Quantum electrodynamics: one- and two-photon processes

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Preface

These are the lecture notes of the five hour course on quantum electrodynamics given during the "Graduate course on Theory and Spectroscopy" in Han-sur-Lesse, Belgium, December 12-16, 2005. This part only treats the vacuum. An updated version that includes the part on the interaction between molecules and fields will be put on the website www.theochem.ru.nl/han

These lecture notes were made while studying the book "*Molecular quantum electrodynamics, An Introduction to Radiation-Molecule Interactions*" by D. P. Craig and T. Thirunamachandran (Academic, London, 1984).

I also made use of the discussion of units in the appendix of the book "*Classical Electrodynamics*", by John David Jackson (Wiley, New York, 1999).

1 Mathematical background: vector algebra

1.1 Scalar and vector fields

A *scalar field* is a real or complex valued function defined on R^3; $\phi(\mathbf{r}) \equiv \phi(x, y, z)$. We will also encounter time-dependent scalar fields $\phi(\mathbf{r}, t)$.

A *vector field* has three components in each point of space:

$$\mathbf{A}(\mathbf{r}) \equiv \begin{bmatrix} A_x(\mathbf{r}) \\ A_y(\mathbf{r}) \\ A_z(\mathbf{r}) \end{bmatrix}. \tag{1}$$

The *gradient* of a scalar field is a vector field defined by

$$\nabla\phi(\mathbf{r}) \equiv \begin{bmatrix} \frac{\partial}{\partial x}\phi(x,y,z) \\ \frac{\partial}{\partial y}\phi(x,y,z) \\ \frac{\partial}{\partial z}\phi(x,y,z) \end{bmatrix}. \tag{2}$$

The *divergence* of a vector field is a scalar field given by

$$\nabla \cdot \mathbf{A}(\mathbf{r}) \equiv \frac{\partial}{\partial x}A_x(\mathbf{r}) + \frac{\partial}{\partial y}A_y(\mathbf{r}) + \frac{\partial}{\partial z}A_z(\mathbf{r}). \tag{3}$$

The *curl* of a vector field is a vector field given by

$$\nabla \times \mathbf{A} \equiv \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix} \times \begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix} = \begin{bmatrix} \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \\ \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \\ \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \end{bmatrix}. \tag{4}$$

1.2 Gauss and Stokes theorems

The *total flux* j_S *of a vector field* $\mathbf{A}$ through a surface S is defined by

$$j_S = \iint_S \mathbf{A} \cdot d\mathbf{S}. \tag{5}$$

The vector $d\mathbf{S}$ is perpendicular to the surface and its length is proportional to the area of a surface element.

The outward flux through a surface S enclosing a volume V is related by *Gauss theorem* to a volume integral over the divergence of the field:

$$\iint_S \mathbf{A} \cdot d\mathbf{S} = \iiint_V \nabla \cdot \mathbf{A} dV. \tag{6}$$

Stokes theorem relates a line integral to a surface integral:

$$\oint \mathbf{A} \cdot d\mathbf{r} = \iint_S (\nabla \times \mathbf{A}) \cdot d\mathbf{S}. \tag{7}$$

A vector field is *singly connected* if each closed line can be contracted continuously to a point. Stokes theorem can be applied to each closed line in such a field.

A vector field is *doubly connected* if each closed surface can be contracted continuously to a point. Gauss theorem can be applied to any such field.

1.3 Solenoidal and irrotational fields

A *solenoidal* or *divergence free* vector field $\mathbf{V}^{\perp}$ is defined by

$$\nabla \cdot \mathbf{V}^{\perp} \equiv 0. \tag{8}$$

An *irrotational* or *curl-free* vector field is defined by

$$\nabla \times \mathbf{V}^{\parallel} \equiv 0. \tag{9}$$

A force field described by an irrotational field is called *conservative*.

The gradient of a scalar field can easily be verified to be irrotational:

$$\nabla \times (\nabla \phi) = \mathbf{0}. \tag{10}$$

The reverse is also true, any irrotational vector field $\mathbf{V}^{\parallel}$ can be written as the gradient of some scalar field ϕ. To show this define

$$\phi(\mathbf{r}) = \int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{V}^{\parallel}(\mathbf{r}') \cdot d\mathbf{r}'. \tag{11}$$

Stokes theorem can be used to show that this definition of ϕ is independent of the path. This requires that the field is singly connected. Taking the gradient of both sides of Eq. 11 gives

$$\nabla \phi = \mathbf{V}^{\parallel}. \tag{12}$$

The divergence of the curl of a vector field can easily be verified to be zero

$$\nabla \cdot (\nabla \times \mathbf{A}) = 0. \tag{13}$$

Again the reverse is also true, any solenoidal (divergence-free) field can be written as the curl of some vector field

$$\mathbf{V}^{\perp} = \nabla \times \mathbf{W}. \tag{14}$$

The field $\mathbf{W}$ is not unique. If the flux through any closed surface is zero the field is called *source free*. If the domain of the field is doubly connected than Gauss theorem can be used to show that a solenoidal field is source free.

A field $\mathbf{V}$ can be both divergence free and curl free. In this case it can be written as $\mathbf{V} = \nabla\phi$, where ϕ is a *harmonic function*, i.e., it satisfies the Laplace equation

$$\nabla \cdot \nabla\phi = \nabla^2\phi = 0. \tag{15}$$

According to the *Helmholz theorem* any singly and doubly connected field can be written as the sum of an irrotational field and a solenoidal field

$$\mathbf{V} = \nabla\phi + \nabla \times \mathbf{A}. \tag{16}$$

This decomposition is not unique: a solution of the Laplace equation (χ) may be added to scalar field ϕ. In this case $\nabla\chi$ is solenoidal and a vector field $\mathbf{B}$ may be found such that $\nabla\chi = \nabla \times \mathbf{A}$ and we have an alternative decomposition

$$\mathbf{V} = \nabla(\phi + \chi) + \nabla \times (\mathbf{A} - \mathbf{B}). \tag{17}$$

The vector field $\mathbf{A}$ in 16 can be chosen to be solenoidal, i.e., $\nabla \cdot \mathbf{A} = 0$. Suppose $\nabla \cdot \mathbf{A} \neq 0$, take

$$\mathbf{A}' = \mathbf{A} - \nabla\phi, \tag{18}$$

where ϕ is the solution of the Poisson equation

$$\nabla^2\phi = \nabla \cdot \mathbf{A} \tag{19}$$

then $\nabla \cdot \mathbf{A}' = 0$ and $\mathbf{V} = \nabla\phi + \nabla \times \mathbf{A}'$. A useful relation to compute the curl of $\mathbf{V}$ is

$$\nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2\mathbf{A}, \tag{20}$$

where in the last term ∇^2 acts on the x, y, and z components of $\mathbf{A}$.

1.4 Continuity equation

The total outward flux $\mathbf{j}_{\mathrm{tot}}$ through a surface S enclosing a volume V is equal to the decrease of the number of particles per time $-\dot{n}(t)$ in that volume.

$$\iint_S \mathbf{j} \cdot d\mathbf{S} = -\dot{n}(t). \tag{21}$$

The number of particles can be written as an integral over the density

$$n(t) = \iiint_V \rho(\mathbf{r}, t)\mathrm{d}^3\mathbf{r} \tag{22}$$

Using Gauss theorem the surface integral in Eq. (21) can be written as a volume integral of the divergence of $\mathbf{j}$ and we can derive

$$\iiint_V [\nabla \cdot \mathbf{j} + \dot{\rho}(\mathbf{r}, t)]\mathrm{d}^3\mathbf{r} = 0. \tag{23}$$

Since this equation must hold for each volume we must have the continuity equation

$$\nabla \cdot \mathbf{j} + \dot{\rho}(\mathbf{r}, t) = 0. \tag{24}$$

If the flux is written as $\mathbf{j} = \mathbf{j}^{\parallel} + \mathbf{j}^{\perp}$ then we may replace $\nabla \cdot \mathbf{j} = \nabla \cdot \mathbf{j}^{\parallel}$.

1.5 The Fourier transform of a field

The Fourier transform of a scalar field is defined by

$$\tilde{\phi}(\mathbf{k}) = (2\pi)^{-3/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi(\mathbf{r}) e^{i\mathbf{kr}} \mathrm{d}^3\mathbf{r} \tag{25}$$

and the inverse is

$$\phi(\mathbf{r}) = (2\pi)^{-3/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{\phi}(\mathbf{k}) e^{-i\mathbf{kr}} \mathrm{d}^3\mathbf{k}. \tag{26}$$

The Fourier transform of a vector field is defined by the Fourier transforms of its components

$$\tilde{\mathbf{A}}(\mathbf{k}) = \begin{bmatrix} \tilde{A}_x(\mathbf{k}) \\ \tilde{A}_y(\mathbf{k}) \\ \tilde{A}_z(\mathbf{k}) \end{bmatrix}. \tag{27}$$

The Fourier transform of the gradient of a scalar field is

$$\widetilde{\nabla\phi}(\mathbf{k}) = -i\mathbf{k}\tilde{\phi}(\mathbf{k}). \tag{28}$$

The Fourier transform of the divergence of a vector field is

$$\widetilde{\nabla\cdot\mathbf{A}}(\mathbf{k}) = -i\mathbf{k}\cdot\tilde{\mathbf{A}}(\mathbf{k}). \tag{29}$$

The Fourier transform of the curl of a vector field is

$$\widetilde{\nabla\times\mathbf{A}}(\mathbf{k}) = -i\mathbf{k}\times\tilde{\mathbf{A}}(\mathbf{k}). \tag{30}$$

For a solenoidal (divergence free) field $\mathbf{A}^{\perp}$ we find from Eq. (29) that $\mathbf{k}\cdot\tilde{\mathbf{A}}^{\perp}(\mathbf{k}) = 0$, i.e.,

$$\mathbf{k} \perp \tilde{\mathbf{A}}^{\perp}(\mathbf{k}), \tag{31}$$

hence a solenoidal field is *transverse* in $\mathbf{k}$-space. Similarly, an irrotational field $\mathbf{A}^{\parallel}$ is *longitudinal* in $\mathbf{k}$-space

$$\mathbf{k} \parallel \tilde{\mathbf{A}}^{\parallel}(\mathbf{k}). \tag{32}$$

In $\mathbf{k}$-space a field can be decomposed in a longitudinal and a transverse part (with $\mathbf{k} = k\hat{\mathbf{k}}$ and $k = |\mathbf{k}|$)

$$\tilde{\mathbf{A}} = \tilde{\mathbf{A}}^{\parallel} + \tilde{\mathbf{A}}^{\perp} \tag{33}$$

$$\tilde{\mathbf{A}}^{\parallel} = \hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\tilde{\mathbf{A}}) \tag{34}$$

$$\tilde{\mathbf{A}}^{\perp} = \tilde{\mathbf{A}} - \tilde{\mathbf{A}}^{\parallel} \tag{35}$$

This decomposition seems to be unique, whereas before we found that the gradient of an harmonic function could be added and subtracted from the solenoidal and irrotational parts. The reason is that the Fourier transform only exists if the contribution of the harmonic functions is zero.

1.6 Levi-Civita tensor

Many vector formulas are most easily derived using the Levi-Civita or permutation tensor ϵ_{ijk}. The indices can be 1, 2, or 3. Furthermore, $\epsilon_{1,2,3} = 1$ and it changes sign when two indices are permuted. Using the Einstein summation convention (summation over any repeated indices) we have three very useful relations for the summation over one, two, or all three indices

$$\begin{aligned} \epsilon_{ijk}\epsilon_{ij'k'} &= \delta_{jj'}\delta_{kk'} - \delta_{jk'}\delta_{kj'} && (36)\\ \epsilon_{ijk}\epsilon_{ijk'} &= 2\delta_{kk'} && (37)\\ \epsilon_{ijk}\epsilon_{ijk} &= 6. && (38) \end{aligned}$$

It can be used to define the cross product of two vectors

$$(\mathbf{x}\times\mathbf{y})_i \equiv \epsilon_{ijk}x_j y_k \tag{39}$$

and the determinant of a 3×3 matrix

$$\det([\mathbf{x}\,\mathbf{y}\,\mathbf{z}]) = \epsilon_{ijk}x_i y_j z_k = \mathbf{x}\cdot(\mathbf{y}\times\mathbf{z}) \tag{40}$$

Use these relations to derive the vector formulas:

$$\begin{aligned} \nabla\times\nabla\phi &= 0 && (41)\\ \nabla\cdot(\nabla\times\mathbf{x}) &= 0 && (42)\\ \nabla\times(\nabla\times\mathbf{x}) &= \nabla(\nabla\cdot\mathbf{x}) - \nabla^2\mathbf{x} && (43)\\ \nabla\cdot(\mathbf{x}\times\mathbf{y}) &= \mathbf{y}\cdot(\nabla\times\mathbf{x}) - \mathbf{x}\cdot(\nabla\times\mathbf{y}) && (44)\\ \mathbf{a}\times(\nabla\times\mathbf{x}) &= \nabla(\mathbf{a}\cdot\mathbf{x}) - (\mathbf{a}\cdot\nabla)\mathbf{x}, \quad \text{where } \mathbf{a} \text{ is a constant vector.} && (45)\\ (\nabla\times\mathbf{x})\cdot(\nabla\times\mathbf{a}) &= (\nabla_i a_j)^2 - (\nabla_i a_j)(\nabla_j a_i) && (46)\\ (\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d}) &= (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}) - (\mathbf{a}\cdot\mathbf{d})(\mathbf{b}\cdot\mathbf{c}). && (47) \end{aligned}$$

2 Classical electromagnetism

2.1 Units

We take as basis dimensions length (l), mass (m), and time (t). Two common unit systems are m.k.s. (meter, kilogram, second), which is used in the S.I. system, and c.g.s. (centimeter, gram, second), which is used in the Gaussian unit system.

The atomic units system has the Bohr radius (a_0) for length and the electron mass (m_e) as unit of mass. The third basic unit is the unit of angular momentum ($\hbar$). Since $[\hbar]$ is l^2m/s the atomic unit of time is $a_0^2 m_e/\hbar$. The atomic unit of energy is $E_h = \hbar^2/(a_0^2 m_e)$.

For the electromagnetic units and dimensions there are various conventions. We will write the equations in a form independent of the unit system. We follow the book of Jackson and introduce several constants that take different values in different unit systems.

2.2 Electrostatics

Coulomb's law gives the force F between two charges q and q' at a distance r

$$F = k_1\frac{qq'}{r^2}. \tag{48}$$

The value and the unit of k_1 can be chosen depending on the convention, which determines the unit of charge. The *electric field* E is defined as the force per charge

$$F = Eq'; \quad E = k_1 \frac{q}{r^2}. \tag{49}$$

The rate of change of charge in a certain volume is equal to the current into that volume ($I = \partial q/\partial t$). Two infinitely long parallel wires separated by a distance d and carrying currents I and I' attract each other with a force per unit length given by Ampère's law

$$\frac{dF}{dl} = 2k_2 \frac{II'}{d}. \tag{50}$$

Combining Coulomb's law and Ampère's law one finds $[k_1/k_2] = l^2/t^2$. In free space the ratio is related to the speed of light

$$\frac{k_1}{k_2} = c^2. \tag{51}$$

Just as the electric field is derived from Coulomb's law we may introduce the magnetic induction B generated by the current

$$\frac{dF}{dl} = \frac{1}{\alpha} BI'; \quad B = 2k_2 \alpha \frac{I}{d}, \tag{52}$$

where the constant α may be chosen for convenience.

If the magnetic flux through a surface S enclosed by a contour C changes in time an electric field is induced along the contour. It is given by the integral form of *Faraday's law*

$$\oint_C \mathbf{E} \cdot d\mathbf{r} + k_3 \frac{d}{\mathrm{d}t} \iint_S \mathbf{B} \cdot d\mathbf{S} = 0. \tag{53}$$

The constant k_3 turns out to be equal to α^{-1}.

The force on a particle moving in an electric and magnetic field is given by *Lorentz* law. According to Ampère's law the force on a piece of the parallel wire of length l if $F = BIl/\alpha$. If in a wire of length l a charge q is moving with a velocity v than the current $I = qv/l$, so $Il = qv$ and

$$\mathbf{F} = q(\mathbf{E} + \frac{1}{\alpha} \mathbf{v} \times \mathbf{B}). \tag{54}$$

2.3 Static electric fields

Consider a particle with charge q and polar coordinates (r, ϕ) moving in the electric field produced by a particle of charge q' in the origin as shown in Fig. 1. Since the Coulomb force is a central force no energy can be gained by moving through a closed loop: in segments where ϕ changes the force is perpendicular to the path so there is no contribution to $\int \mathbf{F} \cdot d\mathbf{r}$ and the energy gained for $r \to r + \Delta r$ is lost in the reverse path. Hence the electric field produced by the charge must be irrotational (see Stokes theorem) and it can be written as the gradient of a scalar potential

$$\mathbf{E}^{\|} = -\nabla \phi(\mathbf{r}). \tag{55}$$

By considering a particle on the z-axis the potential is found to be

$$\phi(\mathbf{r}) = k_1 \frac{q}{r}. \tag{56}$$

The divergence of $\mathbf{E}$ can be found be direct differentiation, using

$$\begin{aligned}\nabla \cdot \mathbf{r} &= 3 &(57)\\ \nabla r &= r^{-1}\mathbf{r} &(58)\\ \nabla r^n &= n r^{n-2}\mathbf{r} &(59)\\ \nabla \cdot \nabla r^{-1} &= 0 \quad (r \neq 0) &(60)\\ \nabla \cdot \mathbf{E}^{\parallel} &= 0 \quad (r \neq 0) &(61)\end{aligned}$$

For the electric field itself we have

$$\mathbf{E}^{\parallel} = k_1 q r^{-3}\mathbf{r}. \tag{62}$$

Using Gauss theorem one finds for a sphere V with radius r that

$$\iiint_V \nabla \cdot \mathbf{E}^{\parallel} dV = \iint_S \mathbf{E}^{\parallel} \cdot d\mathbf{S} = 4\pi k_1 q. \tag{63}$$

Since $\nabla \cdot \mathbf{E}^{\parallel} = 0$ in regions where there is no charge this relation holds for any volume V that contains the charge q. If there is more then one point charge the electric field is the sum of the fields generated by the individual charges. Hence q may be replaced by the sum of all point charges within the volume V or by the integral of the charge density $\rho(\mathbf{r})$ over the volume

$$\iiint_V \nabla \cdot \mathbf{E} dV = 4\pi k_1 \iiint_V \rho(\mathbf{r}) \mathrm{d}^3\mathbf{r}. \tag{64}$$

This hold for any volume V, so we arrive at the differential form of *Gauss' law* for electric fields

$$\nabla \cdot \mathbf{E}^{\parallel} = 4\pi k_1 \rho(\mathbf{r}). \tag{65}$$

With $\mathbf{E}^{\parallel} = -\nabla\phi(r)$ this gives the Poisson equation

$$\nabla^2\phi(r) = -4\pi k_1 \rho(r) \tag{66}$$

For a single point particle in the origin the charge density is a delta function $\rho(\mathbf{r}) = \delta(x)\delta(y)\delta(z) \equiv \delta(\mathbf{r})$ and we find

$$\nabla^2 \frac{1}{r} = -4\pi\delta(\mathbf{r}). \tag{67}$$

2.4 Static magnetic fields

The magnetic flux through a closed surface is zero. This can be readily verified for the magnetic field produced by an infinite long wire carrying a current I, but it holds for any magnetic field. Using Gauss theorem we thus find

$$\nabla \cdot \mathbf{B} = 0. \tag{68}$$

This law is sometimes referred to as the "no magnetic monopoles" law. Because of this law we always have

$$\mathbf{B} = \mathbf{B}^{\perp}. \tag{69}$$

Let C be a circle with radius r around a wire that carries a current I. From Ampère's law one can compute the contour integral

$$\oint_C \mathbf{B} \cdot d\mathbf{l} = 4\pi k_2 \alpha I. \tag{70}$$

For any contour that does not go around the current on can find that the contour integral is zero (see Fig. 2), hence Eq. (70) holds for any contour. If the contour encloses several wires the currents may be added, so we can replace the current I by a surface integral over the current density $\mathbf{j}$. Using Stokes theorem we can replace the contour integral by a surface integral so we find

$$\iint_S \nabla \times \mathbf{B} d\mathbf{S} = \iint_S 4\pi k_2 \alpha \mathbf{j} \cdot d\mathbf{S} \tag{71}$$

Since this result must hold for any surface S we have

$$\nabla \times \mathbf{B}^{\perp} = 4\pi k_2 \alpha \mathbf{j}. \tag{72}$$

Hence for *static* fields we have $\mathbf{j} = \mathbf{j}^{\perp}$.

2.5 Time dependent fields, Maxwell's equations

For a capacitor consisting of two plates with an area A with charges $+Q$ and $-Q$ we find from Gauss' law for electric fields

$$\iint_S \mathbf{E} \cdot d\mathbf{S} = AE = 4\pi k_1 Q. \tag{73}$$

If a capacitor is placed in a wire that carries a constant current I then between the plates there is no current, but instead an electric field that increases linearly in time. With $A = \iint_S d\mathbf{S}$ and Eq. 73 we find that

$$\iint_S \mathbf{j} \cdot d\mathbf{S} = I = \frac{\partial Q}{\partial t} = \frac{A}{4\pi k_1}\frac{\partial E}{\partial t} = \iint_S \frac{1}{4\pi k_1}\frac{\partial \mathbf{E}}{\partial t} \cdot d\mathbf{S} \tag{74}$$

The integrand of the right hand side is called the *displacement current.* It must be added to the current density in Ampere's law [Eq. (72)] to make the law independent whether the surface S is chosen between the capacitor plates of crossing the wire. So we arrive at Ampere's law modified for time dependent fields

$$\nabla \times \mathbf{B}^{\perp} = 4\pi k_2 \alpha \mathbf{j} + \frac{k_2 \alpha}{k_1}\frac{\partial \mathbf{E}}{\partial t}. \tag{75}$$

Faraday's law already deals with time dependent magnetic fields. Using stokes theorem for the first term in Eq. (53) we may write it in differential form

$$\nabla \times \mathbf{E}^{\perp} + k_3 \frac{\partial \mathbf{B}}{\partial t} = 0, \quad \textbf{Faraday} \tag{76}$$

These two laws together with Gauss' law for electric and magnetic fields,

$$\nabla \cdot \mathbf{E}^{\parallel} = 4\pi k_1 \rho \quad \textbf{Gauss} \tag{77}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{78}$$

are Maxwell's equations.

Ampère's law may also be split in a transverse and longitudinal components

$$\mathbf{E} = \mathbf{E}^{\parallel} + \mathbf{E}^{\perp} \tag{79}$$

$$\mathbf{j} = \mathbf{j}^{\parallel} + \mathbf{j}^{\perp} \tag{80}$$

$$0 = \mathbf{j}^{\parallel} + \frac{1}{4\pi k_1}\frac{\partial \mathbf{E}^{\parallel}}{\partial t} \quad \textbf{Ampère} \tag{81}$$

$$\nabla \times \mathbf{B}^{\perp} = 4\pi k_2 \alpha \mathbf{j}^{\perp} + \frac{k_2 \alpha}{k_1}\frac{\partial \mathbf{E}^{\perp}}{\partial t}. \tag{82}$$

Table 1: Magnitudes and dimensions of the electromagnetic constants in several unit systems. The constant $\alpha = 1/k_3$. In SI the dimension of k_1 is $ml^3t^{-4}I^{-2}$, and the dimension of k_2 is $mlt^{-2}I^{-2}$.

System	k_1	k_2	k_3
SI	$\frac{1}{4\pi\epsilon_0} = 10^{-7}c^2$	$\frac{\mu_0}{4\pi} = 10^{-7}$	1
Electrostatic (esu)	1	c^{-2}	1
Atomic units	1	c^{-2}	1
Electromagnetic (emu)	c^2	1	1
Gaussian	1	c^{-2}	c^{-1}
Heaviside-Lorentz	$\frac{1}{4\pi}$	$\frac{1}{4\pi c^2}$	c^{-1}

Taking the divergence of Ampeŕe's law, which is the same as taking the divergence of the irrotational part, combining it with Gauss' law electric fields gives the continuity equation [Eq. (24)]

$$\nabla \cdot \mathbf{j} + \dot{\rho}(\mathbf{r}, t) = 0. \tag{83}$$

2.6 Plane waves

In a source free region, i.e., a region with no charges ρ or currents $\mathbf{j}$ we can combine Ampère's law and Faraday's law by taking the time derivate of either and using the vector identity

$$\nabla \times (\nabla \times \mathbf{a}) = \nabla(\nabla \cdot \mathbf{a}) - \nabla^2 \mathbf{a} \tag{84}$$

to find the wave equations for electric (and magnetic) fields

$$\nabla^2 \mathbf{E} - \frac{k_2 k_3 \alpha}{k_1} \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0. \tag{85}$$

The solutions are plane waves

$$\mathbf{E} = \mathbf{E}_0 e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}. \tag{86}$$

Experimentally it is found that electromagnetic waves travel with the speed of light c. That means that for $\mathbf{r} = \mathbf{r}_0 + c\hat{\mathbf{k}}$ the exponent is constant, i.e., $kc = \omega$. Substituting the plane waves in the wave equation gives

$$\frac{k_1}{k_2 k_3 \alpha} = c^2 \tag{87}$$

Since we already have from comparing Coulomb's law and Ampères law that

$$\frac{k_1}{k_2} = c^2 \tag{88}$$

we find

$$k_3 \alpha = 1. \tag{89}$$

The choices for the constants in several unit systems are shown in table 1. This derivation suggest that two observations are needed to find the two restrictions on the constants k_1, k_2, k_3, and α. However, according to Jackson the last equation can also be derived from the Galilean invariance of the equations. Similarly, for the magnetic field we find

$$\mathbf{B} = \mathbf{B}_0 e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}. \tag{90}$$

and by substituting both B and E into Faraday's law we find

$$\mathbf{B}_0 = \frac{1}{k_3 c}\hat{\mathbf{k}} \times \mathbf{E}_0, \tag{91}$$

which also implies

$$\hat{\mathbf{k}} \times \mathbf{B}_0 = -\frac{1}{k_3 c}\mathbf{E}_0. \tag{92}$$

From Gauss' law we actually already knew $\mathbf{E} \perp \mathbf{k}$ and $\mathbf{B} \perp \mathbf{k}$.

2.7 The energy density of an electric field

The energy required to put a charge Q on a capacitor can be considered to be stored in the electric field E between the plates. We already found the relation

$$E = \frac{4\pi k_1 Q}{A} \tag{93}$$

The energy dU_E required to increase the charge separation dQ is

$$dU_E = E\, l\, dQ, \tag{94}$$

where l is the distance between the plates. From Eq. (93) we have

$$dQ = \frac{A}{4\pi k_1} dE \tag{95}$$

hence

$$dU_E = \frac{E\, l\, A}{4\pi k_1} E dE \tag{96}$$

Integrating this equation gives the energy density U_E/V, where the volume $V = l\, A$,

$$u_E \equiv \frac{U_E}{V} = \frac{1}{4\pi k_1}\frac{1}{2}E^2. \tag{97}$$

2.8 The energy density of a magnetic field

Consider a coil with diameter d, with N turns over a distance l carrying a current I. Neglecting the field outside the coil gives

$$B\, l = 4\pi k_2 \alpha N I. \tag{98}$$

From the integral form of Faraday's law we find for the voltage $\Delta V = -\oint_C \mathbf{E} \cdot d\mathbf{r}$

$$\Delta V = N k_3 A \frac{\partial B}{\partial t} \tag{99}$$

For the energy per time loaded into the coil we find, combining the last two equations,

$$\frac{\partial U_B}{\partial t} = \Delta V\, I = N k_3 A \frac{\partial B}{\partial t}\frac{B\, l}{4\pi k_2 \alpha N}. \tag{100}$$

Integrating this equation, using $V = A\, l$, gives

$$u_B \equiv \frac{U_B}{V} = \frac{k_3}{4\pi k_2 \alpha}\frac{1}{2}B^2 = \frac{c^2}{4\pi k_1 \alpha^2}\frac{1}{2}B^2 \tag{101}$$

2.9 Energy flux

We compute the time derivative of the energy density $u = u_E + u_B$ in a free field. We have

$$\frac{\partial}{\partial t}E^2 = \frac{\partial}{\partial t}(E_x^2 + E_y^2 + E_z^2) = 2E_x\dot{E}_x + 2E_y\dot{E}_y + 2E_z\dot{E}_z = 2\mathbf{E}\cdot\dot{\mathbf{E}} \tag{102}$$

and similarly for B^2. For the free field we use Ampère's law and Faraday's law to rewrite $\dot{\mathbf{E}}$ and $\dot{\mathbf{B}}$ and we obtain

$$\dot{u} = \frac{1}{4\pi k_2\alpha}(\mathbf{E}\cdot\nabla\times\mathbf{B} - \mathbf{B}\cdot\nabla\times\mathbf{E}) = \frac{1}{4\pi k_2\alpha}\nabla\cdot(\mathbf{B}\times\mathbf{E}) \tag{103}$$

Defining the Pointing vector

$$\mathbf{G} = \frac{1}{4\pi k_2\alpha}\mathbf{E}\times\mathbf{B} \tag{104}$$

we obtain the continuity equation for energy

$$\nabla\cdot\mathbf{G} + \frac{\partial u}{\partial t} = 0. \tag{105}$$

This shows the $\mathbf{G}$ is an energy flux density. For complex fields we may derive

$$\mathbf{G} = \frac{1}{4\pi k_2\alpha}\frac{1}{2}(\mathbf{E}^*\times\mathbf{B} + \mathbf{E}\times\mathbf{B}^*). \tag{106}$$

For a plane wave we have

$$\mathbf{G} = \frac{1}{4\pi k_1}cE_0^2\hat{\mathbf{k}}. \tag{107}$$

The energy density of a plane wave is

$$u = \frac{1}{4\pi k_1}E_0^2 \tag{108}$$

Together the last two equations give $\mathbf{G} = uc\hat{\mathbf{k}}$, i.e., the energy is moving with the speed of light in the direction $\hat{\mathbf{k}}$.

2.10 The vector and scalar potentials A and ϕ

Since by Gauss' law the magnetic field is solenoidal (transverse) it may be written, according to Helmholz theorem as

$$\mathbf{B} = \nabla\times\mathbf{A} \equiv \nabla\times\mathbf{A}^{\perp} \tag{109}$$

This relation puts no restriction on $\mathbf{A}^{\parallel}$. Substituting it into Faraday's law gives

$$\nabla\times\left(\mathbf{E}^{\perp} + k_3\frac{\partial\mathbf{A}^{\perp}}{\partial t}\right) = 0, \tag{110}$$

so the sum is both divergence free ($\perp$) and irrotational and we may define the scalar potential ϕ' such that

$$\mathbf{E}^{\perp} + k_3\frac{\partial\mathbf{A}^{\perp}}{\partial t} = -\nabla\phi'. \tag{111}$$

Since $\mathbf{E}^{\parallel}$ and $\mathbf{A}^{\parallel}$ can be written as gradients by definition we may also define a scalar potential ϕ and a irrotational component $\mathbf{A}^{\parallel}$ such that

$$\mathbf{E} + k_3 \frac{\partial \mathbf{A}}{\partial t} = -\nabla \phi. \tag{112}$$

The fields $\mathbf{B}$ and $\mathbf{E}$ are invariant if $\mathbf{A}$ and ϕ are replaced by

$$\begin{aligned} \tilde{\mathbf{A}} &= \mathbf{A} + \nabla \chi & (113)\\ \tilde{\phi} &= \phi - \frac{\partial \chi}{\partial t}, & (114) \end{aligned}$$

where χ may be any function. This is called the *gauge invariance* of the fundamental vector fields. We may choose χ such that $\nabla \cdot \mathbf{A} = 0$ which is called the *Coulomb gauge*. An alternative is the Lorentz gauge which we will not discuss here. In Coulomb's gauge we may choose ϕ such that

$$\begin{aligned} \mathbf{E}^{\parallel} &= -\nabla \phi & (115)\\ \mathbf{E}^{\perp} &= -k_3 \frac{\partial \mathbf{A}^{\perp}}{\partial t} & (116) \end{aligned}$$

Substituting $\mathbf{B}^{\perp}$ and $\mathbf{E}$ expressed $\mathbf{A}^{\perp}$ and ϕ into Maxwell's equations gives

$$\begin{aligned} \nabla^2 \phi &= -4\pi k_1 \rho & (117)\\ \left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \mathbf{A}^{\perp} &= -4\pi k_2 \alpha \mathbf{j} + \frac{k_2 \alpha}{k_1} \nabla \dot{\phi}. & (118) \end{aligned}$$

In free space we find $\phi = 0$, $\rho = 0$, $\mathbf{j} = \mathbf{0}$, and

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \mathbf{A}^{\perp} = 0. \tag{119}$$

The solutions are transverse ($\mathbf{A}_0 \perp \mathbf{k}$) plane waves ($\omega = kc$)

$$\mathbf{A}^{\perp} = \mathbf{A}_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} \tag{120}$$

from which we find

$$\begin{aligned} \mathbf{E}^{\perp} &= -\frac{\partial \mathbf{A}^{\perp}}{\partial t} = i\omega \mathbf{A}^{\perp} & (121)\\ \mathbf{B}^{\perp} &= \nabla \times \mathbf{A}^{\perp} = i\mathbf{k} \times \mathbf{A}^{\perp}. & (122) \end{aligned}$$

2.11 Mode expansion of electromagnetic waves in a box

Quantization of electromagnetic fields is done most easily for fields defined in a cube of dimension $L \times L \times L$, with periodic boundary conditions. The boundary conditions restrict the plane wave solutions to modes for which

$$\mathbf{k} = \frac{2\pi}{L} \mathbf{n} \tag{123}$$

where the vector $\mathbf{n}$ has only integer components. An arbitrary vector potential $\mathbf{A}^{\perp}(\mathbf{r}, t)$ can be expanded as a Fourier series in those modes. Since the Lorentz force must be real, both $\mathbf{E}$ and $\mathbf{B}$ must be real, which means the $\mathbf{A}$ must be real. Since $\mathbf{A}^{\perp}$ is a transverse field we define two *polarization* directions $\{\mathbf{e}_{\mathbf{k},\lambda}, \lambda = x, y\}$, for each mode $\mathbf{k}$. The polarization vectors have orthonormal and perpendicular to $\mathbf{k}$, and $\mathbf{e}_{\mathbf{k},x}, \mathbf{e}_{\mathbf{k},y}$, and $\hat{\mathbf{k}}$ form a right-handed triad,

$$\mathbf{e}_{\mathbf{k},\lambda} \cdot \mathbf{e}^*_{\mathbf{k},\lambda'} = \delta_{\lambda,\lambda'} \tag{124}$$

$$\mathbf{k} \cdot \mathbf{e}_{\mathbf{k},\lambda} = 0 \tag{125}$$

$$\tag{126}$$

Here use a dot product defined without complex conjugation. The polarization vectors are actually real, but the above relations also hold if for the complex polarization vectors associated with left ($\lambda = +1$) and right ($\lambda = -1$) circularly polarized modes

$$\mathbf{e}_{\mathbf{k},\pm} = \frac{1}{\sqrt{2}}(\mathbf{e}_{\mathbf{k},1} \pm i\mathbf{e}_{\mathbf{k},2}). \tag{127}$$

The expansion reads

$$\mathbf{A}^{\perp}(\mathbf{r}, t) = \sum_{\mathbf{k},\lambda} \{\mathbf{a}_{\mathbf{k},\lambda}(\mathbf{r}, t) + \mathbf{a}^*_{\mathbf{k},\lambda}(\mathbf{r}, t)\}, \tag{128}$$

with

$$\mathbf{a}_{\mathbf{k},\lambda}(\mathbf{r}, t) = a_{\mathbf{k},\lambda}(t)\mathbf{e}_{\mathbf{k},\lambda}e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{129}$$

For the free field we have $\mathbf{a}_{\mathbf{k},\lambda}(t)$ is proportional to $e^{-i\omega t}$ and

$$\dot{\mathbf{a}}_{\mathbf{k},\lambda}(t) = -i\omega \mathbf{a}_{\mathbf{k},\lambda}(t). \tag{130}$$

3 Quantization of a system of point charges

Before we will quantize the electromagnetic fields we briefly review the quantization of a single particle system. Classically the system is described by the time-dependent position of the particle $\mathbf{q}(t)$ and the mass μ. Newton's equations of motion for the particle moving in a potential $V(\mathbf{r})$ are

$$\ddot{\mathbf{q}}(t) = -\frac{1}{\mu}\nabla V(\mathbf{q}) = -\frac{1}{\mu}\frac{\partial V(\mathbf{q})}{\partial \mathbf{q}} \tag{131}$$

3.1 The Lagrangian

The first step is to find the *Lagrangian* $L(\mathbf{q}, \dot{\mathbf{q}}, t)$ of the system. For any physical or unphysical path $\mathbf{q}(t)$, for $t_1 \leq t \leq t_2$ the *action integral* $S[\mathbf{q}(t)]$ is defined by

$$S([\mathbf{q}(t)] = \int_{t_1}^{t_2} L(\mathbf{q}, \dot{\mathbf{q}}, t)\mathrm{d}t. \tag{132}$$

According to Hamilton's principle the path taken by the system is the one for which the action integral is minimized. It is assumed that the Lagrangian is a convex function of $\dot{\mathbf{q}}$, which guarantees that any stationary point is actually a minimum (see below). Consider a variation of $\mathbf{q}(t)$ for which $\mathbf{q}(t_1)$ and $\mathbf{q}(t_2)$ are fixed

$$\mathbf{q}(t) \to \mathbf{q}(t) + \delta\mathbf{q}(t) \tag{133}$$

$$\delta\mathbf{q}(t_1) = \delta\mathbf{q}(t_2) = 0 \tag{134}$$

Figure 1: Legendre transform of a function

This results in a variation of the action integral

$$\delta S = \int_{t_1}^{t_2} L(\mathbf{q} + \delta\mathbf{q}, \dot{\mathbf{q}} + \delta\dot{\mathbf{q}}, t)\mathrm{d}t = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial \mathbf{q}} \cdot \delta\mathbf{q} + \frac{\partial L}{\partial \dot{\mathbf{q}}} \cdot \delta\dot{\mathbf{q}} \right] \mathrm{d}t. \tag{135}$$

Using

$$\delta\dot{\mathbf{q}} = \frac{\partial}{\partial t}\delta\mathbf{q} \tag{136}$$

and integration by parts

$$\int_{t_1}^{t_2} \frac{\partial L}{\partial \dot{\mathbf{q}}} \cdot \left(\frac{\partial}{\partial t}\delta\mathbf{q} \right) \mathrm{d}t = \frac{\partial L}{\partial \dot{\mathbf{q}}}\delta\mathbf{q}\bigg|_{t_1}^{t_2} - \int_{t_1}^{t_2} \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\mathbf{q}}} \right) \cdot \delta\mathbf{q}\,\mathrm{d}t \tag{137}$$

and dropping the surface term because of Eq. (134) we find

$$\delta S = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial \mathbf{q}} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\mathbf{q}}} \right) \cdot \delta\mathbf{q}\,\mathrm{d}t. \tag{138}$$

The Lagrangian equations of motion are obtained for $\delta S = 0$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L(\mathbf{q}, \dot{\mathbf{q}}, t)}{\partial \dot{\mathbf{q}}} = \frac{\partial L(\mathbf{q}, \dot{\mathbf{q}}, t)}{\partial \mathbf{q}}. \tag{139}$$

For our one-particle system it is readily verified that the Lagrangian

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{1}{2}\mu\dot{\mathbf{q}} \cdot \dot{\mathbf{q}} - V(\mathbf{q}) \tag{140}$$

reproduces Newton's equation of motion.

3.2 Legendre transform

Let $f(x)$ be a *strictly convex* function on the open interval (x_1, x_2), i.e.,

$$\lambda f(x_1) + (1-\lambda) f(x_2) < f\left(\lambda x_1 + (1-\lambda) x_2\right), \quad \text{for } 0 < \lambda < 1. \tag{141}$$

For each slope p there is exactly one $x(p)$ for which $p = f'(x)$ (see Fig. 1). The Legendre transform $g(p)$ is defined by

$$g(p) = x(p)p - f(x(p)) \tag{142}$$

For the first derivative $g'(p)$ we find

$$\frac{dg(p)}{dp} = \frac{dx(p)}{dp}p + x(p) - \frac{dx(p)}{dp}f'\left(x(p)\right) = x(p). \tag{143}$$

Hence, when taking the derivative $\frac{dg(p)}{dp}$ the terms containing $x'(p)$ cancel and we can treat x and p as independent variables.

3.3 Classical Hamiltonian

The Lagrangian equations of motion are second order. To convert them to first order equations we define the conjugate momenta

$$\mathbf{p} = \frac{\partial L(\mathbf{q}, \dot{\mathbf{q}}, t)}{\partial \dot{\mathbf{q}}} \tag{144}$$

so we have

$$\dot{\mathbf{p}} = \frac{\partial L(\mathbf{q}, \dot{\mathbf{q}}, t)}{\partial \mathbf{q}}. \tag{145}$$

In order to eliminate $\dot{\mathbf{q}}$ from the equations we define the Legendre transform of the Lagrangian with respect to $\dot{\mathbf{q}}$

$$H(\mathbf{q}, \mathbf{p}, t) = \mathbf{p} \cdot \dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t) \tag{146}$$

Strictly, $\dot{bfq}$ is a function of $(\mathbf{q}, \mathbf{p})$. However, because the Hamiltonian is a Legendre transform of the Lagrangian we can treat $\dot{\mathbf{q}}$ and $\mathbf{p}$ as independent variables and we find the (first order) Hamiltonian equations of motion

$$\dot{\mathbf{q}} = \frac{\partial H(\mathbf{q}, \mathbf{p}, t)}{\partial \mathbf{p}} \tag{147}$$

$$\dot{\mathbf{p}} = -\frac{\partial H(\mathbf{q}, \mathbf{p}, t)}{\partial \mathbf{q}} \tag{148}$$

The total time derivative of any function $A(\mathbf{q}, \mathbf{p}, t)$ is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} A(\mathbf{q}, \mathbf{p}, t) = \dot{\mathbf{q}} \cdot \frac{\partial A}{\partial \mathbf{q}} + \dot{\mathbf{p}} \cdot \frac{\partial A}{\partial \mathbf{p}} + \frac{\partial A}{\partial t} = \frac{\partial H}{\partial \mathbf{p}} \cdot \frac{\partial A}{\partial \mathbf{q}} - \frac{\partial H}{\partial \mathbf{p}} \cdot \frac{\partial A}{\partial \mathbf{q}} + \frac{\partial A}{\partial t} \equiv \{H, A\} + \frac{\partial A}{\partial t}. \tag{149}$$

The *Poisson bracket* $\{H, H\}$ is zero, so if the Hamiltonian has no explicit time dependence then it is a constant of the motion. For the one particle system we have

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}} = \mu \dot{\mathbf{q}}, \qquad \dot{\mathbf{q}} = \tfrac{1}{\mu} \mathbf{p} \tag{150}$$

and

$$H = \mathbf{p} \cdot \dot{\mathbf{q}} - \frac{1}{2} \mu \dot{\mathbf{q}} \cdot \mathbf{q} + V(\mathbf{q}) = \frac{1}{2\mu} p^2 + V(\mathbf{q}), \tag{151}$$

i.e., H is the total energy of the system.

3.4 Quantization of Harmonic oscillator

To quantize the one particle system the time dependent variables $q_i(t)$ and it's conjugate momenta $p_i(t)$ are replaced by operators with the commutation relations

$$[\hat{q}_i, \hat{q}_j] = 0, \quad [\hat{p}_i, \hat{p}_j] = 0, \quad [\hat{q}_i, \hat{p}_j] = i\hbar \delta_{i,j}. \tag{152}$$

i.e., $\hat{p}_i = \frac{\hbar}{i} \frac{\partial}{\partial q_i}$.

Commutator algebra

$$
\begin{aligned}
[\hat{a}, \hat{b}] &\equiv \hat{a}\hat{b} - \hat{b}\hat{a} && (153)\\
[\hat{a}, \hat{b}\hat{c}] &= [\hat{a}, \hat{b}]\hat{c} + \hat{b}[\hat{a}, \hat{c}] && (154)\\
[\hat{a}\hat{b}, \hat{c}] &= \hat{a}[\hat{b}, \hat{c}] + [\hat{a}, \hat{b}]\hat{c} && (155)\\
[\hat{a}\hat{b}, \hat{c}\hat{d}] &= \hat{a}\hat{c}[\hat{b}, \hat{d}] + \hat{a}[\hat{b}, \hat{c}]\hat{d} + \hat{c}[\hat{a}, \hat{d}]\hat{b} + [\hat{a}, \hat{c}]\hat{d}\hat{b} && (156)
\end{aligned}
$$

If $[\hat{a}, [\hat{a}, \hat{b}]] = [\hat{b}, [\hat{a}, \hat{b}]] = 0$ then

$$[\hat{a}, \hat{b}^n] = n\hat{b}^{n-1}[\hat{a}, \hat{b}] \quad \text{and} \quad [\hat{a}, e^{\hat{b}}] = [\hat{a}, \hat{b}]e^{\hat{b}} \tag{157}$$

One dimensional harmonic oscillator (In atomic units, mass and force constant unity, $\hat{q}$ and $\hat{p}$ are Hermitian)

$$
\begin{aligned}
[\hat{q}, \hat{p}] &= i && (158)\\
\hat{H} &\equiv \frac{1}{2}(\hat{p}^2 + \hat{q}^2) && (159)\\
[\hat{H}, \hat{p}] &= i\hat{q}, \qquad [\hat{H}, \hat{q}] = -i\hat{p} && (160)\\
\hat{a} &\equiv \tfrac{1}{\sqrt{2}}(\hat{q} + i\hat{p}), \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p}) && (161)\\
[\hat{a}, \hat{a}^\dagger] &= 1 && (162)\\
\hat{N} &\equiv \hat{a}^\dagger\hat{a} = \frac{1}{2}(\hat{q}^2 + \hat{p}^2) - \frac{1}{2} && (163)\\
\hat{H} &= \hat{N} + \frac{1}{2} && (164)\\
[\hat{H}, \hat{a}] &= [\hat{N}, \hat{a}] = -\hat{a}, \qquad [\hat{H}, \hat{a}^\dagger] = [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger && (165)\\
\hat{H}|n\rangle &\equiv \epsilon_n|n\rangle, \qquad \hat{N}|n\rangle = (\epsilon_n - \frac{1}{2})|n\rangle && (166)\\
\hat{H}\hat{a}^\dagger|n\rangle &= (\epsilon_n + 1)\hat{a}^\dagger|n\rangle, \qquad \hat{H}\hat{a}|n\rangle = (\epsilon_n - 1)\hat{a}|n\rangle && (167)\\
\hat{a}|n\rangle &\equiv c_n|n-1\rangle, && (168)
\end{aligned}
$$

To show that there must be a lowest eigenvalue ϵ_0 we note that the norm of the vector $\hat{a}|n\rangle$ can not be negative

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle n|\hat{N}|n\rangle = (\epsilon_n - \frac{1}{2})\langle n|n\rangle \geq 0 \tag{169}$$

so $\epsilon_0 = \frac{1}{2}$ and because of Eq. 167

$$\epsilon_n = n + \frac{1}{2}, \qquad n = 0, 1, \ldots \tag{170}$$

and for the *number* operator we have

$$\hat{N}|n\rangle = n|n\rangle \tag{171}$$

The eigenfunction $|n\rangle$ can be found recursively from

$$|n\rangle = c_n\hat{a}^\dagger|n-1\rangle. \tag{172}$$

Using the relation

$$\hat{a}\hat{a}^\dagger = [\hat{a}, \hat{a}^\dagger] + \hat{a}^\dagger\hat{a} = 1 + \hat{N} \tag{173}$$

we find

$$\langle n|n\rangle = |c_n|^2\langle n-1|\hat{a}\hat{a}^\dagger|n-1\rangle = |c_n|^2 n = 1 \tag{174}$$

The phase is a matter of convention and we take $c_n = \frac{1}{\sqrt{n}}$ and we find

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle. \tag{175}$$

It is left as an exercise for the reader to show:

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{176}$$

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle. \tag{177}$$

For a general harmonic oscillator we have

$$\hat{H}' = \frac{1}{2\mu}\hat{P}^2 + \frac{1}{2}k\hat{Q}^2, \quad \text{with, } [\hat{Q},\hat{P}] = i\hbar \tag{178}$$

The following transformation

$$\hat{q} = \beta\hat{Q}, \qquad \beta = \sqrt{\mu\omega/\hbar}, \ \ \omega = \sqrt{k/\mu} \tag{179}$$

$$\hat{p} = \frac{1}{\beta\hbar}\hat{P} \tag{180}$$

gives $[\hat{q},\hat{p}] = 1$ and

$$\hat{H}' = \hbar\omega(\hat{N} + \frac{1}{2}) \tag{181}$$

and the eigenvalues are

$$\epsilon'_n = \hbar\omega(n + \frac{1}{2}). \tag{182}$$

3.5 A system of uncoupled harmonic oscillators

The hamiltonian is given by

$$\hat{H} = \sum_i \frac{1}{2}\hbar\omega_i(\hat{p}_i^2 + \hat{q}_i^2) = \sum_i \hbar\omega_i(\hat{N}_i + \frac{1}{2}) \tag{183}$$

where

$$\hat{N}_i = \hat{a}_i^\dagger\hat{a}_i \tag{184}$$

$$\hat{a}_i = \frac{1}{\sqrt{2}}(\hat{q}_i + i\hat{p}_i) \tag{185}$$

$$[\hat{a}_i,\hat{a}_j] = 0 \tag{186}$$

$$[\hat{a}_i^\dagger,\hat{a}_j^\dagger] = 0 \tag{187}$$

$$[\hat{a}_i,\hat{a}_j^\dagger] = \delta_{ij}. \tag{188}$$

The eigenvalues are the sum of the individual oscillator energies

$$\hat{H}|n_1,n_2,\ldots\rangle = \sum_i \hbar\omega_i(\epsilon_i + \frac{1}{2})\ |n_1,n_2,\ldots\rangle \tag{189}$$

and the eigenfunctions are direct products

$$|n_1, n_2, \ldots\rangle = \Pi_i \frac{(\alpha_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0, 0, \ldots\rangle. \tag{190}$$

For the ground state

$$\hat{a}_i |0, 0, \ldots\rangle = 0 \quad \text{for all } i. \tag{191}$$

3.6 Lagrangian and classical Hamiltonian of a particle in a field

The Lagrangian for a particle with mass m, charge q, position $\mathbf{q}$, velocity $\dot{\mathbf{q}}$, in an external field described by a vector potential $\mathbf{A}(\mathbf{q}, t)$ and a scalar potential $\phi(\mathbf{q}, t)$ is

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{1}{2} m \dot{\mathbf{q}} \cdot \dot{\mathbf{q}} + q k_3 \mathbf{A}(\mathbf{q}, t) \cdot \dot{\mathbf{q}} - q\phi(\mathbf{q}, t). \tag{192}$$

This Lagrangian correctly reproduces the Lorentz force: The Euler-Lagrange equations of motion are

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{\mathbf{q}}} = \frac{\partial L}{\partial \mathbf{q}}. \tag{193}$$

This gives

$$\begin{aligned}
\frac{\partial L}{\partial \mathbf{q}} &= q k_3 \nabla \left(\mathbf{A}(\mathbf{q}, t) \cdot \dot{\mathbf{q}} \right) - q \nabla \phi(\mathbf{q}) && (194) \\
\frac{\partial L}{\partial \dot{\mathbf{q}}} &= m \dot{\mathbf{q}} + q k_3 \mathbf{A}(\mathbf{q}, t) && (195) \\
\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{\mathbf{q}}} &= m \ddot{\mathbf{q}} + q k_3 \frac{\partial r_i}{\partial t} \frac{\partial \mathbf{A}(\mathbf{q}, t)}{\partial r_i} + q k_3 \frac{\partial \mathbf{A}(\mathbf{q}, t)}{\partial t} && (196) \\
&= m \ddot{\mathbf{q}} + q k_3 (\dot{\mathbf{q}} \cdot \nabla) \mathbf{A} + q k_3 \dot{\mathbf{A}}. && (197)
\end{aligned}$$

Hence

$$m \ddot{\mathbf{q}} \quad = \quad q k_3 [\nabla(\mathbf{A} \cdot \dot{\mathbf{q}}) - (\dot{\mathbf{q}} \cdot \nabla) \mathbf{A}] - q k_3 \dot{\mathbf{A}} - q \nabla \phi \tag{198}$$

Using Eq. (45) the term in the brackets can be rewritten as $\dot{\mathbf{q}} \times (\nabla \times \mathbf{A})$ and together with Eqs. (109) and (112), and Newtons $\mathbf{F} = m\ddot{\mathbf{q}}$ this gives Lorentz Eq. (54)

$$\mathbf{F} = q[\mathbf{E} + k_3 \dot{\mathbf{q}} \times \mathbf{B}]. \tag{199}$$

To obtain the Hamiltonian we define the conjugate momentum

$$\mathbf{p} \equiv \frac{\partial L}{\partial \dot{\mathbf{q}}} \tag{200}$$

It is left as an exercise to work out the Hamiltonian

$$H(\mathbf{q}, \mathbf{p}, t) = \mathbf{p} \cdot \dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{1}{2m} (\mathbf{p} - q k_3 \mathbf{A}(\mathbf{q}, t))^2 + q\phi(\mathbf{q}, t). \tag{201}$$

4 Field quantization

4.1 Lagrangian of a field

The Lagrangian of a field described by a vector potential $\mathbf{a}(\mathbf{r}, t)$ is the integral of Langrangian density

$$L = \int \mathcal{L}(\mathbf{a}, \nabla\mathbf{a}, \dot{\mathbf{a}}) \mathrm{d}^3\mathbf{r}. \tag{202}$$

The action integral is

$$S = \int_{t_1}^{t_2} L \, \mathrm{d}t. \tag{203}$$

The equations of motion for the field are found using Hamilton's principle $\delta S = 0$. We have

$$\begin{aligned} \delta S &= \int_{t_1}^{t_2} \int \mathcal{L}(\mathbf{a} + \delta\mathbf{a}, \nabla\mathbf{a} + \nabla\delta\mathbf{a}, \dot{\mathbf{a}} + \delta\dot{\mathbf{a}}) \mathrm{d}^3\mathbf{r} \, \mathrm{d}t - S && (204) \\ &= \int_{t_1}^{t_2} \int \left[\frac{\partial\mathcal{L}}{\partial a_i}\delta a_i + \frac{\partial\mathcal{L}}{\partial(\frac{\partial a_i}{\partial x_j})} \frac{\partial\delta a_i}{\partial x_j} + \frac{\partial\mathcal{L}}{\partial\dot{a}_i}\delta\dot{a}_i \right] \mathrm{d}^3\mathbf{r} \, \mathrm{d}t = 0. && (205) \end{aligned}$$

The second term can be integrated by parts, assuming $\delta\mathbf{a} \to 0$ for $\mathbf{r} \to \infty$ we find

$$\int \frac{\partial\mathcal{L}}{\partial(\frac{\partial a_i}{\partial x_j})} \frac{\partial}{\partial x_j}\delta a_i \mathrm{d}^3\mathbf{r} = -\int \left(\frac{\partial}{\partial x_j} \frac{\partial\mathcal{L}}{\partial(\frac{\partial a_i}{\partial x_j})} \right) \delta a_i \mathrm{d}^3\mathbf{r}. \tag{206}$$

For the third term we use integration by parts with respect to t and we use $\delta\mathbf{a}(t_1) = \delta\mathbf{a}(t_2) = 0$ and $\delta\dot{a}_i = \frac{\partial}{\partial t}\delta a_i$,

$$\int_{t_1}^{t_2} \frac{\partial\mathcal{L}}{\partial\dot{a}_i}\delta\dot{a}_i \mathrm{d}t = -\int_{t_1}^{t_2} \left(\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial\mathcal{L}}{\partial\dot{a}_i} \right) \delta a_i \mathrm{d}t. \tag{207}$$

Hence we arrive at the Euler-Lagrange equations of motion of the vector potential $\mathbf{a}(\mathbf{r}, t)$

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial\mathcal{L}}{\partial\dot{a}_i} = \frac{\partial\mathcal{L}}{\partial a_i} - \frac{\partial}{\partial x_j} \frac{\partial\mathcal{L}}{\partial(\frac{\partial a_i}{\partial x_j})}. \tag{208}$$

4.2 The Lagrangian density for a field in free space

The Langrangian density for an electromagnetic field in free space is given by

$$\mathcal{L} = \frac{1}{2} C \left\{ \dot{\mathbf{a}}^2 - c^2 (\nabla \times \mathbf{a})^2 \right\}, \tag{209}$$

with

$$C = \frac{k_3^2}{4\pi k_1} = \begin{cases} \epsilon_0 & \text{SI} \\ \frac{1}{4\pi c^2} & \text{Gaussian} \\ \frac{1}{4\pi} & \text{atomic units} \end{cases} \tag{210}$$

We derive the corresponding Euler-Langrange equations:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial\mathcal{L}}{\partial\dot{a}_i} &= \frac{\mathrm{d}}{\mathrm{d}t} C\dot{a}_i = C\ddot{a}_i && (211) \\ \frac{\partial\mathcal{L}}{\partial a_i} &= 0. && (212) \end{aligned}$$

With the notation $\nabla_l = \frac{\partial}{\partial x_l}$ we have from Eq. (46)

$$(\nabla \times \mathbf{a}) \cdot (\nabla \times \mathbf{a}) = (\nabla_l a_m)^2 - (\nabla_l a_m)(\nabla_m a_l) \tag{213}$$

and for the last term in the Euler Langrange equation we need

$$\frac{\partial}{\partial \nabla_j a_i}(\nabla_l a_m)^2 = 2\nabla_j a_i \tag{214}$$

$$\frac{\partial}{\partial \nabla_j a_i}(\nabla_l a_m)(\nabla_m a_l) = 2\nabla_i a_j, \tag{215}$$

so we find

$$\frac{\partial}{\partial x_j}\frac{\partial}{\partial(\frac{\partial a_i}{\partial x_j})}(\nabla \times \mathbf{a}) \cdot (\nabla \times \mathbf{a}) = 2\nabla_j \nabla_j a_j - 2\nabla_j \nabla_i a_j = 2[\nabla^2 a_i - \nabla_i(\nabla \cdot \mathbf{a})] \tag{216}$$

Combining all the terms we find

$$\ddot{a}_i - c^2 a_i + c^2 \nabla_i(\nabla \cdot \mathbf{a}) = 0 \tag{217}$$

or, in the Coulomb gauge ($\nabla \cdot \mathbf{a} = 0, \mathbf{a} = \mathbf{a}^\perp$)

$$\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right)\mathbf{a}^\perp = 0. \tag{218}$$

4.3 The classical Hamiltonian for a field in free space

The conjugate momentum density for the Lagrangian density of Eq. (209) is

$$\Pi(\mathbf{r}) = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{a}}} = C\dot{\mathbf{a}} \tag{219}$$

so $\dot{\mathbf{a}} = C^{-1}\Pi$ and the Hamiltonian density is

$$\mathcal{H} = \Pi \cdot \dot{\mathbf{a}} - \mathcal{L} = \frac{1}{2C}\Pi^2 + \frac{1}{2}Cc^2(\nabla \times \mathbf{a})^2. \tag{220}$$

Using the free-field relations

$$\dot{\mathbf{a}} = -\frac{1}{k_3}\mathbf{e}, \quad \Pi(\mathbf{r}) = -\frac{C}{k_3}\mathbf{e} \tag{221}$$

$$\nabla \times \mathbf{a} = \mathbf{b} \tag{222}$$

we can express the Hamiltonian density in electric and magnetic fields

$$\mathcal{H} = \frac{1}{4\pi k_1}\frac{1}{2}(\mathbf{e}^2 + c^2 k_3^2 \mathbf{b}^2), \tag{223}$$

which is in agreement with Eqs. (97) and (101) (use $k_3 = 1/\alpha$).

The mode expansion of the free field Hamiltonian. In order to quantize we will first work out the mode expansion of the fields and the Hamiltonian density. The mode expansion of $\mathbf{a}(\mathbf{r}, t)$ is given in Eqs. (128) and (129). Using Eq. (130) and $\omega = kc$ we find

$$\Pi = C\dot{\mathbf{a}} = -icC \sum_{\mathbf{k},\lambda} k \left\{ \mathbf{a}_{\mathbf{k},\lambda}(\mathbf{r}, t) - \mathbf{a}^*_{\mathbf{k},\lambda}(\mathbf{r}, t) \right\} \tag{224}$$

The Hamiltonian is the integral of the Hamiltonian density

$$\hat{H} = \int \mathcal{H} \mathrm{d}^3\mathbf{r}. \tag{225}$$

To work out the integral we use

$$\int e^{i(\mathbf{k}+\mathbf{k}')} \mathrm{d}^3\mathbf{r} = \begin{cases} V & \text{if } \mathbf{k} = -\mathbf{k}' \\ 0 & \text{otherwise} \end{cases} \tag{226}$$

and

$$(a + a^*)(b + b^*) = ab + ab^* + \text{c.c.} \tag{227}$$

where c.c. means complex conjugate. Furthermore, we use Eq. (47) to simplify

$$(\hat{\mathbf{k}} \times \mathbf{e}_{\mathbf{k},\lambda}) \cdot (\hat{\mathbf{k}} \times \mathbf{e}_{-\mathbf{k},\lambda'}) = \mathbf{e}_{\mathbf{k},\lambda} \cdot \mathbf{e}_{-\mathbf{k},\lambda} \tag{228}$$

$$(\hat{\mathbf{k}} \times \mathbf{e}_{\mathbf{k},\lambda}) \cdot (\hat{\mathbf{k}} \times \mathbf{e}^*_{\mathbf{k},\lambda'}) = \mathbf{e}_{\mathbf{k},\lambda} \cdot \mathbf{e}^*_{\mathbf{k},\lambda} = \delta_{\lambda\lambda'} \tag{229}$$

and we obtain after quite some work

$$\hat{H} = 2c^2 CV \sum_{\mathbf{k},\lambda} k^2 a_{\mathbf{k},\lambda} a^*_{\mathbf{k},\lambda} = \sum_{\mathbf{k},\lambda} \hbar\omega \frac{2\omega VC}{\hbar} a_{\mathbf{k},\lambda} a^*_{\mathbf{k},\lambda} \tag{230}$$

so with the normalization

$$\alpha_{\mathbf{k},\lambda} = \sqrt{\frac{2\omega VC}{\hbar}} a_{\mathbf{k},\lambda} \tag{231}$$

we obtain, using a symmetrized expression to prepare for quantization,

$$\hat{H} = \sum_{\mathbf{k},\lambda} \hbar\omega \frac{\alpha_{\mathbf{k},\lambda}\alpha^*_{\mathbf{k},\lambda} + \alpha^*_{\mathbf{k},\lambda}\alpha_{\mathbf{k},\lambda}}{2} \tag{232}$$

4.4 Quantization of the free field

The expansion coefficients $\alpha_{\mathbf{k},\lambda}$ are replaced by operators with the commutation relations

$$[\hat{\alpha}_{\mathbf{k},\lambda}, \hat{\alpha}_{\mathbf{k}',\lambda'}] = 0 \tag{233}$$

$$[\hat{\alpha}^\dagger_{\mathbf{k},\lambda}, \hat{\alpha}^\dagger_{\mathbf{k}',\lambda'}] = 0 \tag{234}$$

$$[\hat{\alpha}_{\mathbf{k},\lambda}, \hat{\alpha}^\dagger_{\mathbf{k}',\lambda'}] = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\lambda,\lambda'} \tag{235}$$

so with

$$\hat{\alpha}_{\mathbf{k},\lambda}\hat{\alpha}^\dagger_{\mathbf{k},\lambda} = \hat{\alpha}^\dagger_{\mathbf{k},\lambda}\hat{\alpha}_{\mathbf{k},\lambda} + 1 \tag{236}$$

we have find the quantum Hamiltonian of the free field

$$\hat{H} = \sum_{\mathbf{k},\lambda} \hbar\omega(\hat{\alpha}^\dagger_{\mathbf{k},\lambda}\hat{\alpha}_{\mathbf{k},\lambda} + \frac{1}{2}). \tag{237}$$

The eigenstates are direct products

$$|n_1(\mathbf{k}_1,\lambda_1), n_2(\mathbf{k}_2,\lambda_2),\ldots\rangle = \frac{(\hat{\alpha}^\dagger_{\mathbf{k}_1,\lambda_1})^{n_1}}{\sqrt{n_1!}}\frac{(\hat{\alpha}^\dagger_{\mathbf{k}_2,\lambda_2})^{n_2}}{\sqrt{n_2!}}\cdots|0,0,\ldots\rangle, \tag{238}$$

where $|0\rangle \equiv |0,0,\ldots\rangle$ is the vacuum state for which

$$a_{\mathbf{k},\lambda}|0\rangle = 0, \quad \text{for all } \mathbf{k} \text{ and } \lambda. \tag{239}$$

With the convention to specify only non-zero quantum numbers

$$|n(\mathbf{k},\lambda\rangle \equiv |\ldots,0,0,n(\mathbf{k},\lambda),0,0,\ldots\rangle \tag{240}$$

we have

$$\begin{aligned}
\hat{\alpha}_{\mathbf{k},\lambda}|\mathbf{k},\lambda\rangle &= \sqrt{n}|(n-1)(\mathbf{k},\lambda)\rangle & (241)\\
\hat{\alpha}^\dagger_{\mathbf{k},\lambda}|\mathbf{k},\lambda\rangle &= \sqrt{n+1}|(n+1)(\mathbf{k},\lambda)\rangle & (242)\\
\hat{\alpha}^\dagger_{\mathbf{k},\lambda}\hat{\alpha}_{\mathbf{k},\lambda}|\mathbf{k},\lambda\rangle &= n|n(\mathbf{k},\lambda)\rangle. & (243)
\end{aligned}$$

The expansion of the (Hermitian) field operators $\hat{\mathbf{a}}(\mathbf{r})$, $\Pi(\mathbf{r})$, $\hat{\mathbf{e}}(\mathbf{r})$, and $\hat{\mathbf{b}}(\mathbf{r})$ is given by

$$\begin{aligned}
\hat{\mathbf{a}}(\mathbf{r}) &= \sum_{\mathbf{k},\lambda}\sqrt{\frac{\hbar}{2\omega VC}}\left\{\hat{\alpha}_{\mathbf{k},\lambda}\mathbf{e}_{\mathbf{k},\lambda}e^{i\mathbf{k}\cdot\mathbf{r}} + \hat{\alpha}^\dagger_{\mathbf{k},\lambda}\mathbf{e}^*_{\mathbf{k},\lambda}e^{-i\mathbf{k}\cdot\mathbf{r}}\right\} & (244)\\
\hat{\Pi}(\mathbf{r}) &= -i\sum_{\mathbf{k},\lambda}\sqrt{\frac{\hbar\omega C}{2V}}\left\{\hat{\alpha}_{\mathbf{k},\lambda}\mathbf{e}_{\mathbf{k},\lambda}e^{i\mathbf{k}\cdot\mathbf{r}} - \hat{\alpha}^\dagger_{\mathbf{k},\lambda}\mathbf{e}^*_{\mathbf{k},\lambda}e^{-i\mathbf{k}\cdot\mathbf{r}}\right\} & (245)\\
\hat{\mathbf{e}}(\mathbf{r}) &= i\sum_{\mathbf{k},\lambda}\sqrt{\frac{4\pi k_1\hbar\omega}{2V}}\left\{\hat{\alpha}_{\mathbf{k},\lambda}\mathbf{e}_{\mathbf{k},\lambda}e^{i\mathbf{k}\cdot\mathbf{r}} - \hat{\alpha}^\dagger_{\mathbf{k},\lambda}\mathbf{e}^*_{\mathbf{k},\lambda}e^{-i\mathbf{k}\cdot\mathbf{r}}\right\} & (246)\\
\hat{\mathbf{b}}(\mathbf{r}) &= i\sum_{\mathbf{k},\lambda}\sqrt{\frac{\hbar\omega}{2Vc^2C}}\left\{\hat{\alpha}_{\mathbf{k},\lambda}\mathbf{b}_{\mathbf{k},\lambda}e^{i\mathbf{k}\cdot\mathbf{r}} - \hat{\alpha}^\dagger_{\mathbf{k},\lambda}\mathbf{b}^*_{\mathbf{k},\lambda}e^{-i\mathbf{k}\cdot\mathbf{r}}\right\}, & (247)
\end{aligned}$$

where

$$\mathbf{b}_{\mathbf{k},\lambda} \equiv \hat{\mathbf{k}} \times \mathbf{e}_{\mathbf{k},\lambda}. \tag{248}$$