7 Quantum Radiation

In this section we study the quantum properties of electromagnetic radiation in free space where we:

(a) Show how classical radiation in an otherwise empty box can be expressed as a superposition of wave modes, for each of which there is a dynamical similarity between the amplitude of the vector potential and the displacement of a simple harmonic oscillator. This view of radiation as oscillators will be the basis for quantizing the EM field.

(b) Review the quantum mechanics of Simple Harmonic Motion (SHM), using the number representation and ladder operators.

(c) Complete the analogy between radiation oscillations in a box and SHM, and carry across the quantization procedure to the waves, revealing photons or radiation quanta.

7.1 The classical radiation field as a set of oscillators

In this part of the course we move from the classical description of electromagnetic radiation and its interaction with matter, which accounts for the continuum emission, to a quantum description which describes line emission and absorption of radiation with matter. To do this we return to Maxwell's equations for radiation in empty space and see how we can use gauge freedom to recast our description in terms of a set of free oscillators which we can quantize.

Let us remind ourselves of Maxwell's equations,

$$\boldsymbol{\nabla}\wedge\mathbf{E} = -\dot{\mathbf{B}} \qquad \boldsymbol{\nabla}\cdot\mathbf{B} = 0 \tag{48}$$

$$\boldsymbol{\nabla}\cdot\mathbf{E} = \rho/\epsilon_0 \qquad \boldsymbol{\nabla}\wedge\mathbf{B} = \mu_0(\mathbf{j} + \epsilon_0\dot{\mathbf{E}}). \tag{49}$$

These allow us to introduce the electromagnetic potentials

$$\mathbf{B} = \boldsymbol{\nabla}\wedge\mathbf{A} \qquad \mathbf{E} = -\boldsymbol{\nabla}\phi - \partial\mathbf{A}/\partial t, \tag{50}$$

which themselves are invariant to the gauge transformations

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \boldsymbol{\nabla}\chi, \qquad \phi \to \phi' = \phi - \partial\chi/\partial t. \tag{51}$$

We can choose a gauge to satisfy the Lorenz gage condition,

$$\frac{1}{c^2}\frac{\partial\phi}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{A} = 0, \tag{52}$$

so the potentials obey the wave equations

$$\Box\mathbf{A} = \mu_0\mathbf{j} \qquad \Box\phi = \rho/\epsilon_0, \tag{53}$$

where $\Box$ is the Lorentz invariant wave operator, or d'Alembertian:

$$\Box \equiv \partial^\mu\partial_\mu = \partial^2/c^2\partial t^2 - \nabla^2. \tag{54}$$

Here, $\partial_\mu \equiv \partial/\partial x^\mu = (\partial/\partial ct, \boldsymbol{\nabla})$ and $\partial^\mu = (\partial/\partial ct, -\boldsymbol{\nabla})$ – the usual relativistic distinction of up and down indices being related by a change of sign in spatial parts of 4-vectors. In the absence of charged sources, we set

$$\rho = 0, \qquad \mathbf{j} = 0. \tag{55}$$

Given gauge freedom, we are able to choose a gauge with $\phi = \boldsymbol{\nabla} \cdot \mathbf{A} = 0$ (consistent with Maxwell's equations, since $\boldsymbol{\nabla} \cdot \mathbf{E} = \boldsymbol{\nabla} \cdot (-\partial \mathbf{A}/\partial t) = 0$). We now have all of the information about the electromagnetic field in just two components of the vector potential (one suppressed by requiring $\boldsymbol{\nabla} \cdot \mathbf{A} = 0$), instead of the four components of the complete set.

The Lorenz condition is still obeyed, so $\mathbf{A}$ obeys the source-free wave equation,

$$\nabla^2 \mathbf{A} - \ddot{\mathbf{A}}/c^2 = 0. \tag{56}$$

We now solve this equation by Fourier analysis. Imagine the radiation inside a very large cube of side L. Then the potential is expressible as a triple Fourier series with amplitudes $\mathbf{A}_\mathbf{k}$:

$$\mathbf{A}(\mathbf{r}, t) = \sum_\mathbf{k} \mathbf{A}_\mathbf{k}(t) e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{57}$$

The allowed wave vectors are those that obey *periodic boundary conditions*, in which whole number of oscillations span the box:

$$\mathbf{k} = (k_x, k_y, k_z) = (2\pi/\lambda)\hat{\mathbf{k}} = (2\pi/L)(n_x, n_y, n_z), \tag{58}$$

where the n_i are positive or negative integers. The summation is over these integers. The volume is assumed to be so large that edge effects are negligible, and that the wavenumbers are very closely spaced, so that sums over these can be approximated by integrals when convenient. As usual, with a real function, the Fourier coefficients must be *Hermitian*: $\mathbf{A}_{-\mathbf{k}} = \mathbf{A}^*_\mathbf{k}$.

The wave equation gives

$$\ddot{\mathbf{A}}_\mathbf{k}(t) + \omega^2 \mathbf{A}_\mathbf{k}(t) = 0, \tag{59}$$

where $\omega = ck$ (because if a Fourier sum is zero, each term vanishes independently), so the possible time dependence is $\exp(\pm i\omega t)$: in combination with the $\exp(i\mathbf{k}\cdot\mathbf{r})$ dependence, the modes are of course travelling waves. At this point, we need a little care over the choice of conventions for the complex representation of travelling waves. A complex disturbance, ψ, can be written either as

$$\psi \propto e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)} \qquad \text{or} \qquad \psi \propto e^{i(\omega t - \mathbf{k}\cdot\mathbf{x})}. \tag{60}$$

Both the real and imaginary parts of these expressions represent waves moving in the direction of $\mathbf{k}$; the real parts are identical, and the imaginary parts just have a relative phase shift of π. Thus these are not independent waves. The conventional solution to this is to represent travelling waves so that the frequency is positive, so that a wave moving in the $\mathbf{k}$ direction is always represented as

$$\psi \propto e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}, \tag{61}$$

with $\omega > 0$. We can therefore represent the vector potential as a sum of travelling waves by writing

$$\mathbf{A}(\mathbf{r}, t) = \sum_\mathbf{k} \mathbf{A}_\mathbf{k} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}. \tag{62}$$

Finally, in order to make the reality of $\mathbf{A}$ explicit, we can add this expression to its complex conjugate (easier than making $\mathbf{X}_\mathbf{k}$ Hermitian):

$$\mathbf{A}(\mathbf{r}, t) = \sum_\mathbf{k} \mathbf{A}_\mathbf{k} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} + \sum_\mathbf{k} \mathbf{A}^*_\mathbf{k} e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega t)}. \tag{63}$$

The condition $\boldsymbol{\nabla} \cdot \mathbf{A} = 0$ leads to $\mathbf{k} \cdot \mathbf{A}_\mathbf{k}(t) = 0$, *i.e.* the waves are transverse. This transverse vector can be expressed as a superposition of two independent vectors (which

we also choose to be orthogonal to each other), representing the polarization components of the field. We therefore define a right-handed triad involving $\mathbf{k}$ and the unit vectors $\mathbf{e}_{\mathbf{k},1}$ and $\mathbf{e}_{\mathbf{k},2}$. The orientation of the $\mathbf{e}_{\mathbf{k},1} - \mathbf{e}_{\mathbf{k},2}$ basis is arbitrary. Finally, then, we can express $\mathbf{A}$ as a sum of wave modes summing over both $\mathbf{k}$ and a polarization index, α. For future convenience, we choose to renormalize the field amplitudes by a factor $\sqrt{(\hbar/(2\epsilon_0 V\omega)}$ and take the exponential time dependence back into the time dependence of the field coefficients:

$$\mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{k},\alpha} \sqrt{\frac{\hbar}{2\epsilon_0 V\omega}}\, \mathbf{e}_{\mathbf{k},\alpha} \left(a_{\mathbf{k},\alpha}(t) e^{i\mathbf{k}\cdot\mathbf{r}} \; + \; a^*_{\mathbf{k},\alpha}(t) e^{-i\mathbf{k}\cdot\mathbf{r}} \right) \,, \tag{64}$$

where the factor e^{iwt} has been absorbed into $a_{\mathbf{k},\alpha}$ and correspondingly e^{-iwt} into $a^*_{\mathbf{k},\alpha}$. This expression is a little messy (life would be easier if EM waves were unpolarized), but it can be written more transparently in the form

$$\mathbf{A}(\mathbf{r},t) = \sum_n (\mathbf{A}_n a_n + \mathbf{A}^*_n a^*_n) \,, \tag{65}$$

where n is a general index labelling the modes: $n \equiv (\mathbf{k},\alpha)$. This general form makes it clear that we could have used basis functions other than plane waves – for instance, spherical waves of given angular momentum.

7.1.1 The oscillator energies

The total field energy, or Hamiltonian, is

$$H = \int \frac{1}{2}(\epsilon_0 E^2 + B^2/\mu_0)\, dV = \int \frac{1}{2}(\epsilon_0 \dot{A}^2 + |\boldsymbol{\nabla}\wedge\mathbf{A}|^{\mathbf{2}}/\mu_0)\, dV. \tag{66}$$

At first sight, this looks a mess: the quadratic terms mix modes of different k and α. But in practice very little of this matters: the polarization states are orthogonal, and mixing modes will give terms with a spatial dependence $\propto \exp(i\boldsymbol{\Delta k}\cdot\mathbf{r})$, which averages to zero over the box. The only way to get a non-zero term is by mixing the $\exp(i\mathbf{k}\cdot\mathbf{r})$ and $\exp(-i\mathbf{k}\cdot\mathbf{r})$ parts of a single mode. This is easy in the $\dot{A}^2$ term, where the effect of the time derivative is

$$\mathbf{A}_n a_n + \mathbf{A}^*_n a^*_n \to (i\omega)\mathbf{A}_n a_n + (-i\omega)\mathbf{A}^*_n a^*_n, \tag{67}$$

and the non-vanishing term is $\omega^2|\mathbf{A}|^2(a_n a^*_n + a^*_n a_n)$. The magnetic term is just a little more work – but it must give the same result as the electric one, since this is radiation. Allowing for the normalization constant, we get

$$H_n = \frac{1}{2}(a_n a^*_n + a^*_n a_n)\, \hbar\omega, \tag{68}$$

where we haven't commuted the a, a^* for future convenience.

What is the linear *momentum density* of the plane wave field? Consider a pulse of radiation in a given direction containing energy E, and for which special relativity requires $E = pc$ as it travels with the speed of light. By measuring the flow of this pulse across a surface we find $SA\Delta t = E$ where S is the magnitude of the Poynting vector, A is the cross section of the pulse, $\Delta t = \ell/c$ is the time for the pulse of length ℓ to pass. Hence $S = c^2 p/(A\ell)$, and is therefore c^2 times the momentum density in the pulse.

A calculation similar to that for energy then gives for total linear momentum

$$\mathbf{p} = c^{-2} \int \mathbf{S}\, dV = \sum \frac{1}{2} \left(a_{\mathbf{k},\alpha} a^*_{\mathbf{k},\alpha} + a^*_{\mathbf{k},\alpha} a_{\mathbf{k},\alpha} \right) \hbar\mathbf{k}. \tag{69}$$

Now introduce real linear combinations of a_n, a_n^*

$$q_n = \sqrt{\hbar/2\omega}(a_n + a_n^*), \quad p_n = \dot{q}_n = -i\omega\sqrt{\hbar/2\omega}(a_n - a_n^*). \tag{70}$$

Then the energy per mode can be written

$$H_n = \frac{1}{2}(p_n^2 + \omega^2 q_n^2). \tag{71}$$

Furthermore p_n and q_n obey

$$\partial H_n/\partial q_n = -\dot{p}_n, \qquad \partial H_n/\partial p_n = \dot{q}_n, \tag{72}$$

so behave as dynamically conjugate momentum and coordinate respectively, with respect to the *Hamiltonian* H; these are Hamilton's equations. Note that the p_n quantities are completely different from $\mathbf{p}$ above.

These equations are identical to the equations of motion of a harmonic oscillator of unit mass and natural frequency $\omega = kc$ (see next section). Each state is formally the same as such an oscillator, each independent of the others. The energy of the electromagnetic field in the box is identical with that of a set of independent oscillators, one for each mode $(\mathbf{k}, \alpha)$.

This was the start of Dirac's breakthrough to quantum electrodynamics.

7.2 Quantized Simple Harmonic Motion

First of all the quantum mechanics of the simple harmonic oscillator will be reviewed from the point of view of annihilation and creation operators. Then the connection noted above with modes of the radiation field is used to quantize the radiation field (*Dirac's second step to quantum electrodynamics, soon after the invention of proper quantum mechanics*).

Assume for simplicity that the oscillating mass of the oscillator is unity. Then the energy equation is

$$H = \frac{1}{2}(p^2 + \omega^2 q^2), \tag{73}$$

where q is the displacement and p is the corresponding canonical momentum (in this case it is v) with respect to the Hamiltonian H. These obey Hamilton's equations

$$\partial H/\partial q = -\dot{p} \quad \partial H/\partial p = \dot{q}. \tag{74}$$

To make this a quantum calculation p, q and therefore H become operators and p, q obey

$$[q, p] = i\hbar. \tag{75}$$

New operators a, $a^\dagger$ are defined by

$$a = (2\hbar\omega)^{-1/2}(\omega q + ip) \quad a^\dagger = (2\hbar\omega)^{-1/2}(\omega q - ip). \tag{76}$$

Here we have used the † notation for the Hermitian conjugate of an operator, which in general means

$$\langle\psi|O^\dagger|\phi\rangle \equiv \langle\phi|O|\psi\rangle^*. \tag{77}$$

A Hermitian operator is self-conjugate, and $(iO)^\dagger = -iO^\dagger$. In these terms,

$$[a,\, a^\dagger] = 1 \quad \text{and} \quad H = \frac{\hbar\omega}{2}\left(aa^\dagger + a^\dagger a\right). \tag{78}$$

These two results allow the most convenient way of writing the Hamiltonian:

$$H = (N + 1/2)\hbar\omega \quad \text{where} \quad N \equiv a^\dagger a, \tag{79}$$

in terms of N, the *number operator*.

Here is Dirac's argument for the states of a harmonic oscillator. We want to find a set of energy eigenstates $|E\rangle$, which are eigenstates of H with eigenvalue E (*i.e.* $H|E\rangle = E|E\rangle$). From above, it is clear that this is equivalent to finding the eigenstates of N: $N|n\rangle = n|n\rangle$, where $E = (n + 1/2)\hbar\omega$. This notation presupposes that the eigenvalues of N are integers, which we now prove. The first step is to establish the raising/lowering properties of the $a^\dagger$ and a operators, which means considering their action on the state $|n\rangle$. This will make a different state: is it possible that this is related to one of the other eigenstates? To test for this, we need to consider $N\,a|n\rangle$; if this is proportional to $a|n\rangle$, then our new state is indeed an eigenstate, and we can figure out which one by reading off the eigenvalue. To carry out this test, use the commutator:

$$N\,a|n\rangle = a^\dagger a\,a|n\rangle = (aa^\dagger - 1)\,a|n\rangle = a(a^\dagger a - 1)|n\rangle = (n - 1)\,a|n\rangle. \tag{80}$$

Thus we see that the action of a is to lower the eigenvalue of N by one, i.e. to lower the energy eigenvalue by $\hbar\omega$. In exactly the same way, $a^\dagger$ raises n by one.

So given a single eigenstate, we can construct a ladder of larger and smaller n eigenvalues; but as yet there is no reason for this ladder to take integer values. The key to proving that it does so is to realise that the series must terminate at the negative end. This makes physical sense: an oscillator has positive kinetic and potential energies, so how can it have negative total energy? For this reason, we would be disturbed to encounter $n < -1/2$. But this result should arise in a more inevitable mathematical way, and it comes from the normalization of the eigenstates. Consider some state $|n\rangle$, and make the new state $a\,|n\rangle$. The integral under the modulus squared of the wavefunction cannot be negative, so that

$$\langle a\,n|a\,n\rangle \geq 0. \tag{81}$$

Now we can rewrite this using the definition of the Hermitian conjugate. Remember this was $\langle\psi|O^\dagger|\phi\rangle \equiv \langle\phi|O|\psi\rangle^*$. We can rewrite this by explicitly associating operators with states, and then realizing that the complex conjugate of a bracket of two wavefunctions just reverses the order:

$$\langle\psi|O\phi\rangle = \langle\phi|O^\dagger\psi\rangle^* = \langle O^\dagger\psi|\phi\rangle. \tag{82}$$

In words, we usually think of O as 'looking right' and operating on the wavefunction there: but this has the same effect as $O^\dagger$ 'looking left'. This is a very important result; if the proof using Dirac notation seems too abstract, write out the steps in explicit integrals.

For our current problem, this says the following:

$$\langle a\,n|a\,n\rangle = \langle n|a^\dagger a|n\rangle = n, \tag{83}$$

where the last step follows because $|n\rangle$ is a normalized eigenstate of $N = a^\dagger a$. But the initial bracket could not be negative, so we must have $n \geq 0$. The only way to prevent this is for it to be impossible to reach negative n, and this is why n has to be an integer. In that case, we find that attempting to lower the $|0\rangle$ state yields zero for the normalization: rather than $a|0\rangle$ generating $|-1\rangle$, it generates no state at all. Thus the allowed number eigenvalues are $n = 0, 1, 2, \cdots$, and the energies of the harmonic oscillator are

$$E_n = (n + 1/2)\hbar\omega; \qquad n = 0, 1, 2, \cdots, \tag{84}$$

so that the ground state has *zero-point energy* $\hbar\omega/2$. This can be seen as an illustration of the uncertainty principle: zero energy would require $x = 0$ and zero momentum.

The same argument as above also tells us that the a and $a^\dagger$ operators do change the normalization of the states. Suppose $\langle n|n\rangle = 1$ for some n, and assume that $a|n\rangle = \alpha|n-1\rangle$, where α is the normalization constant that we want to find. Now we have

$$\langle a\, n|a\, n\rangle = |\alpha|^2 = \langle n|a^\dagger a\, n\rangle = n, \tag{85}$$

so that $|\alpha| = \sqrt{n}$, although the phase is undetermined (but unobservable, in any case). The normalization of $a^\dagger$ is derived in the same way, although now we need to use the commutator to re-express $aa^\dagger = N + 1$.

In summary, we have derived the following properties for our operators:

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle. \tag{86}$$

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle. \tag{87}$$

The operator $a^\dagger$ increases the energy by one quantum (creates a quantum) and amplifies the state by $\sqrt{n+1}$ and the operator a decreases the energy (annihilates a quantum) and amplifies the state by $\sqrt{n}$ (automatically preventing attempts to lower below $n = 0$). The operators are thus known as *raising and lowering operators* or *creation and annihilation operators* or collectively as *ladder operators*. The operator $N \equiv a^\dagger a$ has eigenvalues n, and is called the *number operator*.

7.3 Quantizing the radiation oscillators

The radiation oscillators are quantized identically to SHM. The classical values for the jth state become non-commuting operators:

$$[q_j, p_j] = i\hbar, \qquad [a_j, a_j^\dagger] = 1 \tag{88}$$

and clearly the amplitudes $a_j, a_j^\dagger$ have become the annihilation and creation operators for this state, which, analogously with the harmonic oscillator case, can be denoted in terms of its number eigenstate $|n_j\rangle$. This explains the strange normalization constant we chose: it was so the complex coefficients $a, a*$ could be immediately replaced by the ladder operators $a_n, a_n^\dagger$ (and this is why we kept aa^* distinct from a^*a).

Therefore, the Hamiltonian of the radiation field is a sum over modes:

$$H = \sum_j (n_j + 1/2)\hbar\omega_j, \tag{89}$$

where we assume that the radiation field sits in an eigenstate $|n_j\rangle$ for each mode. A puzzling aspect of this expression is the *zero-point energy* $\hbar\omega/2$. This is present even in the vacuum state ($|0\rangle$ for all modes), and the sum is infinite. For field theory, this constant offset is generally ignored; but it is a big problem in cosmology, where the gravitational effects of the zero-point energy should be apparent. The lack of such an effect is a big problem.

Photons It is convenient to talk of the energy quanta in these states as *photons*, with *energy* $\hbar\omega$ and *linear momentum* $\hbar\mathbf{k}$ in the case of plane waves, or *angular momentum* $\ell\hbar$ in the case of spherical waves, as specified by the state. The same physical system is being described whether we specify the numbers of photons in each momentum and polarization

state, or specify the energy (quantized) of all oscillators, identified by their momentum and polarization. The eigenvalue n_j is called the *occupation number*, to denote the fact that there are n_j photons in mode j. But this description conflicts with the common picture of photons as distinct particles: where are they? The best we can say is that the particles are delocalized over the size of the box we used to analyse the field. By the uncertainty principle, we should then expect a momentum uncertainty $\sim \hbar/L$, and this is indeed the spacing of the modes.