Chapter XIX

Quantization of electromagnetic radiation

Introduction

This chapter presents a quantum description of the electromagnetic field and its interactions with an ensemble of charged particles. Such a description is necessary for interpreting certain physical phenomena such as the spontaneous emission of a photon by an excited atom, which cannot be carried out with the semiclassical treatments we have used previously[1] (classical description for the field, and quantum description for the

[1]See for example in Complement A_{XIII} the study of the interaction between an atom and an electromagnetic wave.

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particles). Imagine, for example, that a monochromatic field with angular frequency ω is described by a classical field $\mathbf{E}_0 \cos \omega t$; its interaction with an atom is then described by the Hamiltonian $\widehat{H}_I = -\widehat{\mathbf{D}} \cdot \mathbf{E}_0 \cos \omega t$, where $\widehat{\mathbf{D}}$ is an operator (the electric dipole moment) whereas $\mathbf{E}_0$ remains a classical quantity[2]. Such a treatment is adequate for understanding how the field can excite the atom from its ground state a with energy E_a towards an excited state b of energy E_b; the processus is resonant if ω is close to the atomic Bohr frequency $\omega_0 = (E_b - E_a)/\hbar$. Imagine now that the atom is initially in the excited state b, in the absence of any incident radiation. The classical field $\mathbf{E}_0$ is then identically zero and, consequently, so is the interaction Hamiltonian $\widehat{H}_I$. The Hamiltonian of the total system is then reduced to the atomic Hamiltonian $\widehat{H}_A$. Since this operator is time-independent, its eigenstates are stationary, including, in particular, the excited state b. The semiclassical theory predicts that an atom, initially excited in a state b in the absence of incident radiation, will remain indefinitely in that state. But this is not what is experimentally observed: after a certain time, the atom spontaneously falls into a lower level a, emitting a photon whose frequency is close to $\omega_0 = (E_b - E_a)/\hbar$. This process is called spontaneous emission and happens after an average time called the *radiative lifetime* of the excited state b. This is a first example of a situation where a radiation quantum treatment is indispensable. It is far from being the only example: numerous experiments, more and more elaborate, have created situations where the quantum description of the electromagnetic field is necessary.

This chapter presents the base of this quantum description, while following an approach that is as simple as possible – a more general presentation of the quantization of the electromagnetic field is possible with the Lagrangian formulation of electrodynamics (Complement $\mathrm{A_{XVIII}}$. In the previous chapter, we underlined the analogy between the eigenmodes of the radiation field vibrations and an ensemble of harmonic oscillators. We shall use this analogy in § A of this chapter, and proceed to a simple quantization of this ensemble of oscillators. With each eigenmode i of the classical field, described by normal variables α_i and α_i^*, we shall associate annihilation $\widehat{a}_i$ and creation $\widehat{a}_i^\dagger$ operators, obeying the well-known commutation relations $\left[\widehat{a}_i, \widehat{a}_i^\dagger\right] = 1$. We shall also propose a plausible form for the quantum Hamiltonian of the system "field + particles", starting from the classical energy of that system established in the previous chapter. We will see that the equations of evolution[3] for these various quantities in the Heisenberg picture (Complement $\mathrm{G_{III}}$) are the transposition of the Maxwell-Lorentz equations to operators describing fields and particles, properly symmetrized. This will yield an a posteriori justification for the simple quantization procedure we used.

Several important properties of the free field (in the absence of sources) are described in § B. The state space of this field has the structure of a tensor product of Fock spaces, analogous to those studied in Chapter XV; the elementary excitations of the field are called photons. A few important states of the field will be described: the photon vacuum, where no photons are present (but where there exists, nonetheless, a fluctuating field throughout the entire space, with a zero average value), the one-photon states, and the quasi-classical states, which reproduce the properties of a given classical field.

Finally, § C studies the interaction Hamiltonian between an electromagnetic field and particles, in particular when those are neutral atoms (such as the Hydrogen atom

[2]For the sake of clarity, we use in the entire chapter and its complements the symbol "hat" to distinguish an operator $\widehat{G}$ from its corresponding classical quantity G.

[3]More concisely, we shall call them Heinsenberg equations.

where the positive and negative charges of the atom's constituents balance each other). It is then possible to distinguish between two types of atomic variables: the center of mass variables (external variables) and the "relative motion" variables in the center of mass frame (internal variables). We shall also study the electric dipole approximation, valid when the radiation wavelength is large compared to the atomic sizes, as well as the selection rules associated with the interaction Hamiltonian.

A. Quantization of the radiation in the Coulomb gauge

A-1. Quantization rules

In the previous chapter, we established in relation (B-26) the following expression for the energy of the classical transverse field:

$$H_{\text{trans}} = \varepsilon_0 \int \mathrm{d}^3k \sum_{\boldsymbol{\varepsilon}} \frac{\omega^2}{4\mathcal{N}^2(k)} \left[\alpha^*_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)\alpha_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t) + \alpha_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)\alpha^*_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)\right] \tag{A-1}$$

where $\alpha_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ and $\alpha^*_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ are the normal variables describing the transverse field, $\omega = ck$, and $\mathcal{N}(k)$ a real normalization constant that appeared in the equations defining the normal variables in terms of the transverse potential vector and its time derivative:

$$\begin{aligned} \boldsymbol{\alpha}(\boldsymbol{k},t) &= \mathcal{N}(k)\left[\tilde{\boldsymbol{A}}_\perp(\boldsymbol{k},t) + \frac{i}{\omega}\dot{\tilde{\boldsymbol{A}}}_\perp(\boldsymbol{k},t)\right] \\ \boldsymbol{\alpha}^*(\boldsymbol{k},t) &= \mathcal{N}(k)\left[\tilde{\boldsymbol{A}}^*_\perp(\boldsymbol{k},t) - \frac{i}{\omega}\dot{\tilde{\boldsymbol{A}}}^*_\perp(\boldsymbol{k},t)\right] \end{aligned} \tag{A-2}$$

The analogy between the free transverse field and an ensemble of classical harmonic oscillators of frequency ω associated with the modes $\{\boldsymbol{k},\boldsymbol{\varepsilon}\}$ is clearly seen in expression (A-1).

To quantize the field, this analogy suggests replacing the normal variables $\alpha_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ and $\alpha^*_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ by annihilation and creations operators. We shall use in this § A the Schrödinger picture where these operators are time-independent and where the time dependence only appears in the evolution of the state vector. The quantization procedure will consist in replacing the $\alpha_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t=0)$ by time-independent annihilation operators $\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})$, and of course the $\alpha^*_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t=0)$ by the adjoint creation operators $\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})$. Once this operation is performed on (A-1), we obtain a quantum Hamiltonian identical to a sum of standard harmonic oscillator Hamiltonians, provided the factor $\omega^2/4\mathcal{N}^2(k)$ multiplying the bracket on the right-hand side of (A-1) is equal to $\hbar\omega/2\epsilon_0$. We therefore choose for $\mathcal{N}(k)$ the value:

$$\mathcal{N}(k) = \sqrt{\frac{\varepsilon_0\, ck}{2\hbar}} = \sqrt{\frac{\varepsilon_0\, \omega}{2\hbar}} \tag{A-3}$$

This relation is the same as relation (69) of Complement $\mathrm{A_{XVIII}}$, obtained from the commutation relations. We now replace in (A-1) the classical normal variables $\alpha_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ and $\alpha^*_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ by the operators $\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})$ and $\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})$ obeying the commutation relations:

$$\left[\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k}), \hat{a}^\dagger_{\boldsymbol{\varepsilon}'}(\boldsymbol{k}')\right] = \delta_{\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}'}\ \delta(\boldsymbol{k}-\boldsymbol{k}') \tag{A-4a}$$

$$\left[\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k}), \hat{a}_{\boldsymbol{\varepsilon}'}(\boldsymbol{k}')\right] = \left[\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k}), \hat{a}^\dagger_{\boldsymbol{\varepsilon}'}(\boldsymbol{k}')\right] = 0 \tag{A-4b}$$

This yields the Hamiltonian operator (as this operator will be frequently used, we simplify the notation and replace $\hat{H}_{\text{trans}}$ by $\hat{H}_R$):

$$\hat{H}_R \equiv \hat{H}_{\text{trans}} = \int \mathrm{d}^3k \sum_{\boldsymbol{\varepsilon}} \frac{\hbar\omega}{2} \left[\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k}) + \hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\right] \tag{A-5}$$

which has the expected form for the quantum Hamiltonian of the transverse field.

Extending this procedure, we now replace the classical normal variables by annihilation and creation operators in all the classical expressions established in the previous chapter for the various physical quantities. The transverse momentum – see equation (B-27) of Chapter XVIII – becomes:

$$\hat{\boldsymbol{P}}_{\text{trans}} = \int \mathrm{d}^3k \sum_{\boldsymbol{\varepsilon}} \frac{\hbar\boldsymbol{k}}{2} \left[\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k}) + \hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\right] \tag{A-6}$$

As for the transverse fields, written in (B-29), (B-30) and (B-28) of Chapter XVIII, they become linear combinations of creation and annihilation operators:

$$\hat{\boldsymbol{E}}_\perp(\boldsymbol{r}) = i \int \frac{\mathrm{d}^3k}{(2\pi)^{3/2}} \sum_{\boldsymbol{\varepsilon}} \left[\frac{\hbar\omega}{2\varepsilon_0}\right]^{1/2} \left[\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\ \boldsymbol{\varepsilon}\ e^{i\boldsymbol{k}\cdot\boldsymbol{r}} - \hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\ \boldsymbol{\varepsilon}^*\ e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\right] \tag{A-7}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r}) = \frac{i}{c} \int \frac{\mathrm{d}^3k}{(2\pi)^{3/2}} \sum_{\boldsymbol{\varepsilon}} \left[\frac{\hbar\omega}{2\varepsilon_0}\right]^{1/2} \left[\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\ \boldsymbol{\kappa}\times\boldsymbol{\varepsilon}\ e^{i\boldsymbol{k}\cdot\boldsymbol{r}} - \hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\ \boldsymbol{\kappa}\times\boldsymbol{\varepsilon}^*\ e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\right] \tag{A-8}$$

$$\hat{\boldsymbol{A}}_\perp(\boldsymbol{r}) = \int \frac{\mathrm{d}^3k}{(2\pi)^{3/2}} \sum_{\boldsymbol{\varepsilon}} \left[\frac{\hbar}{2\varepsilon_0\omega}\right]^{1/2} \left[\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\ \boldsymbol{\varepsilon}\ e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\ \boldsymbol{\varepsilon}^*\ e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\right] \tag{A-9}$$

Comment:

As in Chapter XVIII, these relations are written in the general case where the polarizations may be complex (elliptical or circular). Complex conjugate $\boldsymbol{\varepsilon}*$ of the polarization vectors are therefore associated with the creation operators. It is of course necessary to check that the quantification procedure is independent of the arbitrary choice of the polarization basis. If a quantization is performed with a given basis of polarizations, by substitution one can calculate the operators multiplying $\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}^*$ in the new basis, and check that the commutation relations of these operators are indeed those of standard creation and annihilation operators. This ensures the polarization basis independence.

Finally, relation (A-48) of Chapter XVIII for the total energy of the system "particles + fields" becomes:

$$\hat{H} = \frac{1}{2m_a} \sum_a \left[\hat{\boldsymbol{p}}_a - q_a \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a)\right]^2 + \hat{V}_{\text{Coul}} + \int \mathrm{d}^3k \sum_{\boldsymbol{\varepsilon}} \frac{\hbar\omega}{2} \left[\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k}) + \hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})\right] \tag{A-10}$$

which is a plausible form for the quantum Hamiltonian of the system "particles + fields". The position $\hat{\boldsymbol{r}}_a$ and momentum $\hat{\boldsymbol{p}}_a$ operators defined using equation (A-47) of Chapter XVIII obey the usual commutation relations:

$$[(\hat{\boldsymbol{r}}_a)_i, (\hat{\boldsymbol{p}}_b)_j] = i\hbar\ \delta_{ab}\ \delta_{ij} \tag{A-11a}$$

$$[(\hat{\boldsymbol{r}}_a)_i, (\hat{\boldsymbol{r}}_b)_j] = [(\hat{\boldsymbol{p}}_a)_i, (\hat{\boldsymbol{p}}_b)_j] = 0 \tag{A-11b}$$

The quantization rules we just heuristically introduced have the advantage of simplicity. We are going to show in addition that the Heisenberg equations for the various operators describing the particles and the fields, deduced from the Hamiltonian (A-10) as well as from the commutation relations (A-4), (A-11a) and (A-11b), are indeed the Maxwell-Lorentz equations for operators. This result justifies a posteriori the quantization procedure exposed in this chapter.

A-2. Radiation contained in a box

If the real space is infinite, $\boldsymbol{k}$ is a continuous variable, and there exists a continuous infinity of modes. However, as we mentioned in § B-3 of Chapter XVIII, it is often more convenient to consider the field to be contained in a cube of edge length L with periodic boundary conditions; the variable $\boldsymbol{k}$ is now discrete:

$$k_{x,y,z} = 2\pi \; n_{x,y,z}/L \tag{A-12}$$

where $n_{x,y,z}$ are positive, negative or zero integers. All the physical predictions must be independent of L when it is large enough. In such an approach, we replace the Fourier integrals by Fourier series and the integrals over $\boldsymbol{k}$ by discrete summations. For a classical field, the continuous variables $\alpha_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ then become discrete variables $\alpha_{\boldsymbol{k},\boldsymbol{\varepsilon}}(t)$. If the field is zero outside the box, relation (B-35) of chapter XVIII indicates the multiplicative factor that must be used to go from one type of variable to the other.

The system is then quantized as we just explained. In the Schrödinger picture, each classical coefficient $\alpha_{\boldsymbol{k},\boldsymbol{\varepsilon}}(t=0)$ in a Fourier series becomes an annihilation operator $\hat{a}_{\boldsymbol{k},\boldsymbol{\varepsilon}}$; each coefficient $\alpha^*_{\boldsymbol{k},\boldsymbol{\varepsilon}}(t=0)$ becomes a creation operator $\hat{a}^\dagger_{\boldsymbol{k},\boldsymbol{\varepsilon}}$. This latter operator creates a quantum in a field mode confined inside the box (instead of spreading over the entire space). The commutation relations (A-4) are then written:

$$\left[\hat{a}_{\boldsymbol{k},\boldsymbol{\varepsilon}}, \hat{a}^\dagger_{\boldsymbol{k},\boldsymbol{\varepsilon}'}\right] = \delta_{\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}'} \; \delta_{\boldsymbol{k},\boldsymbol{k}'} \tag{A-13a}$$

$$\left[\hat{a}_{\boldsymbol{k},\boldsymbol{\varepsilon}}, \hat{a}_{\boldsymbol{k}',\boldsymbol{\varepsilon}'}\right] = \left[\hat{a}^\dagger_{\boldsymbol{k},\boldsymbol{\varepsilon}}, \hat{a}^\dagger_{\boldsymbol{k}',\boldsymbol{\varepsilon}'}\right] = 0 \tag{A-13b}$$

Relation (B-36) of Chapter XVIII indicates that once the discrete variables have been inserted in the expressions for the fields, the following rule must be applied to go from a continuous to a discrete summation:

$$\int \mathrm{d}^3k \implies \left(\frac{2\pi}{L}\right)^{3/2} \sum_{\mathbf{k}} \tag{A-14}$$

Expressions (A-7) to (A-9) must be modified. As an example, relation (A-7) becomes:

$$\hat{\boldsymbol{E}}_\perp(\boldsymbol{r}) = i \sum_{\boldsymbol{k},\boldsymbol{\varepsilon}} \left[\frac{\hbar\omega}{2\varepsilon_0 L^3}\right]^{1/2} \left[\hat{a}_{\boldsymbol{k},\boldsymbol{\varepsilon}} \; \boldsymbol{\varepsilon} \; e^{i\boldsymbol{k}\cdot\boldsymbol{r}} - \hat{a}^\dagger_{\boldsymbol{k},\boldsymbol{\varepsilon}} \; \boldsymbol{\varepsilon}^* \; e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\right] \tag{A-15}$$

This means that in addition to replacing the integral by a discrete summation, and multiplying by a factor $(2\pi)^{3/2}$, one must divide the field expansion by the square root of the volume L^3. Both relations (A-8) and (A-9) undergo the same changes.

A-3. Heisenberg equations

A-3-a. Heisenberg equations for massive particles

We start with the equation for the evolution of $\hat{\boldsymbol{r}}_a(t)$:

$$\dot{\hat{\boldsymbol{r}}}_a(t) = \frac{1}{i\hbar}\left[\hat{\boldsymbol{r}}_a(t), \hat{H}\right] \tag{A-16}$$

The only term in Hamiltonian (A-10) that does not commute with $\hat{\boldsymbol{r}}_a$ is the first one. Using the commutation relation deduced from (A-11a) and (A-11b) :

$$[(\hat{\boldsymbol{r}}_a)_i, f((\hat{\boldsymbol{p}}_a)_j)] = \delta_{ij}\ \hbar \frac{\partial f}{\partial(\hat{\boldsymbol{p}}_a)_i} \tag{A-17}$$

we get:

$$\begin{aligned}\dot{\hat{\boldsymbol{r}}}_a(t) &= \frac{1}{i\hbar}\left[\hat{\boldsymbol{r}}_a(t), \frac{1}{2m_a}\left(\hat{\boldsymbol{p}}_a(t) - q_a\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a, t)\right)^2\right] \\ &= \frac{1}{m_a}\left[\hat{\boldsymbol{p}}_a(t) - q_a\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a, t)\right]\end{aligned} \tag{A-18}$$

This equality is simply the operator form:

$$\hat{\boldsymbol{p}}_a(t) = m_a\dot{\hat{\boldsymbol{r}}}_a(t) + q_a\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a, t) \tag{A-19}$$

of the classical equation relating the generalized (or canonical) momentum $\boldsymbol{p}_a$ and the mechanical momentum $m_a\dot{\boldsymbol{r}}_a$. We then define the velocity operator $\hat{\boldsymbol{v}}_a$ of particle a by:

$$\hat{\boldsymbol{v}}_a(t) = \frac{1}{m_a}\left[\hat{\boldsymbol{p}}_a(t) - q_a\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a, t)\right] \tag{A-20}$$

Consider now the Heisenberg equation for the evolution of this operator. It yields the equation of motion of that particle:

$$m_a\dot{\hat{\boldsymbol{v}}}_a(t) = m_a\ddot{\hat{\boldsymbol{r}}}_a(t) = \frac{m_a}{i\hbar}\left[\hat{\boldsymbol{v}}_a(t), \hat{H}\right] \tag{A-21}$$

We shall compute below the commutator $\left[\hat{\boldsymbol{v}}_a(t), \hat{H}\right]$; it leads to the quantum equation of motion for particle a:

$$m_a\ddot{\hat{\boldsymbol{r}}}_a = q_a\hat{\boldsymbol{E}}(\hat{\boldsymbol{r}}_a) + \frac{q_a}{2}\left[\hat{\boldsymbol{v}}_a \times \hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a) - \hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a) \times \hat{\boldsymbol{v}}_a\right] \tag{A-22}$$

which is simply the quantum Lorentz equation describing the motion of particles interacting with the magnetic field $\hat{\boldsymbol{B}}$ and the total electric field $\hat{\boldsymbol{E}} = \hat{\boldsymbol{E}}_{\|} + \hat{\boldsymbol{E}}_\perp$. The special form of the magnetic force $q_a\left[\hat{\boldsymbol{v}}_a \times \hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a) - \hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a) \times \hat{\boldsymbol{v}}_a\right]/2$ comes, as shown in the computation below, from using the Heisenberg equations, and from the fact that the operator $\hat{\boldsymbol{v}}_a \times \hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a)$ is not Hermitian. To make that operator Hermitian, we must add its adjoint $\left(\hat{\boldsymbol{v}}_a \times \hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a))\right)^\dagger$, which is simply $-\hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a) \times \hat{\boldsymbol{v}}_a$, and divide the result by 2.

Demonstration of equation (A-22)

To compute the commutator of $m_a\hat{\boldsymbol{v}}_a/i\hbar$ with the first term of $\hat{H}$, it is useful to first calculate the following commutators:

$$\begin{aligned} m_a^2\left[(\hat{\boldsymbol{v}}_a)_j,(\hat{\boldsymbol{v}}_a)_l\right] &= -q_a\left[(\hat{\boldsymbol{p}}_a)_j,(\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a))_l\right]-q_a\left[(\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a))_j,(\hat{\boldsymbol{p}}_a)_l\right] \\ &= i\hbar q_a\left[\partial_j(\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a))_l-\partial_l(\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a))_j\right] \\ &= i\hbar q_a\sum_k\epsilon_{jlk}(\hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a))_k, \end{aligned} \tag{A-23}$$

where ϵ_{jkl} is the completely antisymmetric tensor that allows writing the cross product components of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ in the form $(\boldsymbol{a}\times\boldsymbol{b})_k=\sum_{jl}\epsilon_{kjl}a_jb_l$. We then get:

$$\begin{aligned} \frac{m_a}{i\hbar}\left[(\hat{\boldsymbol{v}}_a)_j,\sum_l m_a(\hat{\boldsymbol{v}}_a)_l^2/2\right] &= \frac{m_a^2}{2i\hbar}\sum_l\left\{(\hat{\boldsymbol{v}}_a)_l\left[(\hat{\boldsymbol{v}}_a)_j,(\hat{\boldsymbol{v}}_a)_l\right]+\left[(\hat{\boldsymbol{v}}_a)_j,(\hat{\boldsymbol{v}}_a)_l\right](\hat{\boldsymbol{v}}_a)_l\right\} \\ &= \frac{q_a}{2}\sum_k\sum_l\epsilon_{jlk}\left\{(\hat{\boldsymbol{v}}_a)_l(\hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a))_k+(\hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a))_k(\hat{\boldsymbol{v}}_a)_l\right\} \end{aligned} \tag{A-24}$$

The last line in (A-24) can be rewritten in the form:

$$\frac{q_a}{2}\left[\hat{\boldsymbol{v}}_a\times\hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a)-\hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a)\times\hat{\boldsymbol{v}}_a\right]_j \tag{A-25}$$

and is thus the component along the j axis of the symmmetrized magnetic force.

The commutator of $m_a\hat{\boldsymbol{v}}_a/i\hbar$ with the second term of $\hat{H}$ is written:

$$\frac{m_a}{i\hbar}\left[(\hat{\boldsymbol{v}}_a)_j,V_{\text{Coul}}\right]=\frac{1}{i\hbar}\left[(\hat{\boldsymbol{p}}_a)_j,V_{\text{Coul}}\right]=-\frac{\partial}{\partial(\hat{\boldsymbol{r}}_a)_j}V_{\text{Coul}}=q_a(\hat{\boldsymbol{E}}_\parallel(\hat{\boldsymbol{r}}_a))_j \tag{A-26}$$

It describes the interaction between particle a and the longitudinal electric field.

We finally have to compute the commutator of $m_a\hat{\boldsymbol{v}}_a/i\hbar$ with the last term of $\hat{H}$. Using the commutation relations (A-4) and expressions (A-9) and (A-7) for $\hat{\boldsymbol{A}}_\perp$ and $\hat{\boldsymbol{E}}_\perp$, we get:

$$\begin{aligned} &\frac{m_a}{i\hbar}\left[(\hat{\boldsymbol{v}}_a)_j,\int\mathrm{d}^3k\sum_{\boldsymbol{\varepsilon}}\hbar\omega\left(\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)+1/2\right)\right] \\ &\quad= iq_a\int\mathrm{d}^3k\sum_{\boldsymbol{\varepsilon}}\omega\left[(\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a))_j,\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)\right] \\ &\quad= q_a(\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{r}}_a))_j \end{aligned} \tag{A-27}$$

This term describes the interaction of particle a with the transverse electric field. Finally grouping (A-25), (A-26) and (A-27) leads to (A-22).

A-3-b. Heisenberg equations for fields

As all the fields are linear combinations of the operators $\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ and $\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$, we simply have to consider the Heisenberg equation for $\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$:

$$\dot{\hat{a}}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)=\frac{1}{i\hbar}\left[\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t),\hat{H}\right] \tag{A-28}$$

We assume that the polarizations $\boldsymbol{\varepsilon}$ are real (linear polarizations). The commutator with the first term of $\hat{H}$ yields, with the use of(A-4a) and (A-20):

$$\frac{1}{i\hbar}\left[\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t),\sum_a \frac{m_a\hat{\boldsymbol{v}}_a^2}{2}\right] = \sum_a \frac{-q_a}{2i\hbar}\left\{\hat{\boldsymbol{v}}_a\cdot\frac{\partial \boldsymbol{A}_\perp}{\partial\alpha^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})}+\frac{\partial \boldsymbol{A}_\perp}{\partial\alpha^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})}\cdot\hat{\boldsymbol{v}}_a\right\}$$
$$= \sum_a \frac{iq_a}{2\hbar}\sqrt{\frac{\hbar}{2\varepsilon_0\omega(2\pi)^3}}\;\boldsymbol{\varepsilon}\cdot\left[\hat{\boldsymbol{v}}_a e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}_a}+e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}_a}\hat{\boldsymbol{v}}_a\right] \qquad \text{(A-29)}$$

where $\partial\boldsymbol{A}_\perp/\partial a^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)$ denotes the coefficient of $\hat{a}^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k})$ in the integral (A-9) of $\hat{\boldsymbol{A}}_\perp(\boldsymbol{r})$, which is nothing but the coefficient of $\alpha^\dagger_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t=0)$ in the classical expression of $\boldsymbol{A}_\perp(\boldsymbol{r})$. We introduce the current operator (symmetrized to make it Hermitian):

$$\hat{\boldsymbol{j}}(\boldsymbol{r}) = \frac{1}{2}\sum_a q_a\left[\hat{\boldsymbol{v}}_a\delta(\boldsymbol{r}-\hat{\boldsymbol{r}}_a)+\delta(\boldsymbol{r}-\hat{\boldsymbol{r}}_a)\hat{\boldsymbol{v}}_a\right] \qquad \text{(A-30)}$$

The right hand side term of equation (A-29) can then be rewritten in the form:

$$\sum_a \frac{iq_a/2}{\sqrt{2\varepsilon_0\hbar\omega(2\pi)^3}}\;\boldsymbol{\varepsilon}\cdot\left[\hat{\boldsymbol{v}}_a e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}_a}+e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}_a}\hat{\boldsymbol{v}}_a\right] = \frac{i}{\sqrt{2\varepsilon_0\hbar\omega(2\pi)^3}}\int \mathrm{d}^3r\; e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{j}}(\boldsymbol{r})$$
$$= \frac{i}{\sqrt{2\varepsilon_0\hbar\omega}}\;\boldsymbol{\varepsilon}\cdot\hat{\bar{\boldsymbol{j}}}(\boldsymbol{k}) \qquad \text{(A-31)}$$

The commutator with the second term of $\hat{H}$ is zero, whereas the commutator with the third term yields, using (A-4):

$$\frac{1}{i\hbar}\left[\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t),\int \mathrm{d}^3k'\;\sum_{\boldsymbol{\varepsilon}'}\hbar\omega\left(\hat{a}^\dagger_{\boldsymbol{\varepsilon}'}(\boldsymbol{k}',t)\hat{a}_{\boldsymbol{\varepsilon}'}(\boldsymbol{k}',t)+1/2\right)\right] = -i\omega\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t) \qquad \text{(A-32)}$$

Finally, regrouping (A-31) and (A-32) yields:

$$\dot{\hat{a}}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t)+i\omega\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k},t) = \frac{i}{\sqrt{2\varepsilon_0\hbar\omega}}\;\boldsymbol{\varepsilon}\cdot\hat{\bar{\boldsymbol{j}}}(\boldsymbol{k},t) \qquad \text{(A-33)}$$

This equation is, for the operator $\hat{a}_\varepsilon(\boldsymbol{k},t)$, an equation of motion of the same form as the equation of motion of the classical normal variables $\boldsymbol{\alpha}(\boldsymbol{k},t)$, which is given by equation (B-19) of Chapter XVIII. As this latter equation is equivalent to Maxwell's equations for the transverse fields, we may conclude that the Heisenberg equations for the quantum transverse fields are simply the usual Maxwell's equations applied to the field operators.

B. Photons, elementary excitations of the free quantum field

We now study a certain number of properties of the electromagnetic field we just quantized, starting with the simplest case: the field in the absence of charged particles.

B-1. Fock space of the free quantum field

The state space of the total system "field + particles" is the tensor product of the particle state space $\mathcal{E}_P$ and the radiation field state space $\mathcal{E}_R$. This latter space is itself the tensor product of the state spaces of the harmonic oscillators associated with the different modes $\{\boldsymbol{k}, \boldsymbol{\varepsilon}\}$:

$$\mathcal{E}_R = \mathcal{E}_{\mathbf{k}_1,\varepsilon_1} \otimes \mathcal{E}_{\mathbf{k}_2,\varepsilon_2} \otimes .... \otimes \mathcal{E}_{\mathbf{k}_i,\varepsilon_i} \otimes ... \tag{B-1}$$

where $\mathcal{E}_{\mathbf{k}_i,\varepsilon_i}$ is the state space of the harmonic oscillator associated with the mode $\{\boldsymbol{k}_i, \boldsymbol{\varepsilon}_i\}$, with frequency ω_i.

As in § A-2, we assume the radiation to be contained in a box of edge length L. The operators $\hat{a}_\varepsilon(\boldsymbol{k})$ depending on the variables $\boldsymbol{k}$ are then transformed into operators $\hat{a}_{\boldsymbol{k}_i,\boldsymbol{\varepsilon}_i}$ depending only on discrete variables. We can even use a more compact notation $\hat{a}_i$, where the index i labels[4] the whole set of indices $\boldsymbol{k}_i, \boldsymbol{\varepsilon}_i$; the operators $\hat{a}_{\boldsymbol{\varepsilon}}(\boldsymbol{k})$ are now simply written $\hat{a}_i$. In this section, it is convenient to use the Heisenberg picture; the time dependence of the $\hat{a}_i$ and $\hat{a}_i^\dagger$ is then particularly simple, since we have:

$$\hat{a}_i(t) = \exp(i\hat{H}_R t/\hbar)\,\hat{a}_i\,\exp(-i\hat{H}_R t/\hbar) = \hat{a}_i\,e^{-i\omega_i t} \tag{B-2}$$

as well as the Hermitian conjugate relation.

Once the discrete variables have been inserted in the continuous expressions of the fields, we must use rule (A-14) to transform the continuous integrals into discrete summations. The expansions of these fields in term of normal variables are then:

$$\hat{\boldsymbol{E}}_\perp(\boldsymbol{r},t) = i\sum_i \left(\frac{\hbar\omega_i}{2\epsilon_0 L^3}\right)^{1/2} \left[\hat{a}_i\boldsymbol{\varepsilon}_i e^{i(\boldsymbol{k}_i\cdot\boldsymbol{r}-\omega_i t)} - \hat{a}_i^\dagger\boldsymbol{\varepsilon}_i^* e^{-i(\boldsymbol{k}_i\cdot\boldsymbol{r}-\omega_i t)}\right] \tag{B-3}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r},t) = i\sum_i \left(\frac{\hbar k_i}{2\epsilon_0 c L^3}\right)^{1/2} \left[\hat{a}_i\boldsymbol{\kappa}_i\times\boldsymbol{\varepsilon}_i e^{i(\boldsymbol{k}_i\cdot\boldsymbol{r}-\omega_i t)} - \hat{a}_i^\dagger\boldsymbol{\kappa}_i\times\boldsymbol{\varepsilon}_i^* e^{-i(\boldsymbol{k}_i\cdot\boldsymbol{r}-\omega_i t)}\right] \tag{B-4}$$

$$\hat{\boldsymbol{A}}_\perp(\boldsymbol{r},t) = \sum_i \left(\frac{\hbar}{2\epsilon_0\omega_i L^3}\right)^{1/2} \left[\hat{a}_i\boldsymbol{\varepsilon}_i e^{i(\boldsymbol{k}_i\cdot\boldsymbol{r}-\omega_i t)} + \hat{a}_i^\dagger\boldsymbol{\varepsilon}_i^* e^{-i(\boldsymbol{k}_i\cdot\boldsymbol{r}-\omega_i t)}\right] \tag{B-5}$$

$$\hat{H}_R = \sum_i \frac{\hbar\omega_i}{2}\left[\hat{a}_i^\dagger\hat{a}_i + \hat{a}_i\hat{a}_i^\dagger\right] = \sum_i \hbar\omega_i\left[\hat{a}_i^\dagger\hat{a}_i + \frac{1}{2}\right] \tag{B-6}$$

$$\hat{\boldsymbol{P}}_{\text{trans}} = \sum_i \frac{\hbar\boldsymbol{k}_i}{2}\left[\hat{a}_i^\dagger\hat{a}_i + \hat{a}_i\hat{a}_i^\dagger\right] = \sum_i \hbar\boldsymbol{k}_i\,\hat{a}_i^\dagger\hat{a}_i \tag{B-7}$$

Note that the last term in (B-7) does not contain the factor 1/2, since $\sum_i \boldsymbol{k}_i = \boldsymbol{0}$.

B-2. Corpuscular interpretation of states with fixed total energy and momentum

Consider first the mode i. The eigenvalues of the operator $\hat{a}_i^\dagger\hat{a}_i$ appearing in expressions (B-6) and (B-7) for $\hat{H}_R$ and $\hat{\boldsymbol{P}}_{\text{trans}}$ are all the positive or zero integers n_i :

$$\hat{a}_i^\dagger\hat{a}_i|n_i\rangle = n_i|n_i\rangle, \quad n_i = 0, 1, 2... \tag{B-8}$$

[4]For each $\boldsymbol{k}_i$, there exists two polarization vectors $\boldsymbol{\varepsilon}_{i1}$ and $\boldsymbol{\varepsilon}_{i2}$ perpendicular to $\boldsymbol{k}_i$ and perpendicular to each other. The compact notation $\sum_i$ must be interpreted as a summation over $\boldsymbol{k}_i$ and, for each value of $\boldsymbol{k}_i$, as a sum over $\boldsymbol{\varepsilon}_{i1}$ and $\boldsymbol{\varepsilon}_{i2}$.

Remember the well-known actions of operators $\hat{a}_i^\dagger$ and $\hat{a}_i$ on the states $|n_i\rangle$:

$$\begin{aligned} \hat{a}_i^\dagger|n_i\rangle &= \sqrt{n_i+1}|n_i\rangle \\ \hat{a}_i|n_i\rangle &= \sqrt{n_i}|n_i-1\rangle \\ \hat{a}_i|0_i\rangle &= 0 \end{aligned} \tag{B-9}$$

As $\hat{a}_i^\dagger\hat{a}_i$ commutes with $\hat{a}_j^\dagger\hat{a}_j$, the eigenstates of $\hat{H}_R$ and $\hat{\boldsymbol{P}}_{\text{trans}}$ are the tensor products of the eigenstates $|n_1...n_i...\rangle = |n_1\rangle\otimes...\otimes|n_i\rangle...$ of the creation and annihilation operators $\hat{a}_1^\dagger\hat{a}_1,....\hat{a}_i^\dagger\hat{a}_i$ ...:

$$\hat{H}_R|n_1...n_i...\rangle = \sum_i \left(n_i+\frac{1}{2}\right)\hbar\omega_i|n_1...n_i...\rangle \tag{B-10a}$$

$$\hat{\boldsymbol{P}}_{\text{trans}}|n_1...n_i...\rangle = \sum_i n_i\hbar\boldsymbol{k}_i|n_1...n_i...\rangle \tag{B-10b}$$

The field's ground state corresponds to all the n_i equal to zero, and will be noted $|0\rangle$:

$$|0\rangle = |0_1...0_i...\rangle \tag{B-11}$$

the states $|n_1...n_i...\rangle$ being obtained by the action of a certain number of creation operators on this $|0\rangle$ state:

$$|n_1...n_i...\rangle = \frac{(\hat{a}_1^\dagger)^{n_1}}{\sqrt{n_1!}}...\frac{(\hat{a}_i^\dagger)^{n_i}}{\sqrt{n_i!}}...|0\rangle \tag{B-12}$$

With respect to the field ground state, the state $|n_1...n_i...\rangle$ has an energy $\sum_i n_i\hbar\omega_i$ and a momentum $\sum_i n_i\hbar\boldsymbol{k}_i$. It can be interpreted as describing an ensemble of n_1 particles of energy $\hbar\omega_1$ and momentum $\hbar\boldsymbol{k}_1$,....., n_i particles of energy $\hbar\omega_i$ and momentum $\hbar\boldsymbol{k}_i$, *etc...* . These particles characterize the elementary excitations of the quantum field and are called *photons*. The quantum number n_i is therefore the number of photons occupying the mode i, so that the ground state $|0\rangle$, corresponding to all the n_i equal to zero, can be called the photon *vacuum*.

Whereas there exists for photons eigenstates of momentum and energy, there are no quantum states of the electromagnetic field where the position can be perfectly known; no position operator is associated with this field. This is a different situation from what we encounter with massive particles, which have both a position and a momentum operator; the wave functions in the two representations are related by a simple Fourier transform. This non-existence of a position operator is linked to the impossibility of building, by a linear superposition of transverse electromagnetic waves, a vector wave perfectly localized at a point in space. The relativistic and transverse character of the electromagnetic field yields commutation relations between its components that involve the transverse delta function (Complement A_{XVIII}, § 2-e) instead of the usual delta function.

B-3. Several examples of quantum radiation states

We now study several examples of states of quantum radiation.

B-3-a. Photon vacuum

The presence of the 1/2 term in the parenthesis on the right-hand side of equation (B-10a) shows that the vacuum state energy is not zero, but equal to $\sum_i \hbar\omega_i/2$; this sum is an infinite quantity. We encounter here a first example of the difficulties linked to the divergences appearing in quantum electrodynamics. They can be resolved by *renormalization* techniques, whose presentation is outside the scope of this book. We shall avoid this difficulty by only considering energy differences with respect to the vacuum.

If we consider a single mode i of the field, the energy $\hbar\omega_i/2$ of the vacuum state for this mode is finite, and reminiscent of the zero-point energy of a harmonic oscillator of frequency ω_i. As you may recall, this zero-point energy is due to the impossibility of having simultaneously zero values for the position x and momentum p of that oscillator, because of the Heisenberg relations. The lowest energy state of the oscillator results from a compromise between the kinetic energy, proportional to p^2, and the potential energy, proportional to x^2 (this problem is discussed in § D-2 of Chapter V). The same arguments can be presented for the contribution, at a given point $\boldsymbol{r}$, of mode i to the electric $\hat{\boldsymbol{E}}_\perp(\boldsymbol{r},t)$ and magnetic $\hat{\boldsymbol{B}}(\boldsymbol{r},t)$ fields; according to (B-3) and (B-4), those fields are represented by two different linear superpositions of operators $\hat{a}_i$ and $\hat{a}_i^\dagger$, which thus do not commute. Consequently, one cannot have simultaneously a zero value for the electric energy proportional to $\hat{\boldsymbol{E}}_\perp^2$, and for the magnetic energy proportional to $\hat{\boldsymbol{B}}^2$.

One can further calculate the average value and variance of the contribution of mode i to the electric field $\hat{\boldsymbol{E}}_\perp(\mathbf{r},t)$ at point $\boldsymbol{r}$. Since $\hat{a}_i$ and $\hat{a}_i^\dagger$ change n_i by ± 1, a simple calculation yields:

$$\langle 0|\hat{\boldsymbol{E}}_\perp(\boldsymbol{r},t)|0\rangle_{\text{mode i}} = 0 \tag{B-13a}$$

$$\langle 0|\hat{\boldsymbol{E}}_\perp^2(\boldsymbol{r},t)|0\rangle_{\text{mode i}} = \frac{\hbar\omega_i}{2\varepsilon_0 L^3} \tag{B-13b}$$

Similar calculations can be done for the magnetic field. They show that in the photon vacuum state, the average value of both the electric and magnetic fields is zero, but not their variance. Since result (B-13b) is proportional to $\hbar$, the non-zero variance of the fields in the vacuum is a quantum effect.

Comments

(i) The summation over all the modes of expressions (B-13) yields, once we have replaced the discrete sum by an integral:

$$\langle 0|\hat{\boldsymbol{E}}_\perp(\boldsymbol{r},t)|0\rangle = 0 \tag{B-14a}$$

$$\langle 0|\hat{\boldsymbol{E}}_\perp^2(\boldsymbol{r},t)|0\rangle = \sum_i \frac{\hbar\omega_i}{2\varepsilon_0 L^3} = \frac{\hbar c}{2\varepsilon_0 \pi^2}\int_0^{k_M} k^3 \mathrm{d}k \tag{B-14b}$$

This means that the variance of the electric field diverges as the fourth power of the upper boundary of the integral over k appearing in the summation of the modes of frequency $\omega = ck$. This divergence is the same as that mentioned above.

(ii) To characterize the dynamics of these field fluctuations, it is possible to compute the field correlation functions in vacuum[5]. This calculation shows that the electric and magnetic fields fluctuate very rapidly around their zero average value. These fluctuations are called the *vacuum fluctuations*. Certain radiative corrections, such as the "Lamb shift"

[5]See for example § III-C-3-c and Complement C_{III} of reference [16].

in atoms, can be interpreted from a physical point of view, as resulting from the vibration of the atom's electron caused by its interaction with this fluctuating electric field. This vibration leads the electron to explore the nucleus Coulomb potential over the range of its vibrational motion. The corresponding correction to its binding energy depends on the energy level it occupies; this explains why the degeneracy between the $2s_{1/2}$ and $2p_{1/2}$ states of the hydrogen atom, predicted by the Schrödinger and Dirac equations, can be lifted by the interaction with the vacuum fluctuations [6].

B-3-b. Field quasi-classical states

The state and observables of a classical field are characterized by the normal variables $\{\alpha_i\}$ introduced in § B-2-b of Chapter XVIII. The coherent states of a one-dimensional harmonic oscillator studied in Complement G_V, can be used to build the field quantum states whose properties are closest to those of the classical field $\{\alpha_i\}$.

The coherent state, supposed to be normalized, of a one-dimensional harmonic oscillator is the eigenstate of the annihilation operator $\hat{a}$, with eigenvalue α:

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \tag{B-15}$$

The eigenvalue α may be a complex number since operator $\hat{a}$ is not Hermitian. Equation (B-15) leads to:

$$\langle\alpha|\hat{a}|\alpha\rangle = \alpha \qquad \langle\alpha|\hat{a}^\dagger|\alpha\rangle = \alpha^* \tag{B-16}$$

More generally, the average value of any function of $\hat{a}$ and $\hat{a}^\dagger$, once put in the *normal* order, i.e. where all the annihilation operators are positioned to the right of the creation operators (Complement B_{XVI}, § 1-a-α), is equal to the expression obtained by replacing operator $\hat{a}$ by α and operator $\hat{a}^\dagger$ by α^*. As an example:

$$\langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle = \alpha^*\alpha \tag{B-17}$$

Consider then the field quantum state:

$$|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \ldots |\alpha_i\rangle \ldots = |\alpha_1, \alpha_2 \ldots \alpha_i \ldots\rangle \tag{B-18}$$

where each mode i is in the coherent state $|\alpha_i\rangle$ corresponding to the classical normal variable α_i. Using equations (B-16) and (B-17), we can obtain the average values of the various field operators (B-3), (B-4) and (B-5) in the state (B-18); they coincide with the values of these various physical quantities for a classical field described by the normal variables $\{\alpha_i\}$. The same is true for the observables (B-6) and (B-7) corresponding to the energy and momentum of the transverse field. This is why the quantum state (B-18), which yields average values identical to all the properties of a classical field, is called a *quasi-classical state*[7]. We shall see later that the correlation functions of the quantum and classical fields involved in various photodetection signals also coincide when the field state is a quasi-classical state.

[6] See for example [17].

[7] For more details on the properties of the radiation quasi-classical states, see § III-C-4 of reference [16].

B-3-c. Single photon state

Consider the state vector:

$$|\Psi\rangle = \sum_i c_i |1_i\rangle \prod_{\otimes j \neq i} |0_j\rangle \tag{B-19}$$

which is a linear superposition of kets where a mode i contains one photon, whereas all the other modes $j \neq i$ are empty. Such a ket is an eigenket of the operator total number of photons $\hat{N} = \sum_i \hat{a}_i^\dagger \hat{a}_i$ with an eigenvalue equal to 1. It is therefore a single photon state. However, except in special cases, it is not a stationary state since it is not an eigenstate of the field energy $\hat{H}_R$. It describes a single photon propagating in space with velocity c. We shall see later (Complement D_{XX}) that, when the field is in the state (B-19), a photodetector placed in a small region of space yields a signal corresponding to the passage, in that region, of a wave packet.

C. Description of the interactions

C-1. Interaction Hamiltonian

The Hamiltonian $\hat{H}$ of the system "particles + field" has been given above. In its expression (A-10), we now separate the terms that depend only on the particle variables or only on the field variables, and those that depend on both. We can then write $\hat{H} = \hat{H}_P + \hat{H}_R + \hat{H}_I$, where the particle Hamiltonian is:

$$\hat{H}_P = \sum_a \frac{\hat{\boldsymbol{p}}_a^2}{2m_a} + \hat{V}_{\text{Coul}} \tag{C-1}$$

whereas the radiation one is:

$$\hat{H}_R = \sum_i \hbar\omega_i \left(\hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \right) \tag{C-2}$$

Finally, the interaction Hamiltonian is the sum:

$$\hat{H}_I = \hat{H}_{I1} + \hat{H}_{I2}, \tag{C-3}$$

with:

$$\hat{H}_{I1} = -\sum_a \frac{q_a}{2m_a} \left[\hat{\boldsymbol{p}}_a \cdot \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a) + \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a) \cdot \hat{\boldsymbol{p}}_a \right] \tag{C-4}$$

$$\hat{H}_{I2} = \sum_a \frac{q_a^2}{2m_a} \left[\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_a) \right]^2 \tag{C-5}$$

(we have separated the linear and quadratic terms with respect to the fields).

To that interaction Hamiltonian, we must further add the term:

$$\hat{H}_{I1}^s = -\sum_a \hat{\boldsymbol{M}}_a^s \cdot \hat{\boldsymbol{B}}(\hat{\boldsymbol{r}}_a) \tag{C-6}$$

describing the interaction of the spin magnetic moments of the various particles with the magnetic field of the radiation (Complement A_{XIII}, § 1-d):

$$\hat{\boldsymbol{M}}_a^s = g_a \frac{q_a}{2m_a} \hat{\boldsymbol{S}}_a \tag{C-7}$$

where g_a is the "Landé g-factor" of particle a whose spin is noted $\hat{\boldsymbol{S}}_a$.

Comment

Even with this additional term, all the possible interactions are not contained in that Hamiltonian: missing for example are the electron spin-orbit coupling, the hyperfine interaction between the electron and the nucleus, etc. – see comment (iii) of § C-5. The Hamiltonian we wrote is however sufficient in a great number of cases.

C-2. Interaction with an atom. External and internal variables

Consider the case where the particle system is a single atom, assumed to be neutral, formed by an electron e and a nucleus N which have opposite charges ($q_e = -q_N = q$) and whose masses are noted m_e and m_N. This is the case for example of the hydrogen atom. It is standard practice (see for example § B of Chapter VII) to separate the variables $\hat{\boldsymbol{R}}$ and $\hat{\boldsymbol{P}}$ of the system's center of mass and the variables $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$ of the relative motion. These two types of variables commute with each other and are given by equations:

$$\begin{cases} \boldsymbol{R} = \dfrac{m_e\ \boldsymbol{r}_e + m_N\ \boldsymbol{r}_N}{M} \\ \boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_N \end{cases} \qquad \begin{cases} \boldsymbol{P} = \boldsymbol{p}_e + \boldsymbol{p}_N \\ \dfrac{\boldsymbol{p}}{m} = \dfrac{\boldsymbol{p}_e}{m_e} - \dfrac{\boldsymbol{p}_N}{m_N} \end{cases} \tag{C-8}$$

where we have noted M the total mass of the system, and m its reduced mass:

$$M = m_e + m_N \qquad ; \qquad m = \frac{m_e m_N}{M} \tag{C-9}$$

Expressed as a function of these new variables, the particle Hamiltonian is written:

$$\hat{H}_P = \frac{\hat{\boldsymbol{P}}^2}{2M} + \frac{\hat{\boldsymbol{p}}^2}{2m} + \hat{V}_{\text{Coul}}(\hat{r}) \tag{C-10}$$

The center of mass variables, also called *external variables*, describe the global motion of the atom, whereas the variables of the relative motion, also called *internal variables*, describe the motion in the center of mass reference frame.

C-3. Long wavelength approximation

The interaction Hamiltonians (C-4), (C-5) and (C-6) contain fields evaluated at the electron $\boldsymbol{r}_e$ and nucleus $\boldsymbol{r}_N$ positions. These positions can be described with respect to the position of the center of mass and we can write for example:

$$\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_e) = \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}} + \hat{\boldsymbol{r}}_e - \hat{\boldsymbol{R}}) \tag{C-11}$$

In an atom, the distance between the position of the electron or the nucleus and the atom's center of mass is of the order of the atom's size, i.e. just a fraction of a nanometer. Now the radiation wavelengths that can have a resonant interaction with the atom are of the order of a fraction of a micron, much larger than the atomic dimension. One can thus neglect the variation of the fields over distances of the order of $|\boldsymbol{r}_e - \boldsymbol{R}|$ (or $|\boldsymbol{r}_N - \boldsymbol{R}|$) and write:

$$\begin{aligned} \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_e) &\simeq \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}}) \\ \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_N) &\simeq \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}}) \end{aligned} \tag{C-12}$$

Such an approximation is called the long wavelength approximation (or dipole approximation).

Using this approximation in the interaction Hamiltonian $\hat{H}_{I1}$, yields:

$$\begin{aligned} \hat{H}_{I1} &= -\frac{q_e}{m_e}\hat{\boldsymbol{p}}_e \cdot \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_e) - \frac{q_N}{m_N}\hat{\boldsymbol{p}}_N \cdot \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{r}}_N) \\ &\simeq -q\left[\frac{\hat{\boldsymbol{p}}_e}{m_e} - \frac{\hat{\boldsymbol{p}}_N}{m_N}\right] \cdot \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}}) \\ &= -\frac{q}{m}\hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}}) \end{aligned} \tag{C-13}$$

We used the relation $q_e = -q_N = q$ as well as definition (C-8) for the relative momentum.

As for Hamiltonian $\hat{H}_{I2}$, it becomes with this approximation:

$$\begin{aligned} \hat{H}_{I2} &= \frac{q_e^2}{2m_e}\hat{\boldsymbol{A}}_\perp^2(\hat{\boldsymbol{r}}_e) + \frac{q_N^2}{2m_N}\hat{\boldsymbol{A}}_\perp^2(\hat{\boldsymbol{r}}_N) \\ &\simeq \frac{q^2}{2m}\hat{\boldsymbol{A}}_\perp^2(\hat{\boldsymbol{R}}) \end{aligned} \tag{C-14}$$

Comment

When we include the Hamiltonian describing the spin magnetic coupling $\hat{H}_{I1}^s$ written in (C-6), we also replace all the $\hat{\boldsymbol{r}}_a$ by $\hat{\boldsymbol{R}}$. This is however insufficient: we must add other terms of the same order, obtained by including first order terms in $\boldsymbol{k}\cdot(\hat{\boldsymbol{r}}_e - \hat{\boldsymbol{R}})$ in $\hat{H}_{I1}$ and $\hat{H}_{I2}$, and representing corrections to the long wavelength approximation. This is because a computation analogous to the one in § 1-d of Complement $\mathrm{A_{XIII}}$ shows that these corrections yield new interaction terms of the same order as $\hat{H}_{I1}^s$: interaction between the atomic orbital momentum $\boldsymbol{L}$ and the radiation magnetic field; electric quadrupole interaction.

C-4. Electric dipole Hamiltonian

Using the long wavelength approximation, the global Hamiltonian for the system atom + field is written:

$$\hat{H} = \frac{\hat{\boldsymbol{P}}^2}{2M} + \frac{1}{2m}\left[\hat{\boldsymbol{p}} - q\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}})\right]^2 + \hat{V}_{\text{Coul}} + \sum_i \frac{\hbar\omega_i}{2}\left[\hat{a}_i^\dagger\hat{a}_i + \hat{a}_i\hat{a}_i^\dagger\right] \tag{C-15}$$

We are going to perform a unitary transformation on this Hamiltonian, leading to a new interaction Hamiltonian, composed of a single term of the form $-\hat{\boldsymbol{D}}\cdot\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})$, where $\hat{\boldsymbol{D}}$ is the electric dipole moment of the atom:

$$\hat{\boldsymbol{D}} = q\ \hat{\boldsymbol{r}} \tag{C-16}$$

and $\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})$, the quantum field given by expression (B-3). This new interaction Hamiltonian is called the *electric dipole Hamiltonian.*

To find this unitary transformation, it is useful to start with the simpler case where the radiation field is treated classically.

C-4-a. Electric dipole Hamiltonian for a classical field

When the radiation field is treated classically, as an external field whose dynamic is externally imposed and hence has a fixed time dependence, the last term of relation (C-15) does not exist; operator $\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}})$, which appears in the second term, must be replaced by the external field $\boldsymbol{A}_{\perp e}(\hat{\boldsymbol{R}}, t)$. The system Hamiltonian is then written:

$$\hat{H} = \frac{\hat{\boldsymbol{P}}^2}{2M} + \frac{1}{2m}\left[\hat{\boldsymbol{p}} - q\boldsymbol{A}_{\perp e}(\hat{\boldsymbol{R}}, t)\right]^2 + \hat{V}_{\text{Coul}} \tag{C-17}$$

We are looking for a unitary transformation that performs a translation of $\hat{\boldsymbol{p}}$ by a quantity $q\boldsymbol{A}_{\perp e}(\hat{\boldsymbol{R}}, t)$, so that the second term in (C-17) is reduced to $\hat{\boldsymbol{p}}^2/2m$. Such a transformation reads:

$$\hat{T}(t) = \exp\left[-\frac{i}{\hbar} q\,\hat{\boldsymbol{r}} \cdot \boldsymbol{A}_{\perp e}(\hat{\boldsymbol{R}}, t)\ \right] \tag{C-18}$$

We can check this since, using $[\hat{\boldsymbol{p}}, f(\hat{\boldsymbol{r}})] = -i\hbar\, \partial f/\partial \hat{\boldsymbol{r}}$ and the fact that the internal variable $\hat{\boldsymbol{r}}$ commutes with the external variable $\hat{\boldsymbol{R}}$, we have:

$$\hat{T}(t)\,\hat{\boldsymbol{p}}\,\hat{T}^\dagger(t) = \hat{\boldsymbol{p}} + q\boldsymbol{A}_{\perp e}(\hat{\boldsymbol{R}}, t) \tag{C-19}$$

As they do not depend on $\hat{\boldsymbol{p}}$, the other terms of (C-17) are unchanged by the transformation. On the other hand, since this transformation has an explicit time dependence via the term $q\boldsymbol{A}_{\perp e}(\hat{\boldsymbol{R}}, t)$, the new Hamiltonian H' that governs the evolution of the new state vector:

$$|\Psi'(t)\rangle = \hat{T}(t)|\Psi(t)\rangle \tag{C-20}$$

is given by:

$$\hat{H}'(t) = \hat{T}(t)\hat{H}(t)\hat{T}^\dagger(t) + i\hbar\left[\frac{\mathrm{d}\hat{T}(t)}{\mathrm{d}t}\right]\hat{T}^\dagger(t) \tag{C-21}$$

As we have in addition:

$$i\hbar\left[\frac{\mathrm{d}\hat{T}(t)}{\mathrm{d}t}\right]\hat{T}^\dagger(t) = q\hat{\boldsymbol{r}} \cdot \frac{\partial \boldsymbol{A}_{\perp e}(\hat{\boldsymbol{R}}, t)}{\partial t} = -\hat{\boldsymbol{D}} \cdot \boldsymbol{E}_{\perp e}(\hat{\boldsymbol{R}}, t) \tag{C-22}$$

where $\hat{\boldsymbol{D}} = q\,\hat{\boldsymbol{r}}$ is the electric dipole moment of the atom, we finally obtain:

$$\hat{H}'(t) = \frac{\hat{\boldsymbol{P}}^2}{2M} + \frac{\hat{\boldsymbol{p}}^2}{2M} + V_{\text{Coul}} - \hat{\boldsymbol{D}} \cdot \boldsymbol{E}_{\perp e}(\hat{\boldsymbol{R}}, t) \tag{C-23}$$

where the last term has the expected form for an electric dipole Hamiltonian.

C-4-b. Electric dipole Hamiltonian for a quantum field

The results we just obtained suggest using the unitary transformation:

$$\hat{T} = \exp\left[-\frac{i}{\hbar} q\,\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}})\right] \tag{C-24}$$

where it is now the operator $\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}})$ that appears in the exponential. One can check that this operator is still a translation operator for $\hat{\boldsymbol{p}}$, so that the second term in (C-15) is now simply of the form $\hat{\boldsymbol{p}}^2/2m$.

As the transformation (C-24) no longer has an explicit time dependence, the term analogous to (C-22) does not exist anymore. On the other hand, we must study the transformation of the last term of (C-15), which represents the energy $\hat{H}_R$ of the transverse quantum field. We therefore rewrite expression (C-24) using the expansion (B-5) of $\hat{\boldsymbol{A}}_\perp(\hat{\boldsymbol{R}})$ as a function of $\hat{a}_i$ and $\hat{a}_i^\dagger$:

$$\hat{T} = \exp\left[\sum_i \left(\lambda_i^*\hat{a}_i - \lambda_i\hat{a}_i^\dagger\right)\right] \tag{C-25}$$

with:

$$\lambda_i = \frac{i}{\sqrt{2\varepsilon_0\hbar\omega_i L^3}}\ \boldsymbol{\varepsilon}_i\cdot\hat{\boldsymbol{D}}\ e^{-i\boldsymbol{k}_i\cdot\hat{\boldsymbol{R}}} \tag{C-26}$$

In this form, operator $\hat{T}$ does appear as a translation operator (Complement G_V, § 2-d); it obeys the equations:

$$\hat{T}\,\hat{a}_j\,\hat{T}^\dagger = \hat{a}_j + \lambda_j \qquad \hat{T}\,\hat{a}_j^\dagger\,\hat{T}^\dagger = \hat{a}_j^\dagger + \lambda_j^* \tag{C-27}$$

To prove relations (C-27), one can use (Complement B_{II} B_{II}, § 5-d) the identity:

$$e^{(A+B)} = e^A e^B e^{-[A,B]/2} \tag{C-28}$$

valid if A and B commute with their commutator $[A,B]$, as well as the commutation relation $\left[\hat{a}, f(\hat{a}^\dagger)\right] = \partial f/\partial\hat{a}^\dagger$. The transformation of the last term in (C-15) then yields:

$$\hat{T}\hat{H}_R\hat{T}^\dagger = \sum_i \frac{\hbar\omega_i}{2}\left[(\hat{a}_i+\lambda_i)(\hat{a}_i^\dagger+\lambda_i^*) + (\hat{a}_i^\dagger+\lambda_i^*)(\hat{a}_i+\lambda_i)\right] \tag{C-29}$$

The terms on the right-hand side of (C-29) that are independent of λ_i and λ_i^* yield again $\hat{H}_R$. The terms linear in λ_i and λ_i^* yield:

$$\begin{aligned}\sum_i \hbar\omega_i\left(\lambda_i\hat{a}_i^\dagger + \lambda_i^*\hat{a}_i\right) &= -\sum_i i\sqrt{\frac{\hbar\omega_i}{2\epsilon_0 L^3}}\left(\hat{a}_i\boldsymbol{\varepsilon}_i e^{i\boldsymbol{k}_i\cdot\hat{\boldsymbol{R}}} - \hat{a}_i^\dagger\boldsymbol{\varepsilon}_i^* e^{-i\boldsymbol{k}_i\cdot\hat{\boldsymbol{R}}}\right)\cdot\hat{\boldsymbol{D}}\\ &= -\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})\cdot\hat{\boldsymbol{D}}\end{aligned} \tag{C-30}$$

where we have used (B-3). We thus get the expected electric dipole form for the interaction Hamiltonian:

$$\hat{H}_I = -\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})\cdot\hat{\boldsymbol{D}} \tag{C-31}$$

Finally, the terms quadratic in λ_i and λ_i^* introduce a term we shall note $\hat{h}_{\text{dip}}$:

$$\hat{h}_{\text{dip}} = \sum_i \hbar\omega_i \lambda_i^* \lambda_i = \sum_i \frac{1}{2\varepsilon_0 L^3} (\boldsymbol{\varepsilon}_i \cdot \hat{\boldsymbol{D}})(\boldsymbol{\varepsilon}_i^* \cdot \hat{\boldsymbol{D}}) \tag{C-32}$$

It represents a dipolar energy intrinsic to the atom.

To sum up, regrouping all the previous terms, we get for the transformed Hamiltonian:

$$\hat{H}' = \frac{\hat{\boldsymbol{P}}^2}{2M} + \frac{\hat{\boldsymbol{p}}^2}{2M} + V_{\text{Coul}} + \hat{H}_R - \hat{\boldsymbol{D}} \cdot \hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}}) + \hat{h}_{\text{dip}} \tag{C-33}$$

This is a form similar to (C-23), with an additional term $\hat{h}_{\text{dip}}$.

Comments

(i) The same mathematical operator does not describe the same physical quantity in two different representations, deduced from one another by a unitary transformation. As an example, the operator $\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})$ appearing in (C-31), does not represent the transverse electric field in the new point of view, which should be $\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})$ transformed by $\hat{T}$, written as $\hat{T}\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})\hat{T}^\dagger$, and hence different from $\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})$. Actually, one can show that the operator $\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})$ represents in the new point of view the physical quantity $\hat{\mathfrak{D}}(\hat{\boldsymbol{R}})/\varepsilon_0$ where $\hat{\mathfrak{D}}(\hat{\boldsymbol{R}})$ is called the *electric displacement field* (see Complement A_{IV} of [16]).

(ii) The intrinsic dipolar energy $\hat{h}_{\text{dip}}$ is given by an integral over k, which diverges at infinity. This integral must however be limited to values of k for which the long wavelength approximation is still valid.

C-5. Matrix elements of the interaction Hamiltonian; selection rules

Consider an initial state where the atom is described by $|\psi_{\text{in}}^{\text{int}}\rangle$ for its internal state, $|\psi_{\text{in}}^{\text{ext}}\rangle$ for its external state, and where the radiation is in the state $|\psi_{\text{in}}^{R}\rangle$. The interaction Hamiltonian (C-31) couples this initial state to a final state where the atomic internal and external variables, as well as the radiation variables are respectively in the states $|\psi_{\text{fin}}^{\text{int}}\rangle$, $|\psi_{\text{fin}}^{\text{ext}}\rangle$, and $|\psi_{\text{fin}}^{R}\rangle$. As the operator $\hat{\boldsymbol{E}}_\perp(\hat{\boldsymbol{R}})$ appearing in (C-31) is a linear superposition of annihilation $\hat{a}_i$ and creation $\hat{a}_i^\dagger$ operators, the matrix element of $\hat{H}_I$ describes two types of processes: the absorption processes associated with operator $\hat{a}_i$ where one photon disappears, and the emission processes associated with operator $\hat{a}_i^\dagger$ where a new photon appears. This matrix element can be factored into a product of three matrix elements concerning the three types of variables; they are written, for the absorption processes:

$$i\sqrt{\frac{\hbar\omega_i}{2\varepsilon_0 L^3}} \left\langle \psi_{\text{fin}}^{\text{int}} \right| \boldsymbol{\varepsilon}_i \cdot \hat{\boldsymbol{D}} \left| \psi_{\text{in}}^{\text{int}} \right\rangle \left\langle \psi_{\text{fin}}^{\text{ext}} \right| \exp(i\,\boldsymbol{k}_i \cdot \hat{\boldsymbol{R}}) \left| \psi_{\text{in}}^{\text{ext}} \right\rangle \left\langle \psi_{\text{fin}}^{R} \right| \hat{a}_i \left| \psi_{\text{in}}^{R} \right\rangle \tag{C-34}$$

and for the emission processes:

$$-i\sqrt{\frac{\hbar\omega_i}{2\varepsilon_0 L^3}} \left\langle \psi_{\text{fin}}^{\text{int}} \right| \boldsymbol{\varepsilon}_i^* \cdot \hat{\boldsymbol{D}} \left| \psi_{\text{in}}^{\text{int}} \right\rangle \left\langle \psi_{\text{fin}}^{\text{ext}} \right| \exp(-i\,\boldsymbol{k}_i \cdot \hat{\boldsymbol{R}}) \left| \psi_{\text{in}}^{\text{ext}} \right\rangle \left\langle \psi_{\text{fin}}^{R} \right| \hat{a}_i^\dagger \left| \psi_{\text{in}}^{R} \right\rangle \tag{C-35}$$

The central term in these expressions is a matrix element concerning the external atomic variables; it expresses the conservation of the global momentum as we now show. Operator $\exp(\pm i\, \boldsymbol{k}_i \cdot \hat{\boldsymbol{R}})$ translates the momentum by a quantity $\pm\hbar \boldsymbol{k}_i$. If the atom's center of mass has an initial momentum $\hbar \boldsymbol{K}_{\text{in}}$, once it absorbs a photon, its final momentum will be $\hbar \boldsymbol{K}_{\text{fin}} = \hbar \boldsymbol{K}_{\text{in}} + \hbar \boldsymbol{k}_i$; the momentum $\hbar \boldsymbol{k}_i$ of the absorbed photon is therefore transferred to the atom during the absorption process. In a similar way, one can show that the atom's momentum decreases by the quantity $\hbar \boldsymbol{k}_i$ when a photon is emitted.

In the first matrix element of (C-34), which concerns the internal atomic variables, operator $\hat{\boldsymbol{D}}$ is an odd operator. The matrix element will be different from zero only if the initial and final internal atomic states have opposite parity, as for instance the $1s$ and $2p$ states of the hydrogen atom. We rediscover here a second conservation law, the conservation of parity. In addition, as the operator $\hat{\boldsymbol{D}}$ is a vector operator, it leads to selection rules on the internal angular momentum which will be studied in Complement C_{XIX}.

Comments

(i) The conservation of the total momentum comes from the central matrix elements in expressions (C-34) and (C-35). One may wonder whether this result is only valid for the approximate form (C-31) of the interaction Hamiltonian used to establish those equations. Actually it can be shown, using the commutation relations $[\boldsymbol{p}_a, F(\boldsymbol{r}_a)] = -i\hbar \partial F/\partial \boldsymbol{r}_a$ and $[\hat{a}_i^\dagger \hat{a}_i, \hat{a}_i] = -\hat{a}_i$, that the interaction Hamiltonian $\hat{H}_{I1}$ written is (C-4) (without the long wavelength approximation) commutes with the system total momentum $\sum_a \hat{\boldsymbol{p}}_a + \sum_i \hbar \boldsymbol{k}_i \hat{a}_i^\dagger \hat{a}_i$. The same result is true for all the terms of the interaction Hamiltonian. Consequently, the exact (without approximation) interaction Hamiltonian has non-zero matrix elements only between states having the same total momentum. The fact that the total momentum commutes with all the terms in the Hamiltonian is related to the system invariance with respect to spatial translation. The properties of the system are unchanged upon the translation by the same quantity of the particles and the fields. Similar considerations apply to the rotational invariance and cause the interaction Hamiltonian to only connect states with the same total angular momentum. These results are important for understanding in a simple fashion the exchanges of linear and angular momenta between atoms and photons, which will be discussed in Complements A_{XIX} and C_{XIX}.

(ii) Conservation of total momentum during the absorption process, combined with total energy conservation, shows that the energy of the absorbed photon is different from the energy separating the two internal levels involved in the transition. Two effects account for this difference: the Doppler effect, and the recoil effect (Complement A_{XIX}); they play an important role in laser cooling methods.

(iii) If we continue the calculations beyond the long wavelength approximation, we find additional terms for the interaction Hamiltonian, describing the interaction between the radiation magnetic field and the atomic orbital or spin magnetic moments (Complement A_{XIII}, § 1). Some of these terms have already been written in (C-6). Transitions, called magnetic dipole transitions, may occur between levels having the same parity, as opposed to the electric dipole transitions studied above. Other types of transitions may also be observed at higher orders, such as the quadrupole transitions.

Note finally that, if the initial radiation state already contains n_i photons, the last two matrix elements of (C-34) and (C-35) are equal to $\langle n_i - 1|\hat{a}_i|n_i\rangle = \sqrt{n_i}$ and $\langle n_i + 1|\hat{a}_i^\dagger|n_i\rangle = \sqrt{n_i + 1}$. In the presence of n_i incident photons, the probability of the absorption process is thus proportional to n_i, whereas the emission probability is proportional to $n_i + 1$. We shall see in Chapter XX that this difference is linked to the existence of two types of emission, the stimulated emission and the spontaneous emission.

With the knowledge of the various Hamiltonians $\hat{H}_A$, $\hat{H}_R$ and $\hat{H}_I$, as well as their matrix elements, we can now solve Schrödinger's equation to compute the transition amplitude between an initial state and a final state of the system "atom + field". This will be done in the next chapter, where we study various processes, such as the absorption or emission of photons for an incident radiation either monochromatic or having a large spectral band, the photoionization phenomenon, multiphoton processes and photon scattering.