|\mathrm{vac}\rangle$ such that $a_\kappa|\mathrm{vac}\rangle = 0$ for all κ. This is an energy eigenstate whose energy is infinity, $\frac{1}{2}\sum_\kappa \hbar\omega_\kappa$, 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

$$\mathbf{A}(\mathbf{x},t) = \sum_\kappa \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa}}\mathbf{f}_\kappa(\mathbf{x})\left(a_\kappa \mathrm{e}^{-\mathrm{i}\omega_\kappa t} + a_\kappa^\dagger \mathrm{e}^{\mathrm{i}\omega_\kappa t}\right). \tag{1.60}$$

We have used here the Heisenberg picture for the vector potential operator. From the Hamiltonian (1.59), it is easy to show that the operator $a_\kappa(t)$ evolves with a complex exponential $\mathrm{e}^{-\mathrm{i}\omega_\kappa t}$. 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 expansion. For completeness, we give here the plane-wave expansion for the field mode functions. These are complex, and therefore they are normalized according to

$$\int \mathrm{d}^3x\, \mathbf{f}_\kappa^*(\mathbf{x})\cdot\mathbf{f}_{\kappa'}(\mathbf{x}) = \delta_{\kappa\kappa'} \tag{1.61}$$

instead of Eq.(1.49). This can be ensured with the choice

$$\mathbf{f}_\kappa(\mathbf{x}) = \frac{1}{\sqrt{V}}\mathbf{u}_\kappa \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{1.62}$$

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 $\mathbf{u}_\kappa$ is a 'transverse' polarization vector with the property $\mathbf{k}\cdot\mathbf{u}_\kappa = 0$. 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 (1.52). The magnetic field is oriented along $\mathbf{k}\times\mathbf{u}_\kappa \equiv (\omega_\kappa/c)\mathbf{v}_\kappa$.

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

$$\mathbf{A}_\perp(\mathbf{x},t) = \sum_\kappa \sqrt{\frac{\hbar}{2\varepsilon_0\omega_\kappa V}}\left(\mathbf{u}_\kappa \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{x}-\omega_\kappa t)}a_\kappa + \text{h.c.}\right). \tag{1.63}$$

$$\mathbf{E}_\perp(\mathbf{x},t) = \sum_\kappa \sqrt{\frac{\hbar\omega_\kappa}{2\varepsilon_0 V}}\left(\mathrm{i}\mathbf{u}_\kappa \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{x}-\omega_\kappa t)}a_\kappa + \text{h.c.}\right). \tag{1.64}$$

$$\mathbf{B}(\mathbf{x},t) = \sum_\kappa \sqrt{\frac{\hbar\omega_\kappa\mu_0}{2V}}\left(\mathrm{i}\mathbf{v}_\kappa \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{x}-\omega_\kappa t)}a_\kappa + \text{h.c.}\right). \tag{1.65}$$

Sometimes, you may encounter these formulas without the factor i in front (and with '$+\mathrm{h.c.}$'). Then the operator $\mathrm{i}a_{\mathbf{k}\lambda}$ is being used instead. Note that Eq.(1.64) gives only the 'transverse' part of the electric field. The 'longitudinal' part, $-\nabla\phi$, is determined according to (1.5) by the charge density.

Note: A useful shortcut to derive the prefactors is the following: for each mode, match the energy density $\frac{1}{2}\varepsilon_0\mathbf{E}^2 + (1/2\mu_0)\mathbf{B}^2$ 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.