

## 5. Elements of quantum electromagnetism

For charged material systems in a classic context electromagnetism provides a descriptive frame. Quantum electromagnetism (QEM) concerns understanding interactions of charged matter with electromagnetic radiations compatible with Planck radiation law.

This chapter initiates an overview of standard Maxwell equation; chemist, biochemists, molecular biologists are not conversant with this domain. We move on to examine some mathematical elements required to enter an elementary study of quantum electrodynamics. This corresponds to a level 1 (see introduction) where no correspondence to laboratory situations is required. We close the chapter with an inquiry about what is required to move into real laboratory processes. No attempt at completeness is made. The reader is referred to de Oliveira's "Intermediate spectral theory and quantum dynamics" (Birkhäuser, Basel, 2009) for an appropriate resource.

### 5.1. Classical Maxwell equations

The electromagnetic field in classical theory appears as two 3-vector fields, the electric  $\mathbf{E}$  and magnetic  $\mathbf{B}$ . The current density  $\mathbf{J}$  relates to the electric field by Ohm's law:  $\mathbf{J} = \sigma \mathbf{E}$ . The symbol  $\sigma$  stands for resistivity. Maxwell equations and gauge invariance (see below) can be used to reduce the fields  $\mathbf{E}$  and  $\mathbf{B}$  degrees of freedom with the help of a single 4-vector field  $A^\mu \equiv (A_0, \mathbf{A})$ , where  $\mathbf{A}$  is a transverse field with two independent components once constraints are made effective; the time component  $A_0$  depends upon the external sources of charge.

Maxwell equations describe classical electromagnetism including charge conservation:

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \rho ; & \nabla \wedge \mathbf{E} &= -(1/c) \partial \mathbf{B} / \partial t ; \\ \nabla \cdot \mathbf{B} &= 0 ; & \nabla \wedge \mathbf{B} &= \mathbf{J} + (1/c) \partial \mathbf{E} / \partial t \end{aligned} \quad (5.1.1)$$

Displacement currents are neglected:  $\mathbf{E} = \mathbf{D}$ ; this is relevant to propagation of EM fields in vacuum. The equations involving curls  $\nabla \wedge \mathbf{B}$  and  $\nabla \wedge \mathbf{E}$  for  $\mathbf{J} = \mathbf{0}$  tell us that

so long there are time dependent electric and magnetic fields their curls do not vanish; electric and magnetic fields are hence coupled to each other; the wedge  $\wedge$  symbol stands for vector product.

The charge density ( $\rho$ ) fulfils a conservation equation:  $\partial\rho/\partial t + \nabla \cdot \mathbf{J} = 0$ . Solutions to these equations characterize specific EM fields. The free space permeability and permittivity constants  $\mu_0$  and  $\epsilon_0$  are subsumed as  $1/\mu_0 \epsilon_0 = c^2$ . The symbol  $c$  is the velocity of light. This theory relates to the speed of light in vacuum electric ( $\epsilon_0$ ) and magnetic ( $\mu_0$ ) magnitudes which was a remarkable achievement.

A change of magnetic field in time,  $\partial\mathbf{B}/\partial t \neq \mathbf{0}$ , is related to the curl of an electric field, i.e.  $\nabla \wedge \mathbf{E}$ . Similarly, a time varying electric field,  $\partial\mathbf{E}/\partial t$ , relates to the curl of a magnetic field minus a current, i.e.  $\nabla \wedge \mathbf{B} - \mathbf{J}$ . Thus, *motion transfers into fields*.

When  $\mathbf{J} \neq 0$  and/or external charges are present electric and magnetic fields are modulated by the response set up by the material surroundings. Particular cases are sketched below.

### E&E.5.1-1 Maxwell equations for stationary media

Medium effects are introduced via two additional field vectors:  $\mathbf{P}$  and  $\mathbf{M}$ ; they correspond to the electric and magnetic polarization of the media, respectively. By definition:

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} \text{ and } \mathbf{B}/\mu_0 = \mathbf{H} + \mathbf{M}$$

The constants appearing in these equations,  $\epsilon_0$  and  $\mu_0$  are vacuum electric susceptibility and magnetic permeability. Equations (5.1.1) read now as:

$$\begin{aligned} \nabla \cdot \mathbf{E} &= (1/\epsilon_0) \rho_{\text{total}} = (1/\epsilon_0) (\rho - \nabla \cdot \mathbf{P}); \\ \nabla \wedge \mathbf{E} &= -(1/c) \partial \mathbf{B} / \partial t; \\ \nabla \cdot \mathbf{B} &= 0; \\ \nabla \wedge \mathbf{B} &= \mu_0 (\mathbf{J} + \partial \mathbf{P} / \partial t + \nabla \wedge \mathbf{M} (1/c) \epsilon_0 \partial \mathbf{E} / \partial t) \end{aligned}$$

Using the definitions relating the fields in vacuum and in the medium, Maxwell equations show a similar form:

$$\begin{aligned} \nabla \cdot \mathbf{D} &= \rho; & \nabla \wedge \mathbf{E} &= -(1/c) \partial \mathbf{B} / \partial t; \\ \nabla \cdot \mathbf{B} &= 0; & \nabla \wedge \mathbf{H} &= \mathbf{J} + (1/c) \partial \mathbf{D} / \partial t \end{aligned} \quad (5.1.1')$$

The equations relating  $\mathbf{E}$  to  $\mathbf{D}$  and  $\mathbf{H}$  to  $\mathbf{B}$  are known as constitutive relationships. At the simplest level they look like:

$$\begin{aligned} \mathbf{D} &= \kappa \epsilon_0 \mathbf{E}; \\ \mathbf{J} &= \boldsymbol{\sigma} \mathbf{E}; \\ \mathbf{H} &= \mathbf{B}/\mu. \end{aligned}$$

A treatment for inhomogeneous media is given in Sections 5.5 and 5.6 below.

The equations above form among other things the core of solvent effect theories on chemical reactions. They indicate that Maxwell equations still holds in an “ordinary” material.

At the Fence, situations where one subsystem is moving with respect to another are commonly found. In the following E&E useful equations are quoted. The reader can consult textbooks on electrodynamics (Jackson, Müller-Kirsten) or electromagnetism (Panofsky & Phillips).

#### E&E.5.1-2 Maxwell equations for moving media

Let  $\mathbf{v}$  be the velocity of a moving media. The constitutive equations are given as:

$$\mathbf{J} = \boldsymbol{\sigma} (\mathbf{E} + \mathbf{v} \wedge \mathbf{P}) = \boldsymbol{\sigma} \mathbf{E}'$$

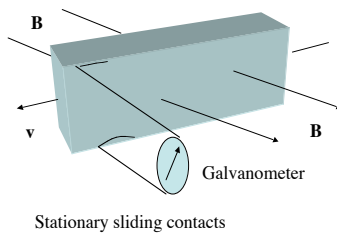
$$\mathbf{P} = \epsilon_0 (\kappa - 1)(\mathbf{E} + \mathbf{v} \wedge \mathbf{B})$$

Maxwell's equations can be written as

$$\begin{aligned} \nabla \cdot \mathbf{D} &= \rho ; \nabla \cdot \mathbf{B} = 0 ; \nabla \wedge \mathbf{E} = -(1/c) \partial \mathbf{B} / \partial t ; \\ \nabla \wedge (\mathbf{B} - \mu_0 \mathbf{P} \wedge \mathbf{v}) &= (1/c) \partial \mathbf{D} / \partial t \end{aligned} \quad (5.1.1'')$$

A moving polarized dielectric is equivalent to a magnetized material of magnetic moment:

$$\mathbf{M}_{\text{eq}} = (\mathbf{P} \wedge \mathbf{v})$$



#### E&E.5.1-3 Conductor motion in a magnetic field

In this figure it is represented a conducting bar moving with velocity  $\mathbf{v}$  in a static magnetic field  $\mathbf{B}$  perpendicular to  $\mathbf{v}$  direction. A meter is connected via sliding contacts; an electric current is detected for  $\mathbf{v} \neq 0$ . From this setup one expects an electric field  $\mathbf{E}' = \mathbf{v} \wedge \mathbf{B}$  so that a current will flow through the contacts and be sensed by a stationary galvanometer. Whether the source of  $\mathbf{B}$  is stationary or is in motion is of no concern.

#### E&E.5.1-4 Classical vector flow

The simplest I-frame system contains a spin vector  $\mathbf{S}$ . For a classical system assume the I-frame carrying a magnetic moment  $\mathbf{m}$  with fixed modulus  $|\mathbf{m}|$  under the motion of the I-frame. To describe the vector flow besides the local vector density  $\mathbf{M} = \rho(\mathbf{r}, t) \mathbf{m}(\mathbf{r}, t)$  there is need of the I-frame linear velocity  $\mathbf{v}(\mathbf{r}, t)$  and its angular velocity  $\boldsymbol{\omega}(\mathbf{r}, t)$ ; the direction of this latter vector is perpendicular to the plane made by  $\mathbf{m}$  and  $\mathbf{v}$ .

Consider a volume element  $\Delta V = \Delta x \Delta y \Delta z$  and the time interval from  $t$  to  $t + dt$  and calculate the change in time of the local vector density:

$$d\mathbf{M}/dt = -\nabla \cdot (\mathbf{v}(\mathbf{r},t)\mathbf{M}(\mathbf{r},t)) + \boldsymbol{\omega}(\mathbf{r},t) \wedge \mathbf{M}(\mathbf{r},t)$$

The term in round parenthesis  $(\mathbf{v}(\mathbf{r},t)\mathbf{m}(\mathbf{r},t))$  is a tensor with elements:

$$(\mathbf{v}(\mathbf{r},t)\mathbf{M}(\mathbf{r},t))_{ij} = v(\mathbf{r},t)_i M(\mathbf{r},t)_j.$$

The equation above is known as vector continuity equation. Here, this continuity equation derives from the kinematics and the invariance of  $|\mathbf{m}|$  only; the equation is independent from dynamic laws. Now, introduce the currents:

$$\begin{aligned} \mathbf{j}_s(\mathbf{r},t) &= \mathbf{v}(\mathbf{r},t)\mathbf{M}(\mathbf{r},t) \text{ and} \\ \mathbf{j}_\omega(\mathbf{r},t) &= \boldsymbol{\omega}(\mathbf{r},t) \wedge \mathbf{M}(\mathbf{r},t) \end{aligned}$$

These are the linear and angular current densities and the equation above takes on the form:

$$d\mathbf{M}/dt = -\nabla \cdot \mathbf{j}_s(\mathbf{r},t) + \mathbf{j}_\omega(\mathbf{r},t)$$

These relationships are of interest for discussing magnetic materials.

#### E&E.5.1-5

A magnetic dipole  $\boldsymbol{\mu}$  (field) arises from a closed loop current ( $i$ ) whose direction is perpendicular to the loop and magnitude is given by

$$\boldsymbol{\mu} = i A$$

The current  $i$  is given in amperes (C/s);  $A$  is the area of the loop ( $m^2$ ). The units of the magnetic dipole are coulombs (C) meters<sup>2</sup> seconds<sup>-1</sup>. For a circular loop with  $v$  standing for the charge velocity and  $r$  the loop radius one has:

$$i = qv/2\pi r$$

The magnetic dipole reads:

$$\boldsymbol{\mu} = i A = (qv/2\pi r) 2\pi r^2 = qrv/2$$

Because the direction of the magnetic dipole is perpendicular to the loop plane one can write with vector notations:

$$\boldsymbol{\mu} = q \mathbf{r} \wedge \mathbf{v} / 2$$

Using the definition of angular momentum  $\mathbf{L} = \mathbf{r} \wedge \mathbf{p}$  and bearing in mind that for a classical mechanical system:  $\mathbf{p} = m\mathbf{v}$

$$\boldsymbol{\mu} = q \mathbf{r} \wedge \mathbf{v} (m/2m) = q \mathbf{r} \wedge \mathbf{p} (1/2m) = q \mathbf{L} / 2m$$

For an electron take  $q = -|e|$  the magnetic moment is just opposite to the direction of the orbital angular momentum:

$$\boldsymbol{\mu} = -(|e|/2m) \mathbf{L}$$

**E&E.5.1-6**

In quantum mechanics the angular momentum is given by:

$$\hat{L}^2 |L, M_L\rangle = \hbar^2 L(L+1) |L, M_L\rangle$$

$\langle L, M_L | \hat{L}^2 |L, M_L\rangle = \hbar^2 L(L+1)$ . The magnetic dipole takes on the form:

$$\boldsymbol{\mu} = -(e\hbar/2m_e) [L(L+1)]^{1/2} = -\beta_e [L(L+1)]^{1/2}$$

The quantity  $\beta_e = (e\hbar/2m_e)$  is known as Bohr magneton for the electron.

Now, the interaction operator for a magnetic dipole in a magnetic field  $\mathbf{B}$  has the form:

$$\hat{V} = -\hat{\boldsymbol{\mu}} \cdot \mathbf{B}$$

The units of the magnetic field are  $\text{J A}^{-1} \text{m}^{-2}$  that is equal to one Tesla (T). Thus,  $1\text{T} = 1 \text{J} \cdot \text{A}^{-1} \cdot \text{m}^{-2}$ . The Bohr magneton units are  $\text{J} \cdot \text{T}^{-1}$ .

Consider a system in absence of material filling the space. The EM field energy for a system in vacuum is given by:

$$E_{\text{EM}} = (1/8\pi) \int (\mathbf{E} \cdot \mathbf{E} + \mathbf{B} \cdot \mathbf{B}) d^3\mathbf{x} \quad (5.1.2)$$

The *energy density* is the function:  $1/2 (\mathbf{E} \cdot \mathbf{E} + \mathbf{B} \cdot \mathbf{B})$ .

The total momentum of the field  $\mathbf{P}_{\text{EM}}$  is obtained with the help of Poynting vector  $\mathbf{S}$  relating electric to magnetic field:

$$\mathbf{P}_{\text{EM}} = (1/4\pi c) \int (\mathbf{E} \wedge \mathbf{B}) d^3\mathbf{x} = \int \mathbf{S} d^3\mathbf{x} \quad (5.1.3)$$

For interactions where the EM field changes, there will be a change in momentum that we have to take into account; note that the wedge product has energy dimension ( $[E]$ ) so that  $[E]/c$  has momentum dimension.

The Poynting vector  $\mathbf{S}$  permits calculating energy flow. Charges in a dielectric piece of matter in motion are accelerated by electromagnetic fields thereby producing radiation; the relative direction of the velocity and electric-field vectors determines the direction of the energy flow between field and matter. For a total field consisting of incident and radiated electromagnetic field, interference term between the two would provide directional emission.

Thus the EM fields determine relevant physical quantities. It is then natural to seek ways and means to calculate them for specific situations.

An appropriate model to describe EM fields is a system with no charges ( $\rho = 0$ ) and no currents ( $\mathbf{J} = \mathbf{0}$ ). The EM fields in terms of the vector potential  $\mathbf{A}(\mathbf{x}, t)$  take on the forms:

$$\begin{aligned}\mathbf{E}(\mathbf{x}, t) &= - (1/c) \partial \mathbf{A}(\mathbf{x}, t) / \partial t \\ \mathbf{B}(\mathbf{x}, t) &= \nabla \wedge \mathbf{A}(\mathbf{x}, t)\end{aligned}\quad (5.1.4)$$

One can sense the economy produced by the introduction of this vector potential.

In reciprocal space, the equations are uncoupled. The reciprocal space representation is introduced via linear superpositions in the base set of plane wave set  $\{\exp(i \mathbf{k} \cdot \mathbf{x})\}_{\mathbf{x}}$ . For fields that can be written  $\mathbf{E}(\mathbf{x}, t) = \mathbf{E}(\mathbf{x}) \exp(i\omega t)$  and  $\mathbf{B}(\mathbf{x}, t) = \mathbf{B}(\mathbf{x}) \exp(i\omega t)$  the Fourier transforms are:

$$\mathcal{E}(\mathbf{k}) = (1/4\pi)^3 \int d^3 \mathbf{x} \mathbf{E}(\mathbf{x}) \exp(i \mathbf{k} \cdot \mathbf{x}) \quad (5.1.5a)$$

$$\mathcal{B}(\mathbf{k}) = (1/4\pi)^3 \int d^3 \mathbf{x} \mathbf{B}(\mathbf{x}) \exp(i \mathbf{k} \cdot \mathbf{x}) \quad (5.1.5b)$$

These relationships can be inverted to get the electric  $\mathbf{E}(\mathbf{x})$  and magnetic  $\mathbf{B}(\mathbf{x})$  fields in the plane wave set  $\{\exp(i \mathbf{k} \cdot \mathbf{x})\}_{\mathbf{k}}$ .

The coupled differential equations (5.1.1) in real space, i.e.  $\nabla \wedge \mathbf{E} = -(1/c) \partial \mathbf{B} / \partial t$  and  $\nabla \wedge \mathbf{B} = \mathbf{J} + (1/c) \partial \mathbf{E} / \partial t$ , in  $\mathbf{k}$ -space are uncoupled. Maxwell equations in  $\mathbf{k}$ -space read:

$$\begin{aligned}i \mathbf{k} \cdot \mathcal{E}(\mathbf{k}) &= 0 ; \\ i \mathbf{k} \wedge \mathcal{E}(\mathbf{k}) &= -(1/c) d\mathcal{B}(\mathbf{k}) / dt\end{aligned}\quad (5.1.6a)$$

$$\begin{aligned}i \mathbf{k} \cdot \mathcal{B}(\mathbf{k}) &= 0 ; \\ i \mathbf{k} \wedge \mathcal{B}(\mathbf{k}) &= (1/c) d\mathcal{E}(\mathbf{k}) / dt.\end{aligned}\quad (5.1.6b)$$

From eqs.(5.1.6) one obtains differential equations for the  $\mathbf{k}$ -fields. Take vector product from the left with  $\nabla$  and use of a vector identity one gets thanks to transverse condition on the electric field (Coulomb gauge):

$$d^2 \mathcal{E}(\mathbf{k}) / dt^2 + c^2 k^2 \mathcal{E}(\mathbf{k}) = 0 \quad (5.1.7a)$$

$$d^2 \mathcal{B}(\mathbf{k}) / dt^2 + c^2 k^2 \mathcal{B}(\mathbf{k}) = 0 \quad (5.1.7b)$$

Similar equations obtain for the transverse potential:  $\mathcal{A}(\mathbf{k})$ .

The import of  $\mathbf{k}$ -equations is enormous. They imply Maxwell equations involve fields at the same point in Fourier space (reciprocal space) defining the EM field in vacuum only; different cases enter via appropriate boundary conditions. Solutions to these equations yield a mode representation for the EM field.

The mode representation is examined with the help of  $\mathbf{A}$ . The vector potential  $\mathbf{A}$  satisfies also the wave equation and a transverse condition:

$$(1/c^2) \partial^2 \mathbf{A} / \partial t^2 - \nabla^2 \mathbf{A} = 0;$$

$$\operatorname{div} \mathbf{A} = \nabla \cdot \mathbf{A} = 0 \quad (5.1.8)$$

The transverse EM (t-EM) fields fulfill the divergence equation in (5.1.8); electric and magnetic fields are transverse as well; this follows from eq.(5.1.1) and the conditions imposed, namely, zero external charge density,  $\rho=0$ .

The vector  $\boldsymbol{\epsilon}_k$  is a unit polarization vector, the wave vector  $\mathbf{k}$  is perpendicular to  $\boldsymbol{\epsilon} = (\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2, \boldsymbol{\epsilon}_3)$ , namely,  $\mathbf{k} \cdot \boldsymbol{\epsilon} = 0$ . In general, two independent vectors  $\boldsymbol{\epsilon}_k$  correspond to each separate vector  $\mathbf{k}$ . For the sake of simplicity we avoid introduction of another index. The vector  $\mathbf{k}$  indicates propagation direction.

#### E&E-5.1-7 Derive equation (5.1.8)

Start from Maxwell equation relating the curl of  $\mathbf{B}$  to the time derivative of the electric field:  $\nabla \wedge \mathbf{B} = \mathbf{J} + (1/c) \partial \mathbf{E} / \partial t$ . The current  $\mathbf{J}$  is zero. Use the definition between  $\mathbf{B}$  and  $\mathbf{A}$  from eq.(5.1.4) to get:

$$\nabla \wedge \nabla \wedge \mathbf{A} = (1/c) \partial[-1/c] \partial \mathbf{A} / \partial t / \partial t = -(1/c^2) \partial^2 \mathbf{A} / \partial t^2$$

From a well-known identity, namely,  $\nabla \wedge \nabla \wedge \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$  and the transverse condition  $\nabla \cdot \mathbf{A} = 0$  by replacement one obtains eq.(5.1.8).

#### E&E.5.1-8 Polarized light representation

A monochromatic light wave propagating in the 3-direction and polarized in 2-direction is given by:

$$\mathbf{E} = E_0 \boldsymbol{\epsilon}_2 \cos(k x_3 - \omega t) \quad (5.1-5.1)$$

For a field polarized along 1-direction you change the polarization vector  $\boldsymbol{\epsilon}_2$  by  $\boldsymbol{\epsilon}_1$ ; the propagation direction still is  $x_3$ . The frequency (pulsation)  $\omega$  is related to the energy quanta ( $\hbar\omega$ ) that this specific type of light can exchange with material systems; the number (intensity) is related to the amplitude ( $|E_0|^2$ ) as shown below.

The vectors  $\mathbf{E}$ ,  $\mathbf{B}$  and  $\mathbf{k}$  are mutually perpendicular; the direction of propagation is given by  $\mathbf{k}$ . The plane perpendicular to  $\mathbf{k}$  is the phase plane.

Note that  $(1/c^2)|\mathbf{E}|^2 = |\mathbf{B}|^2$ . The vectors  $\boldsymbol{\epsilon}_1$  and  $\boldsymbol{\epsilon}_2$  span the plane orthogonal to  $\mathbf{k}$ . For the plane wave  $\mathbf{E} = E_0 \exp(i(\mathbf{k} \cdot \mathbf{x} - \omega t))$  the vector  $E_0$  defines the direction of oscillation.

If  $E_0$  is constant, the wave is linearly polarized. The transport of energy takes place in the direction of the propagation vector  $\mathbf{k}$  and is proportional to  $\mathbf{E} \wedge \mathbf{B}$ . A general case corresponds to a decomposition of the electric and magnetic vectors along the polarization directions:  $\mathbf{E} = \mathbf{E}_1 + \mathbf{E}_2$ ;  $\mathbf{B} = \mathbf{B}_1 + \mathbf{B}_2$ ; obviously,  $|\mathbf{E}| = |E_0|$  and with  $i=,2$ :

$$\begin{aligned} \mathbf{E}_i(\mathbf{x}, t) &= \boldsymbol{\epsilon}_i E_i \exp(i(\mathbf{k} \cdot \mathbf{x} - \omega t)) ; \\ \mathbf{B}_i(\mathbf{x}, t) &= \boldsymbol{\epsilon}_i B_i \exp(i(\mathbf{k} \cdot \mathbf{x} - \omega t)) \end{aligned} \quad (5.1-5.2)$$

Because  $\mathbf{E}$  and  $\mathbf{B}$  are perpendicular one can take  $\mathbf{E}$  as the representative of the whole wave. The  $E_i$  are complex numbers, and can be written as:

$$E_i = |E_i| \exp(i\theta_i) \text{ and } E_2 = |E_2| \exp(i\theta_2) \quad (5.1-5.3)$$

It is a usual practice to take  $\theta_1=0$  and  $\theta_2=\theta$  because only the relative phase makes sense. With this convention,  $\theta=0$  corresponds to a linearly polarized wave:

$$\mathbf{E} = (|E_1| \boldsymbol{\epsilon}_1 + |E_2| \boldsymbol{\epsilon}_2) \exp(i(\mathbf{k}\cdot\mathbf{x} - \omega t)) \quad (5.1-5.4)$$

The real part (Re) of  $\mathbf{E}$  is given by

$$\text{Re}\mathbf{E} = (|E_1| \boldsymbol{\epsilon}_1 + |E_2| \boldsymbol{\epsilon}_2) \cos(\mathbf{k}\cdot\mathbf{x} - \omega t) \quad (5.1-5.5)$$

This latter equation corresponds to our first one with a more detailed content. For  $\theta=\phi\neq 0$  the wave is elliptically polarized:

$$\mathbf{E} = |E_1| \boldsymbol{\epsilon}_1 \exp(i(\mathbf{k}\cdot\mathbf{x} - \omega t)) + |E_2| \boldsymbol{\epsilon}_2 \exp(i(\mathbf{k}\cdot\mathbf{x} - \omega t + \phi)) \quad (5.1-5.6)$$

A circularly polarized wave obtains when  $|E_1|=|E_2|$  and  $\phi=\pm\pi/2$ , i.e.

$$\mathbf{E} = |E_1| (\boldsymbol{\epsilon}_1 + \boldsymbol{\epsilon}_2 \exp(\pm i\pi/2)) \exp(i(\mathbf{k}\cdot\mathbf{x} - \omega t)) = |E_1| (\boldsymbol{\epsilon}_1 \pm \boldsymbol{\epsilon}_2) \exp(i(\mathbf{k}\cdot\mathbf{x} - \omega t)) \quad (5.1-5.7)$$

The real part of the electric field vector reads:

$$\text{Re}\mathbf{E} = |E_1| \boldsymbol{\epsilon}_1 \cos(\mathbf{k}\cdot\mathbf{x} - \omega t) \pm |E_1| \boldsymbol{\epsilon}_2 \sin(\mathbf{k}\cdot\mathbf{x} - \omega t) \quad (5.1-5.8)$$

The formalism presented so far will be adapted to quantize the t-EM field. The simple model of radiation enclosed in a box is used to this end; from now on  $\mathbf{A}(\mathbf{x},t)$  is a transverse vector potential for which no special symbol is used to alleviate notations. Periodic boundary conditions with a cubic box of length  $L$ , turns now the transverse potential into a Fourier series:

$$\mathbf{A}(\mathbf{x},t) = \sum_{\mathbf{k}} \sqrt{(4\pi c/L^3 k_k)} \boldsymbol{\epsilon}_{\mathbf{k}} a_{\mathbf{k}}(t) \exp(i \mathbf{k}_{\mathbf{k}} \cdot \mathbf{x}) \quad (5.1.9)$$

The problem is the determination of the time dependence for the amplitudes  $a_{\mathbf{k}}(t)$ ;  $|\mathbf{k}_{\mathbf{k}}|=k_{\mathbf{k}}$ . Combining the last two equations one gets a harmonic oscillator equation for each field mode with wave vector  $\mathbf{k}_{\mathbf{k}}$ :

$$\ddot{a}_{\mathbf{k}} + \omega_{\mathbf{k}}^2 a_{\mathbf{k}}(t) = 0 \quad (5.1.10)$$

The frequency  $\omega_{\mathbf{k}}$  equals to  $c k_{\mathbf{k}}$ ; a time dependent solution reads:

$$a_{\mathbf{k}}(t) = a_{\mathbf{k}} \exp(-i \omega_{\mathbf{k}} t) \quad (5.1.11)$$

For each frequency there is a normal mode equation describing time dependence.



**E&E-5.1-9 Show that solutions given in eq, (5.1.11) fulfill differential eq,(5.1.10)**

To show this, take the first time derivative of the equation (5.1.11):

$$da_k(t)/dt = d\{ a_k \exp(-i \omega_k t)\}/dt = -i \omega_k a_k \exp(-i \omega_k t)$$

The second derivative  $\ddot{a}_k$  yields

$$\begin{aligned} \ddot{a}_k &= d\{da_k(t)/dt\}/dt = (-i \omega_k)^2 a_k \exp(-i \omega_k t) = \\ &= -\omega_k^2 a_k \exp(-i \omega_k t) = -\omega_k^2 a_k(t) \end{aligned} \quad (5.1-7.1)$$

Sum now  $\omega_k^2 a_k(t)$  to the first and last terms above to get equation (5.1.10).

The set of time independent amplitudes  $\{a_k\}$  completely defines the space part of the time independent vector potential:

$$\begin{aligned} \mathbf{A}(\mathbf{x}) &= \sum_j \sqrt{(4\pi c/L^3 k_j)} [\boldsymbol{\epsilon}_j a_j \exp(i \mathbf{k}_j \cdot \mathbf{x}) + \boldsymbol{\epsilon}_j a_j^* \exp(-i \mathbf{k}_j \cdot \mathbf{x})] \\ \mathbf{A}(\mathbf{x}) &= \mathbf{A}^+(\mathbf{x}) + \mathbf{A}^-(\mathbf{x}) \end{aligned} \quad (5.1.12)$$

The sum is over positive and negative  $\mathbf{k}$ -vectors is represented by  $\mathbf{A}^+(\mathbf{x})$  and  $\mathbf{A}^-(\mathbf{x})$ , respectively. Conventionally, the plane waves in  $\mathbf{A}^+(\mathbf{x})$  are moving from left to right, while in  $\mathbf{A}^-(\mathbf{x})$  they do from right to left. Thus, given a set of  $\{a_k\}$ , the vector potential  $\mathbf{A}(\mathbf{x})$  is fixed once the polarization vectors are known; this would reflect the experimental setup used to prepare the electromagnetic field. Moreover, from eq.(5.1.4) the electric and magnetic fields can be calculated for specific cases.

The energy expression eq.(5.1.2) can be transformed by introducing the definitions from eq.(5.1.4) and the Fourier expansion of  $\mathbf{A}(\mathbf{x},t)$  from eq.(5.1.9) the electromagnetic energy can be written as sum of EM modes:

$$E_{EM} = \sum_k \omega_k |a_k|^2 \quad (5.1.13)$$

The total momentum of the field  $\mathbf{P}_{EM}$  is obtained taking into account that the scalar product  $\mathbf{k} \cdot \mathbf{a}_k = 0$ , the momentum is given the form:

$$\mathbf{P}_{EM} = \sum_k \mathbf{k}_k |a_k|^2 \quad (5.1.14)$$

These are the results for the energy and momentum of the electromagnetic field in absence of external sources of radiation or absorption (or scattering). Each  $k$ -mode contributes independently from others to energy and momentum. In absence of matter, there is no mixing of frequencies. A particular field is characterized by the non-zero amplitudes  $|a_k|^2$ .

The energy formula eq.(5.1.2) is a quadratic real form. The energy is not reckoned from the field directly but from their square modulus. A similar expression obtains from the mode decomposition, eq.(5.1.13). This latter faintly suggests a quantum mechanical kinship.

But light was considered as the paradigm of a classical wave. The wave picture replaced Newton's classical particle description. The surprise came after Planck discovery that the EM field *exchange* energy with sources in finite amounts, i.e. quanta. This energy quantum is proportional to a frequency; Planck constant ( $h$ ) was born in 1900. Quantum physics started to be on the move ever since changing the face of physics and chemistry; later on is changing the face of biological sciences.

### E&E-5.1-10 Gauge transformation

The description of t-EM fields in terms of potentials introduces extra degrees of freedom that cannot be independent. While the fields ( $\mathbf{E}$  and  $\mathbf{B}$ ) remain unchanged under a so-called gauge transformation the potentials change:

$$\begin{aligned}\mathbf{A}(\mathbf{x},t) &\rightarrow \mathbf{A}(\mathbf{x},t) + \nabla\Gamma(\mathbf{x},t) \\ \phi^0(\mathbf{x},t) &\rightarrow \phi^0(\mathbf{x},t) - (1/c) \partial \Gamma(\mathbf{x},t)/\partial t\end{aligned}\quad (5.1-10.1)$$

The gauge function  $\Gamma(\mathbf{x},t)$  is an arbitrary function of  $\mathbf{x}$  and  $t$ . We are in real space. When a particular gauge is selected to handle a type of problem, the unwanted degrees of freedom can be eliminated using the constraint relations introduced by the choice of gauge.

The pair then ( $\mathbf{A}(\mathbf{x},t)$ ,  $\phi^0(\mathbf{x},t)$ ) is referred to as a gauge. There is infinity of gauges leaving invariant the electric and magnetic field. Remember that

$$\begin{aligned}\mathbf{E} &= -\partial\mathbf{A}/\partial t - \nabla_x \phi^0(\mathbf{x},t) \text{ and} \\ \mathbf{B} &= -\nabla_x \wedge \mathbf{A}(\mathbf{x},t),\end{aligned}$$

so that these potentials are handy when one is to calculate the electric and magnetic fields for a given situation.

To find out a specific gauge one has to find out the gauge function  $\Gamma(\mathbf{x},t)$ . This result obtains by imposing supplemental conditions that are known as gauge conditions.

For the Coulomb gauge, the condition is  $\nabla_x \cdot \mathbf{A}(\mathbf{x},t) = 0$ . Then, the vector  $\mathbf{A}$  turns into a transverse vector  $\mathbf{A}_\perp$  that is perpendicular to the propagation vector  $\mathbf{k}$ . By taking  $\phi^0(\mathbf{x},t)=0$  we have the electromagnetic gauge. In this case,

$$\mathbf{E}(\mathbf{x},t) = -\partial\mathbf{A}(\mathbf{x},t)/\partial t.$$

*Göppert-Mayer gauge.* This gauge is particularly useful in molecular quantum mechanics. If the origin of the I-frame system is indicated by  $\mathbf{x}_0$  let us define  $\Gamma(\mathbf{x},t)$  for this case:

$$\Gamma(\mathbf{x},t) = -(\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{A}_\perp(\mathbf{x}_0,t) \quad (5.1-10.2)$$

The transformation may give a special role to an origin in the material system; for us it will be the origin of the I-frame to which the quantum molecular system is attached. The transformed transverse vector potential reads:

$$\mathbf{A}'(\mathbf{x},t) = \mathbf{A}_\perp(\mathbf{x},t) - \mathbf{A}_\perp(\mathbf{x}_0,t) \quad (5.1-10.3)$$

$$\phi'^0(\mathbf{x},t) = U_{Coul}(\mathbf{x}) - ((\mathbf{x} - \mathbf{x}_0)/c) \cdot \partial \mathbf{A}_\perp(\mathbf{x}_0,t)/\partial t \quad (5.1-10.4)$$

The Hamiltonian in this gauge takes on the form:

$$\hat{H} = (1/2M) [ \hat{\mathbf{p}} - q \mathbf{A}'(\hat{\mathbf{x}},t) ]^2 + U_{Coul}(\hat{\mathbf{x}}) - q (\hat{\mathbf{x}} - \mathbf{x}_0) \cdot \partial \mathbf{A}_\perp(\mathbf{x}_0,t)/\partial t \quad (5.1-10.5)$$

The last term is the electric dipole moment operator:  $\hat{\boldsymbol{\mu}} = q (\hat{\mathbf{x}} - \mathbf{x}_0)$ . The interaction operator is known as the electric dipole Hamiltonian:

$$\hat{H}'_1 = \hat{\boldsymbol{\mu}} \cdot \partial \mathbf{A}_\perp(\mathbf{x}_0,t)/\partial t = - \hat{\boldsymbol{\mu}} \cdot \mathbf{E}(\mathbf{x}_0,t) \quad (5.1-10.6)$$

In the long wave length approximation, the external potentials associated to the radiation field can be calculated at  $\mathbf{x}_0$  and, consequently, from eq. (5.1-8.3) one obtains  $\mathbf{A}'(\mathbf{x}_0,t) = 0$ . The approximate Hamiltonian takes on the form:

$$\hat{H} = (1/2M) ( \hat{\mathbf{p}}^2 + U_{Coul}(\hat{\mathbf{x}}) ) - \hat{\boldsymbol{\mu}} \cdot \mathbf{E}(\mathbf{x}_0,t) \quad (5.1-10.7)$$

This operator is extensively used in molecular quantum mechanics. In the long wave length model the interaction operators,  $\hat{\boldsymbol{\mu}} \cdot \mathbf{E}(\mathbf{x}_0,t)$  and  $\hat{\mathbf{p}} \cdot \mathbf{A}$  yield equivalent results.

The word photon is used here mostly in the sense of amount of energy and linear momentum that can be exchanged with material systems at Fences. Albeit the particle idea smuggles all the time, one should be aware that it is a way of talking; you cannot “travel” with a photon because this is massless ( $M_{\text{photon}} = 0$ ) and there is no I-frame where to hang this “particle” (states); the I-frame that makes sense is the one for the sources or sinks or scatter center in real space. The expression: “create a photon at a point in real space” is a way of talking. The meaning will be clear, we hope, once you have gone over the next chapters.

Hint: Before entering Section 5.2 pay a visit to the harmonic oscillator in Section 4.4 again.

We are about to jump into quantum dynamical aspects concerning EM radiation. It is thus advisable to pause and signal some important features of

quantum physical formalisms. All possibilities a physical system may have are coded in one stroke, as it were. The base set must be complete so that any possible quantum state can be represented as a linear superposition. The EM field carries energy and signals. But an appropriate Hilbert space does not carry energy is just an abstract space. At the Fence the projected theory must take into account this experimental fact in one way or another. This is the issue examined below.

## 5.2. Quantum electrodynamics: elements

The construction of base sets able to represent quantum states for the t-EM field in a space where energy available to be transferred that is the issue; these amounts of energy must be *reckoned*.

The amplitudes fulfilling eq.(5.1.10) are replaced by operators:

$$a_{k\alpha} \rightarrow \hat{a}_{k\alpha}^+ \quad \& \quad a_{k\alpha} \rightarrow \hat{a}_{k\alpha} \quad (5.2.1)$$

Remember, the functions  $a_{k\alpha}$  and  $a_{k\alpha}^+$  fulfill harmonic oscillator equations. From Section 4.5.1 we know that a simple translation of these symbols into annihilation and creation operators is possible. These operators must fulfill commutation relations of the kind:

$$\begin{aligned} [\hat{a}_{i\alpha}, \hat{a}_{j\alpha'}] &= [\hat{a}_{i\alpha}^+, \hat{a}_{j\alpha'}^+] = 0 \\ [\hat{a}_{i\alpha}, \hat{a}_{j\alpha'}^+] &= \delta_{ij} \delta_{\alpha\alpha'} \end{aligned} \quad (5.2.2)$$

These operators act in Fock space formed by base state the *label* of which count number of energy quanta in the field.

Before constructing Fock space let us obtain physical operators related to t-EM fields. The operator form for transverse electric  $\mathbf{E}_\perp(\mathbf{x})$ , magnetic  $\mathbf{B}(\mathbf{x})$  and  $\mathbf{A}_\perp(\mathbf{x})$  fields at  $\mathbf{x}$ , a point in real space, are obtained by using eq.(5.2.1) in conjunction with eq.(5.1.12) and, once  $\hat{\mathbf{A}}_\perp(\mathbf{x})$  is obtained, eqs.(5.1.2) is used to get the field operators:

$$\begin{aligned} \hat{\mathbf{A}}_\perp(\mathbf{x}) &= \sum_j \mathcal{A}_{\omega_j} [\hat{a}_j \mathbf{e}_j \exp(i \mathbf{k}_j \cdot \mathbf{x}) + \hat{a}_j^+ \mathbf{e}_j \exp(-i \mathbf{k}_j \cdot \mathbf{x})] = \\ &\hat{\mathbf{A}}_\perp^+(\mathbf{x}) + \hat{\mathbf{A}}_\perp^-(\mathbf{x}) \end{aligned} \quad (5.2.3)$$

$$\begin{aligned} \hat{\mathbf{E}}_\perp(\mathbf{x}) &= \sum_j i \mathcal{E}_{\omega_j} [\hat{a}_j \mathbf{e}_j \exp(i \mathbf{k}_j \cdot \mathbf{x}) - \hat{a}_j^+ \mathbf{e}_j \exp(-i \mathbf{k}_j \cdot \mathbf{x})] = \\ &\hat{\mathbf{E}}_\perp^+(\mathbf{x}) + \hat{\mathbf{E}}_\perp^-(\mathbf{x}) \end{aligned} \quad (5.2.4)$$

$$\begin{aligned} \hat{\mathbf{B}}(\mathbf{x}) &= \sum_j i \mathcal{B}_{\omega_j} [\hat{a}_j (\boldsymbol{\kappa} \wedge \mathbf{e}_j) \exp(i \mathbf{k}_j \cdot \mathbf{x}) - \\ &\hat{a}_j^+ (\boldsymbol{\kappa} \wedge \mathbf{e}_j) \exp(-i \mathbf{k}_j \cdot \mathbf{x})] = \hat{\mathbf{B}}^+(\mathbf{x}) + \hat{\mathbf{B}}^-(\mathbf{x}) \end{aligned} \quad (5.2.5)$$

From the above definitions show that  $(\hat{A}_{\perp}^+(\mathbf{x}))^\dagger = \hat{A}_{\perp}^-(\mathbf{x})$ ;  $(\hat{B}_{\perp}^+(\mathbf{x}))^\dagger = \hat{B}_{\perp}^-(\mathbf{x})$ ;  $(\hat{E}_{\perp}^+(\mathbf{x}))^\dagger = \hat{E}_{\perp}^-(\mathbf{x})$ . The amplitudes are defined by:

$$\begin{aligned}\mathcal{E}_{\omega_j} &= [(\hbar \omega_j)/2L^3]^{1/2}; \\ \mathcal{B}_{\omega_j} &= \mathcal{E}_{\omega_j}/c; \\ \mathcal{A}_{\omega_j} &= \mathcal{E}_{\omega_j}/\omega_j\end{aligned}\quad (5.2.6)$$

Note that the product  $\mathcal{E}_{\omega_j}^* \mathcal{E}_{\omega_j}$  has dimension of energy density. The dimension of  $\mathcal{A}_{\omega_j}$  corresponds to a linear momentum.  $L$  is the cubic box length.

#### E&E5.2-1 Show $\mathcal{A}_{\omega_j}$ actually has linear momentum dimension

To get a start we must remind that due to the unit chosen, the electron charge ( $e$ ) and the speed of light ( $c$ ) have the numerical values:  $e=c=1$ . The amplitude actually looks like  $(e/c)\mathcal{A}_{\omega_j}$ . From eq.(5.2.6) we deduce that  $\dim[(\hbar \omega_j)/2L^3]^{1/2} = [(\text{Energy} \times T^2)/L^3]^{1/2}$ . The dimension of  $e/c$  can be obtained by using Coulomb law:  $\dim(e) = [(\text{Energy} \times L)]^{1/2}$ . We rearrange the dimension of  $\dim[(\hbar \omega_j)/2L^3]^{1/2}$  to make explicit the charge first, to get:  $\dim(e)/\dim L \dim[T^2/L^2]^{1/2} = [\text{Energy}]/[\text{speed}]$ . This latter corresponds to the dimension of linear momentum. It is important to remember that the momentum of a charged particle interacting with an electromagnetic field in part it is mechanical and in part electrodynamics. This is the reason for the difficulties found in separating charges from electromagnetic fields. The operators just reflect this type of situations.

### 5.3. Operators in Fock space

The energy operator  $\hat{H}_{EM}$  obtains after replacing in eq.(5.1.13) the fields in terms of creation and annihilation operators given above:

$$\begin{aligned}\hat{H}_{EM} &= \sum_j (\hbar \omega_j / 2) (\hat{a}_j^+ \hat{a}_j + \hat{a}_j \hat{a}_j^+) = \\ &\sum_j (\hbar \omega_j) (\hat{a}_j^+ \hat{a}_j + 1/2)\end{aligned}\quad (5.3.1)$$

The second equality follows from the commutation relationships. Naturally, this equation has the same form as eq.(4.5.1.9). All these operator symbols make sense when they act on the vacuum state; the sum  $\sum_j (\hbar \omega_j)/2$  is necessarily infinite because quantum mechanics takes care of all possibilities, that in this case are infinite, but this energy is not a term at the Fence; it only makes sense in Fock space. It is the wave function at the Fence that mediates both worlds. Keep this caveat always in mind as it applies in abstract quantum physics. Compare with results of Sect.4.4.1.

The impulse operator of the transverse field  $\hat{P}_\perp$  is given from eq.(5.1.14):

$$\hat{P}_t = \frac{\sum_j (\hbar \mathbf{k}_j / 2) (\hat{a}_j^+ \hat{a}_j + \hat{a}_j \hat{a}_j^+)}{\sum_j \hbar \mathbf{k}_j \hat{a}_j^+ \hat{a}_j} = \quad (5.3.2)$$

The second equality follows from  $\sum_j (\hbar \mathbf{k}_j / 2) = 0$ . The global system is not moving. We have it referred to an I-frame.

Let us introduce spin angular momentum operator. Gauge invariance requires deletion of two degrees of freedom from the field  $\mathbf{A}$ . This amounts to remove  $A^0$  (Coulomb potential) and  $A^3$  for the case where the momentum ( $\mathbf{k}$ ) is aligned in the 3-rd direction (usually referred to as the z-axis in real space). This leaves only two independent polarization states.

The commutation relationships including polarization are given in eq.(5.2.2); the polarization labels can take two values only, say 1 and 2.

The expressions for the energy and momentum are a little more involved but we do not need to write them down. Instead, angular momentum operators do require polarization labels for their definition. The i-th component of the angular momentum operator for the t-EM field is given by:

$$\hat{\Omega}^i = \int d^3r [ \hat{r} \wedge :(\hat{E}_\perp \wedge \hat{B}): ]^i \quad (5.3.3)$$

The operator products in the round bracket between colons (:...:) must be put in normal order, i.e. all creation operators to the left of annihilation ones; e.g.  $\hat{a}^+ \hat{a}$ . In tensorial notation:

$$\hat{\Omega}^j = -i \int d^3r : \partial \hat{A}^b / \partial t (L^j \hat{A}^b - i \epsilon_{jbc} \hat{A}^c) : \quad (5.3.4)$$

The orbital angular momentum  $\hat{L} = -i(\hat{r} \wedge \nabla)$ ; note  $\hbar=1$ . The spin of the field quantum base state, named as photon without implying a particle picture (only particle-state), is given as:

$$\hat{\Omega}_{\text{spin}}^j = - \int d^3r : \partial A^k / \partial t \epsilon_{jkl} \hat{A}^l : \quad (5.3.5)$$

Introducing the creation and annihilation operators in the Coulomb gauge,  $\nabla \cdot \mathbf{E} = 0$ , the spin operator reads as:

$$\hat{\Omega}_{\text{spin}} = \sum_{n, \alpha \neq \alpha'} (\epsilon_n^\alpha \wedge \epsilon_n^{\alpha'}) \hat{a}_{n\alpha}^+ \hat{a}_{n\alpha} \quad (5.3.6)$$

The wedge (cross) product can be simplified by recalling  $(\epsilon^1 \wedge \epsilon^2) = \hat{k}$ . Sum over polarization leads to

$$\hat{\Omega}_{\text{spin}} = \sum_n \hat{k}_n (\hat{a}_{n2}^+ \hat{a}_{n1} - \hat{a}_{n1}^+ \hat{a}_{n2}) \quad (5.3.7)$$

Introducing now a new polarization base, namely, circular or helicity base, defined by:

$$\begin{aligned}\varepsilon^+ &= -(1/\sqrt{2}) (\varepsilon^1 + i \varepsilon^2) \\ \varepsilon^- &= -(1/\sqrt{2}) (\varepsilon^1 - i \varepsilon^2)\end{aligned}\quad (5.3.8)$$

The plus component has the spin in  $+\hat{k}$ -direction and the minus component in  $-\hat{k}$ -direction. Now we define new operators that eliminate the mix of 1,2 sub index in eq.(5.3.7) such that

$$\hat{\Omega}_{\text{spin}} = \sum_n \hat{k}_n (\hat{a}_{n+}^+ \hat{a}_{n+} - \hat{a}_{n-}^+ \hat{a}_{n-}) \quad (5.3.9)$$

There is something unusual with the photon spin. We learn that a system with spin quantum number  $s$  has a  $2s+1$  multiplicity. For  $s=1$ , there should be three orthogonal base states. The photon base states only show two out of three states, only helicity states  $\pm s$  are allowed; the other state is just forbidden. This is taken to be indication for the zero mass of photon forbids helicity zero; the Coulomb gauge imposes a transverse field.

Finally, let us check the mode energy derived from classical EM. The classical formula for  $E_{\text{EM}} = (1/8\pi) \int (\mathbf{E}^* \mathbf{E} + \mathbf{B}^* \mathbf{B}) d^3\mathbf{x}$  and replace by the operators  $\hat{E}_\perp(\mathbf{x})$  and  $\hat{B}(\mathbf{x})$  from eqs. (5.2.4) and (5.2.5). If one uses a time dependent form, this one will be average out over a cycle. Here one gets for mode  $k$ :

$$\begin{aligned}\hat{E}_k &= i \mathcal{E}_{\omega k} [\hat{a}_k \mathbf{e}_k \exp(i \mathbf{k} \cdot \mathbf{x}) - \hat{a}_k^+ \mathbf{e}_k \exp(-i \mathbf{k} \cdot \mathbf{x})] \\ \hat{B}_k &= i \mathcal{B}_{\omega k} [\hat{a}_k (\mathbf{k} \wedge \mathbf{e}_k) \exp(i \mathbf{k} \cdot \mathbf{x}) - \hat{a}_k^+ (\mathbf{k} \wedge \mathbf{e}_k) \exp(-i \mathbf{k} \cdot \mathbf{x})]\end{aligned}$$

Take average over base state  $|n_k\rangle$  one gets the result:

$$\begin{aligned}\varepsilon_k &= (1/2) \int_{\text{cavity}} dV \langle n_k | (\varepsilon_0 |\hat{E}_k|^2 + \mu_0 |\hat{B}_k|^2) | n_k \rangle = \\ &= (n_k + 1/2) \hbar \omega_k\end{aligned}\quad (5.3.10)$$

The radiation Hamiltonian can be written as

$$\hat{H}_R = \int dV \left( \varepsilon_0 \hat{E}_T^2 + (1/\mu_0) \hat{B}^2 \right) \quad (5.3.11)$$

This closes a connection loop between Fock photon view and classical form for the energy. The result is important because for particular photon quantum states one can find the classical Maxwell equation for the energy. In simple words, classical behavior is expressing special quantum states where the photon number density is very large (see below).

Beyond all this tangle-tangle with formalisms, there is an important practical result: If, for a given process at a Fence, a photon is, say absorbed, the spin must be

compensated due to angular momentum conservation. The transition in the absorber must be associated to an increase of angular momentum by one unit. This put forward a rule of selection. A change from an S-state must end up in a P-state; similarly, a P-state into a D-state; and so on and so forth. For emission of a photon, the opposite rule holds: P-state to S-state; D-state to P. These rules follow from angular momentum conservation.

The import of EM quantum states resides in their ability to yield values to the operators such as linear momentum, angular momentum, energy, electric and magnetic fields. We move on to examining some quantum states of interest.

## 5.4. Basis functions

Let us now construct the quantum physical space where the operators defined above must operate. The generic component,  $\hat{a}_j^+ \hat{a}_j$ , has no dimension; Planck's constant permits introducing specific dimensions as it can be seen above. The space where these operators would act is the abstract Fock space. When we move on to the Fence, the base states will be referring to energy quanta associated to specific quantum base states. To construct quantum states there is need for a complete set of base states. We follow the algebraic treatment of the quantum harmonic oscillator using ladder operators. Because the field operators are all frequency uncoupled, consider each oscillator independently; drop thence the index  $j$  for simplicity (note, we can put it back if necessary), the Hamiltonian for an oscillator of frequency  $\omega = ck$  is given by:

$$\hat{H}_{ho} = (\hbar ck)(\hat{a}^+ \hat{a} + 1/2) = (\hbar \omega)(\hat{a}^+ \hat{a} + 1/2) \quad (5.4.1)$$

The operator nature of the field magnitudes is located at the level of creation/annihilation operators; to alleviate notation we use same global symbols for t-EM fields. This equation stands for a generic *monochromatic* model system.

The energy associated to a vacuum state is  $\langle 0 | \hat{H}_{ho} | 0 \rangle$  that equals to  $(\hbar \omega)/2$ . Yet, at the EM field there is no energy that can be traded. This subtlety should be kept in mind.

### 5.4.1. Fock space

As we have already hinted at in Chapter 3 (Sect.3.10) the number  $n$  of quanta in the field is one variable of interest; let  $|n\rangle$  be a base state for  $n$  quanta of given



frequency; for the time being instead of  $n_\omega$  we use  $n$ , and understand that  $n$ -quanta can be exchanged, each of energy ( $\hbar\omega$ ). This type of base set is known as a Fock space.

The annihilation operator  $\hat{a}$  acting on  $|n\rangle$  relates to a state proportional to  $|n-1\rangle$ ; it is common to say: generates thereby implying objects. If now we let  $\hat{a}^+$  to act on  $|n-1\rangle$  by definition it will relate (or create a quanta so that  $\hat{a}^+|n-1\rangle$  would be proportional) to  $|n\rangle$ .

What is the eigenvalue of the product operator  $\hat{a}^+\hat{a}$  acting on  $|n\rangle$ ? From the preceding analysis we got the information  $\hat{a}^+\hat{a}|n\rangle = C_n|n\rangle$ . If  $|n\rangle$  is an eigenvector of  $\hat{a}^+\hat{a}$  then  $C_n = n$ . In general,

$$\langle n|\hat{a}^+\hat{a}|n\rangle = n \langle n|n\rangle \Rightarrow n \geq 0. \quad (5.4.1.1)$$

This  $n$  positive-ness is an important property of the harmonic oscillator. It introduces the zero-point energy,  $n=0$  in eq. (5.4.1). Energy differences are reckoned from this point upwards.

Now, because

$$[\hat{a}^+\hat{a}, \hat{a}] = -\hat{a} \quad (5.4.1.2)$$

You can show that

$$\begin{aligned} \hat{a}^+\hat{a}(\hat{a}|n\rangle) &= \hat{a}\hat{a}^+\hat{a}|n\rangle - \hat{a}|n\rangle = \\ \hat{a}n|n\rangle - \hat{a}|n\rangle &= (n-1)(\hat{a}|n\rangle) \end{aligned} \quad (5.4.1.3)$$

This procedure shows that  $(\hat{a}|n\rangle)$  is proportional to an eigenvector with eigenvalue  $(n-1)$ , or equivalently that the operator  $\hat{a}$  shift down by one quanta and relates to a system having amplitude for a base state  $|n-1\rangle$ ; i.e. annihilates a quantum, that is a colloquial way to say it.

If we keep applying  $\hat{a}$  to  $|n\rangle$  successively, eventually a negative value is attained. But from eq.(5.3.11) negative values are forbidden. Then there must be an integer  $m$  for which  $\hat{a}^m|n\rangle$  does not vanish while  $\hat{a}^{m+1}|n\rangle$  does:

$$\hat{a}^+\hat{a}(\hat{a}^m|n\rangle) = (n-m)(\hat{a}^m|n\rangle) \quad (5.4.1.4)$$

So that  $n=m$  leading to  $\hat{a}^n|n\rangle = 0$ . In other words, the eigenvalues of  $\hat{a}^+\hat{a}$  are all positive integers. The lowest one being  $n=0$  that corresponds to the base state defined by

$$\hat{a}|0\rangle = \hat{a}|\text{vacuum}\rangle = 0 \quad (5.4.1.5)$$

The absence of excitations in the field that could eventually be traded with another system is a realization of the vacuum state  $|0\rangle$  or  $|\text{vacuum}\rangle$ . Thus, fulfillment of eq. (5.4.1.5) is logically consistent.

From this base state -the vacuum (of actual excitations)- any other base state can be generated by applying  $\hat{a}^+$  a sufficient number of times. To show this let us first give the normalized vectors obtained from applying creation and annihilation operators on an arbitrary base state  $|n\rangle$ :

$$\begin{aligned}\hat{a}^+ |n\rangle &= \sqrt{(n+1)} |n+1\rangle \text{ and} \\ \hat{a} |n\rangle &= \sqrt{(n)} |n-1\rangle\end{aligned}\quad (5.4.1.6)$$

The number operator  $\hat{N} = \hat{a}^+ \hat{a}$  acts as follows:

$$\begin{aligned}\hat{N} |n\rangle &= \hat{a}^+ (\hat{a} |n\rangle) = \hat{a}^+ \sqrt{(n)} |n-1\rangle = \\ \sqrt{(n)} (\hat{a}^+ |n-1\rangle) &= \sqrt{(n)} (\sqrt{(n)} |n\rangle) = n |n\rangle\end{aligned}\quad (5.4.1.7)$$

The Hamiltonian reads as:

$$\hat{H}_{ho} = (\hbar \omega) (\hat{N} + 1/2) \quad (5.4.1.8)$$

Now, it can be shown that the base state  $|n\rangle$  can be obtained by successive application of the creation operator:

$$(1/\sqrt{n!}) (\hat{a}^+)^n |0\rangle = |n\rangle \quad (5.4.1.9)$$

In one word, the creation/annihilation operators open a simple way *to construct base functions* referring to varied number of excitations for a given frequency. Do not believe that by playing with these operators you will be creating or annihilating energy in a physical field! This is an abstract Fock space that is used in many different physical chemical contexts.

#### **E&E-5.4-1 Field magnitudes for defined quantum states**

At this point it is important to realize the difference between general field operators and the physical magnitudes related to them. The operators cover all possible levels that might be found and expressed in the spectra of particular material systems. Physical states are specific to given systems; you can prepare them in a laboratory. The energy of a particular quantum state (linear superposition) is the average value of the Hamiltonian operator with respect to that physical state. For example, if we prepare a quantum state with the energy equivalent to one photon per cubic centimeter it does not mean that all amplitudes of the row-vector ought to be zero except that one the system was prepared. See below for further discussions (See also Chapter 9).

## 5.4.2 Quantum physical states

A simple didactic picture retains the amplitudes as the place where a physical state is controlled, e.g. let  $\dots + C_{k-1}|k-1\rangle + C_k|k\rangle + \dots$  be the states where two Fock space basis will be involved in describing a given process. In the first step we have  $C_{k-1}=1$  and  $C_k=0$  after interaction we find  $C_{k-1}=0$  and  $C_k=1$ . Thus, the EM got a photon. The process seen from the Fence is an emission from the material system coupled to the t-EM field. This is all there is. A description using populations of the energy levels of the field modes may be obvious in this case, but in general, things are somewhat more complicated because mechanisms develop inside Hilbert or Fock space where we have the mathematical rules to operate. The point to retain is that the base states inform about the label of energy at disposal; it is a reckoning help. It is the particular quantum state that informs us about the material system under study.

An arbitrary quantum state of the t-EM, say  $|\Xi\rangle$ , is represented by a row vector of complex numbers:  $\langle n_k | \Xi \rangle$  :

$$|\Xi\rangle = \sum_k \langle n_k | \Xi \rangle |n_k\rangle \quad (5.4.2.1)$$

The average energy for this state is given by  $\langle \Xi | \hat{H}_{ho} | \Xi \rangle$ . Introducing the definitions given in eq.(5.1.19) and (5.4.2.1) we get:

$$\begin{aligned} \langle \Xi | \hat{H}_{ho} | \Xi \rangle &= \langle \Xi | \sum_j (\hbar \omega_j) (\hat{a}_j^\dagger \hat{a}_j + 1/2) | \Xi \rangle = \\ &= \sum_{jkl} \langle n_l | \Xi \rangle^* \langle n_k | \Xi \rangle (\hbar \omega_j) \langle n_l | (\hat{a}_j^\dagger \hat{a}_j + 1/2) | n_k \rangle \end{aligned} \quad (5.4.2.2)$$

For the constant term we have  $\langle n_l | (1/2) | n_k \rangle = (1/2)\delta_{lk}$ ; for occupation number one gets:  $\langle n_l | \hat{N}_j | n_k \rangle = n_j \langle n_l | n_k \rangle \delta_{jk}$ , thus there are two Kronecker delta,  $\delta_{jk} \delta_{nl nk}$  eliminating two sum signs to get the average energy for the quantum state  $|\Xi\rangle$  given by:

$$\langle \Xi | \hat{H}_{EM} | \Xi \rangle = \sum_j |\langle n_j | \Xi \rangle|^2 (\hbar \omega_j) (n_j + 1/2) \quad (5.4.2.3)$$

The average energy depends upon the amplitudes that are different from zero in the quantum state via  $|\langle n_j | \Xi \rangle|^2$ , the squared amplitudes and the energy that can be exchanged amounting to:  $n (\hbar \omega)$ .

Take our little example above and call  $|\Xi_1\rangle$  the case for which  $C_{k-1}=1$  and  $C_k=0$  and  $|\Xi_2\rangle$  for  $C_{k-1}=0$  and  $C_k=1$ ; all other modes have zero amplitudes. Thus,

$$\begin{aligned} \langle \Xi_1 | \hat{H}_{EM} | \Xi_1 \rangle &= (\hbar \omega_k) (n_{k-1} + 1/2) |C_{k-1}|^2 \text{ and} \\ \langle \Xi_2 | \hat{H}_{EM} | \Xi_2 \rangle &= (\hbar \omega_k) (n_k + 1/2) |C_k|^2. \end{aligned}$$

The difference in average energy  $\langle \Xi_1 | \hat{H}_{EM} | \Xi_1 \rangle - \langle \Xi_2 | \hat{H}_{EM} | \Xi_2 \rangle = -(\hbar \omega_k)$ .

The initial state lost one photon of energy ( $\hbar \omega_k$ ). Observe the sum in (5.4.2.3) is generic; for each frequency there is a Fock space implied.

*The zero-point energy cancels out when energy differences are calculated.* Such is the case of all physical process involving the t-EM; there is an initial and a final state, even if the latter may be the same as the initial one. Of course, the operator form contains an infinite term for the simple reason we just pointed out above: the operators are there to represent all the possibilities a quantum material system may have. At the Fence you must respect energy conservation.

For a general quantum state, referring to 1-system, the amplitudes are not integers;  $0 \leq |\langle n_j | \Xi \rangle|^2 \leq 1$ . The use of a population picture is not adequate as the energy quanta would have to be divided in fractions  $|\langle n_j | \Xi \rangle|^2 n_j$  in contradiction with a plain (exchanged) particle picture. The energy would be “spread”, as it were, in the field, and it is only interaction with a material system that make energy exchange at the Fence to be in finite quanta. But, again, we are mixing the descriptive levels. The linear superposition  $|\Xi\rangle$  is a coherent state in Hilbert or Fock space; at the Fence, the system is in an energy shell.

An incoherent state will be a statistical ensemble of N copies, where for a base state that had non-zero amplitude in  $|\Xi\rangle$  it must be unity; then there will be  $N_k$  elements of the ensemble that only have amplitude one for that case and statistically  $N_k/N \rightarrow |\langle n_k | \Xi \rangle|^2$  when  $N \rightarrow \infty$ . The population picture is akin to this statistical view.

There are then two parts to the average energy, one determined by the quantum structure of the system, n times ( $\hbar \omega$ ) or total energy that can be exchanged by quanta  $\hbar \omega$ , the other depends upon how do you prepare the system in the laboratory, that is the set of  $|\langle n | \Xi \rangle|$  and phases. Remember that the quantum state is determined by laboratory preparations. If they are to be mapped on to Hilbert space then they have to be normalized to unity.

Let us calculate with eq.(5.4.2.2) the case where all amplitudes are zero except for the base state  $n=50$ . From  $|\langle n=50 | \Xi \rangle|^2 = 1$ , the equation reduces to:  $(50 + 1/2) (\hbar \omega)$ . Now, if a physical process leads to a new state, say  $n=40$  ( $|\langle n=40 | \Xi \rangle|^2 = 1$ ) the energy exchanged  $|(50 + 1/2) - (40 + 1/2)|$  equals 10 photons; the zero point energy is irrelevant for this count.

The amplitudes indicate the possibility to measure a response from n-excitations Fock space base state. Let us take an illustration. Prepare the system in such a way we have  $\langle n | \Xi \rangle$  that for  $n=20$  is different from zero only. If you want to measure a response from the base state  $|n-1\rangle$  there will be no intensity as its amplitude by construction is zero.

The quantum state after interaction leading to 1-quanta “emission”,  $\hat{a} |\Xi\rangle$  is:

$$\hat{a} |\Xi\rangle = \sum_n \langle n | \Xi \rangle \hat{a} |n\rangle = \sum_n \sqrt{n} \langle n | \Xi \rangle |n-1\rangle \quad (5.4.2.4)$$

The new quantum state,  $\hat{a}|\Xi\rangle = |\Xi'\rangle$ , can be expanded as in eq. (5.4.1.6). We can see that the following relation holds:  $\langle n-1|\Xi'\rangle \rightarrow \sqrt{n} \langle n|\Xi\rangle$ .

If a quantum state has been prepared in the laboratory to show a very high number of quantum excitations we can apply the annihilation operator  $m$ -times so that the sum in  $\hat{a}^m|\Xi\rangle$  will start at the term  $n-m$ :  $\hat{a}^m|\Xi\rangle = \sqrt{m!} |n-m\rangle + \sqrt{(m+1)!} |n-m+1\rangle + \sqrt{(m+2)!} |n-m+2\rangle + \dots$ . For  $n-m=1$ , one can cast this sum into:

$$(1/\sqrt{m!})(\hat{a})^m |\Xi\rangle = \sum_{g=1} \sqrt{g!} \langle g+n-m|\Xi\rangle |g+n-m\rangle \quad (5.4.2.5)$$

### 5.4.3. Quantum model for classical EM field

We define now a classical-like t-EM field if for a typical number of quanta that are involved in a measurement of the field (say  $m$  excitations) the remaining t-EM field cannot be distinguished from the initial one. Observe that different subspaces may be identified with phase relations. The classic-like field must show random phases and the frequency range ought to be well defined.

Any standard t-EM detector device would detect the energy quanta by “destroying” them (actually, they can be scattered in direction differing from the one you put the detector). In this case let

$$(1/\sqrt{m!})(\hat{a})^m |\Xi\rangle \sim |\Xi\rangle \text{ for } m \ll N \quad (5.4.3.1)$$

$N$  is an average number over energy quanta in the t-EM field and  $m$  is the number of quanta required to excite the photo-detector, photo-multiplier, photographic plate or your eyes if working in the visible.

Remember that the geometric arrangement of detectors, sources and measured systems is located in real space. The direction of a photon beam is determined by the position of the source and the detector. The emission/absorption processes are local; this is what it makes the difference between the Fence and the abstract domains.

So, we have both, a fully quantized field theory as well as Maxwell equations to handle problems related to energy exchange, interactions, etc. between electromagnetic systems. Before fully exploiting these concepts in a fully quantized scheme, we introduce new aspects of material systems where classical and quantum aspects of electrodynamics appear to be the adequate way to go.

### 5.4.4. Coherent photon states

Consider an arbitrary quantum state given by the linear superposition over the number state basis (given frequency):

$$|A\rangle = \sum_n \langle n|A\rangle |n\rangle \quad (5.4.4.1)$$

Take a special quantum state that is eigenstate of the annihilation operator:

$$\hat{a} |\alpha\rangle = \alpha |\alpha\rangle \quad (5.4.4.2)$$

Recalling (5.4.1.9) we express the number eigenvectors as:  $(1/\sqrt{n!}) (\hat{a}^+)^n |0\rangle$  and changing the label A by the complex number  $\alpha$  one can obtain:

$$\langle n|\alpha\rangle = \exp(-|\alpha|^2) \alpha^n / \sqrt{n!} \quad (5.4.4.3)$$

The coherent state  $|\alpha\rangle$  takes on the form:

$$|\alpha\rangle = \sum_n \langle n|\alpha\rangle |n\rangle = \exp(-|\alpha|^2/2) \sum_n \alpha^n / \sqrt{n!} |n\rangle \quad (5.4.4.4)$$

It is not difficult to check that (5.4.4.2) holds when one uses the expression above.

The relative response towards a probe from root state  $|n\rangle$  takes on the form:

$$|\langle n|\alpha\rangle|^2 = \exp(-|\alpha|^2) |\alpha|^{2n} / n! \quad (5.4.4.5)$$

This is Poisson distribution with mean value  $|\alpha|^2$ .

By construction, the quantum state given by eq. (5.4.4.4) is an eigenstate of  $\hat{a}$ , (annihilation operator). Noting that  $\exp(-\alpha^* \hat{a}) |0\rangle = |0\rangle$ , the coherent quantum state is written as:

$$|\alpha\rangle = \exp(\alpha \hat{a}) |0\rangle \exp(-|\alpha|^2/2) = \hat{D}(\alpha) |0\rangle \quad (5.4.4.6)$$

The operator  $D(\alpha)$  is given by:

$$\hat{D}(\alpha) = \exp(-|\alpha|^2/2) \exp(\alpha \hat{a}^+) \exp(-\alpha^* \hat{a}) = \exp(\alpha \hat{a}^+ - \alpha^* \hat{a}) \quad (5.4.4.7)$$

The average energy associated to this k-mode coherent state obtains by using eq.(5.4.2.3) and (5.4.4.5):

$$\langle \alpha | \hat{H}_{EM} | \alpha \rangle / (\hbar \omega_k) = \sum_n \exp(-|\alpha|^2) |\alpha|^{2n} / n! (n+1/2) = \sum_n \{ \exp(-\langle n \rangle) \langle n \rangle^n / n! \} (n+1/2) \quad (5.4.4.8)$$

The average photon number  $\langle n \rangle = |\alpha|^2$ . This equation includes zero-point energy that can be subtracted so that available energy in the field is reckoned, the result is  $\Delta E_{EM}(\alpha) = \sum_n \{ \exp(-\langle n \rangle) \langle n \rangle^n / n! \} n$ .

Thus,

$$|\langle n | \alpha \rangle|^2 = (1/n!) \langle n \rangle^n \exp(-\langle n \rangle) = p(n) \quad (5.4.4.9)$$

The response in intensity regime from the root state  $|n\rangle$  is given by a Poisson distribution about a mean  $|\alpha|^2$ . It is then  $|\alpha|$  that determines the physical problem by fixing the average photon number.

For  $|\alpha| \leq 1$ ,  $p(n)$  has a maximum at  $n=0$ . While for  $|\alpha| > 1$ ,  $p(n)$  shows a peak at  $n=|\alpha|^2$ .

The complex number  $\alpha$  can be written in terms of an amplitude and a phase:

$$\alpha = |\alpha| \exp(i\theta) \quad (5.4.4.10)$$

This relationship will be useful in what follows.

### 5.4.5. Squeezed photon states

Linear superposition states always show dispersion on conjugated non-commuting operators. In Chapter 3 we saw a typical example. Here, the electric field operator permits construct a pair of Hermitian non-commuting operators of interest when seeking to extract properties of photon quantum states. For the k-mode one has:

$$\hat{E}(t) = i \mathcal{E}_\omega \mathbf{e} [ \hat{a} \exp(-i \nu t) - \hat{a}^+ \exp(i \nu t) ] \quad (5.4.5.1)$$

Introduce Hermitian amplitude operators:

$$\hat{X}_1 = (1/2) (\hat{a} + \hat{a}^+) \quad (5.4.5.2)$$

$$\hat{X}_2 = (1/2) (\hat{a} - \hat{a}^+) \quad (5.4.5.3)$$

These two operators do not commute,

$$[\hat{X}_1, \hat{X}_2] = i/2 \quad (5.4.5.4)$$

And

$$\hat{E}(t) = 2\epsilon_0 \mathbf{e} [\hat{X}_1 \cos vt + \hat{X}_2 \sin vt] \quad (5.4.5.5)$$

The two Hermitian operators  $\hat{X}_1$  and  $\hat{X}_2$  are then quadratures amplitudes of the field having a phase difference  $\pi/2$ . It can be shown that

$$\langle \Delta \hat{X}_1 \Delta \hat{X}_2 \rangle \geq 1/4 \quad (5.4.5.6)$$

A squeezed state of the radiation field obtains if  $(\langle \Delta \hat{X}_i \rangle)^2 < 1/4$  for  $i=1,2$ . The quantum averages correspond to:

$$(\langle \Delta \hat{X}_i \rangle)^2 = \langle \alpha | \hat{X}_i^2 | \alpha \rangle - (\langle \alpha | \hat{X}_i | \alpha \rangle)^2 \quad (5.4.5.7)$$

A straightforward calculation for the coherent state yield  $(\langle \Delta \hat{X}_i \rangle)^2 = 1/4$ ,  $i=1,2$ .

A coherent state  $|\alpha\rangle$  has mean complex amplitude  $\alpha$ , and it is a minimum-uncertainty state for  $\hat{X}_1$  and  $\hat{X}_2$  with equal uncertainties in the two quadratures phases.

Quantum states for which  $(\langle \Delta \hat{X}_1 \rangle)^2$  differs from  $(\langle \Delta \hat{X}_2 \rangle)^2$  while conserving invariant their product are known as *squeezed* states. This is another set of useful quantum states. Using unitary squeeze operators can generate them:

$$\begin{aligned} \hat{S}(\zeta) &= \exp(1/2 (\zeta^* \hat{a}^2 - \zeta (\hat{a}^\dagger)^2)) \\ \zeta &= r \exp(i\theta) \end{aligned} \quad (5.4.5.8)$$

As seen above,  $\zeta$  is an arbitrary complex number. The squeezed state is label with  $\alpha$  and  $r \exp(i\theta)$ :  $|\alpha, r \exp(i\theta)\rangle$  or simply  $|\alpha, \zeta\rangle$ .

Quadrature operators for the squeezed state read  $\hat{Y}_1$  and  $\hat{Y}_2$ . They are related to  $\hat{X}_1$  and  $\hat{X}_2$  as follows:

$$\langle \hat{X}_1 + i \hat{X}_2 \rangle = \langle \hat{Y}_1 + i \hat{Y}_2 \rangle \exp(i\theta/2) = \alpha \quad (5.4.5.9)$$

The difference between these two classes of states lies in the unequal uncertainties for  $\hat{Y}_1$  and  $\hat{Y}_2$ . In the complex-amplitude plane, a coherent-state error circle has



been squeezed into an error ellipse of the same area. The principal axes of the ellipse lie along  $\hat{Y}_1$  and  $\hat{Y}_2$  axes, and the principal radii are  $\Delta \hat{Y}_1$  and  $\Delta \hat{Y}_2$ .

## 5.5. Quantum states: Gauges and phases

At a Fence, quantum states are projected on configuration coordinate spaces. For charged systems the four potential  $A=(A_0,A_1,A_2,A_3)$  under infinitesimal coordinate transformations

$$\begin{aligned} x^\mu &\rightarrow x^\mu + \delta_f x^\mu, \quad \delta_f x^\mu = -f^\mu(x) \\ A_\mu &\rightarrow A_\mu + \delta_f A_\mu = \\ &A_\mu + f^\alpha \partial_\alpha A_\mu + (\partial_\mu f^\alpha) A_\alpha \end{aligned} \quad (6.5.1)$$

These transformations represent freedom of choice of coordinate system rather than redundancy in physical variables. For space coordinates:  $\mathbf{A}(\mathbf{r})=(A_1(\mathbf{r}),A_2(\mathbf{r}),A_3(\mathbf{r}))$ . The time component is the Coulomb potential:  $A_0(\mathbf{r})$ . In E&E-5.1-10 above gauge transformations were introduced, Cf. eq. (5.1-10.1).

$$\begin{aligned} \mathbf{A}(\mathbf{r},t) &\rightarrow \mathbf{A}(\mathbf{r},t) + \nabla \Gamma(\mathbf{r},t) \\ A_0(\mathbf{r},t) &\rightarrow A_0(\mathbf{r},t) - (1/c) \partial \Gamma(\mathbf{r},t)/\partial t \end{aligned}$$

A quantum state projected at a Fence on a coordinate system (configuration space) is transformed according to:

$$\Psi(\mathbf{r},t) \rightarrow \exp(i e \Gamma(\mathbf{r},t)/\hbar c) \Psi'(\mathbf{r},t) \quad (5.5.2)$$

What the gauge is able to sense is presence of external interaction acting on the quantum state. Thus, consider a case where there is a splitting of the quantum state after interaction such as the gauge may take a positive sign when displacing to say upwards ( $+\Gamma(\mathbf{r},t)$ ), namely  $(\exp(+i e \Gamma(\mathbf{r},t)/\hbar c) \Psi_U(\mathbf{r},t)$  and negative when it is downward:  $(\exp(-i e \Gamma(\mathbf{r},t)/\hbar c) \Psi_D(\mathbf{r},t)$ . The left/right quantum states can be bent so that at a common space point one get the quantum mechanical superposition:

$$\Phi(\mathbf{r},t) = \exp(i e \Gamma(\mathbf{r},t)/\hbar c) \Psi_U(\mathbf{r},t) + \exp(-i e \Gamma(\mathbf{r},t)/\hbar c) \Psi_D(\mathbf{r},t) \quad (5.5.3)$$

The phase is no longer global, there is a relative phase  $(2e\Gamma(\mathbf{r},t)/\hbar c)$  that is the cause for interference at the point where upper and lower states converge.

It is the quantum state  $\Psi(\mathbf{r},t)$  that is splitted to get  $\Phi(\mathbf{r},t)$ , the material system is not involved in the splitting. Whatever the path it could have taken the point is that it must be there at the interference zone.

A conspicuous example is the Aharonov-Bohm effect. (See Webb et al. Phys. Rev.Lett. 54(1985) 2696 for an experimental proof.)

## 5.6. At a Fence and beyond

The interaction between a quantum state and a recording device due to elementary energy exchange would appear as an event (“click”). The event belongs to a world beyond the Fence. Interestingly, for quantum events, energy, linear and angular momentum are conserved. To an external observer the events will appear as localized in space-time.

The coefficients  $|a_k|^2$  are real numbers; they define the classical physical state of the system and can be laboratory manipulated to the extent that the power put in the field is controlled. The energy  $E_{EM}$  is in the field and the transport momentum  $\mathbf{P}_{EM}$  can change continuously due to changes of  $|a_k|^2$ .

To turn a continuous view into a picture where exchange of energy takes on discrete amounts demands a change in the representation of the amplitudes  $\{a_k\}$ . For now, there will be variable numbers of energy quanta that t-EM fields can exchange with matter fields, this requires a quantum physical approach where the number of excitations is a variable (degree of freedom).

The picture where light was thought of in terms of particles transported in space is old: Newton’s picture dates back to 17<sup>th</sup> century; In our terms the problem is that there is no place where to put an I-frame origin propagating wit the speed of light and “riding” a photon. The particle picture is flawed because it is not possible to explain diffraction and interference phenomena. From Fresnel description of diffraction and interferences phenomena a wave perspective follows; the bottom line is continuous energy exchange between matter and light waves.

But Planck tells us that exchanges are quantized which produces a puzzling situation. With hindsight, the quantum harmonic oscillator will help us with formalisms able to cope with this problem.

Where does the quantum nature hide in Maxwell equations? Again, with hindsight one can see that the fundamental relationship between frequency, wavelength and speed of light hides a message, namely,  $v \lambda = c$ . This equality can be decrypted with Planck’s constant  $h$ . For now multiplying by  $h$  both sides one gets  $(h v) \lambda = hc$  and the energy quanta associated to the field appears neatly:  $h v$ . Now we better use reciprocal space;  $(1/\lambda)$  is the wave number, and find that the energy quanta relate to the momentum  $(h/\lambda)$ , namely,  $h v = c(h/\lambda)$ . If we call  $k=(1/\lambda)$  and if you want to give it a direction in 3-space with a unit vector  $\mathbf{n}$  then

we have  $\mathbf{k}=(1/\lambda)\mathbf{n}$ ; the energy that can be exchanged is Maxwell relation written with a quantum decoder:  $E_\nu = k_\nu hc$ . At the end we recover the fundamental “classical” relation:  $k_\nu = \nu/c$ : the momentum transported by the excitation being  $hk_\nu$  or  $h\nu/c$ . In special relativity energy is proportional to momentum. These heuristic statements must be changed into a more formal approach that includes quantum physical aspects compatible with the framework developed so far.