Microscopic theory of radiation

On October 19, 1900, Max Planck proposed an explanation of the blackbody radiation spectrum involving a new fundamental constant of nature, $h = 6.626 \times 10^{-34}$ J s [Planck, 1901]. Although Planck's result precipitated the development of quantum mechanics (i.e. the quantum mechanics of electrons), his original observation was about the quantum nature of light, which is a topic for quantum field theory. Thus, radiation is a great motivation for the development of a quantum theory of fields. This introductory topic involves a little history, a little statistical mechanics, a little quantum mechanics, and a little quantum field theory. It provides background and motivation for the systematic presentation of quantum field theory that begins in Chapter 2.

1.1 Blackbody radiation

In 1900, no one had developed a clear explanation for the spectrum of radiation from hot objects. A logical approach at the time was to apply the equipartition theorem, which implies that a body in thermal equilibrium should have energy equally distributed among all possible modes. For a hot gas, the theorem predicts the Maxwell–Boltzmann distribution of thermal velocities, which is in excellent agreement with data. When applied to the spectrum of light from a hot object, the equipartition theorem leads to a bizarre result.

A **blackbody** is an object at fixed temperature whose internal structure we do not care about. It can be treated as a hot box of light (or Jeans cube) in thermal equilibrium. Classically, a box of size L supports standing electromagnetic waves with angular frequencies

$$\omega_n = \frac{2\pi}{L}|\vec{n}|c \tag{1.1}$$

for integer 3-vectors $\vec{n}$, with c being the speed of light. Before 1900, physicists believed you could have as much or as little energy in each mode as you want. By the (classical) equipartition theorem, blackbodies should emit light equally in all modes with the intensity growing as the differential volume of phase space:

$$I(\omega) \equiv \frac{1}{V}\frac{d}{d\omega}E(\omega) = \text{const} \times c^{-3}\omega^2 k_B T \quad \text{(classical)}. \tag{1.2}$$

More simply, this classical result follows from dimensional analysis: it is the only quantity with units of energy $\times$ time $\times$ distance^{-3} that can be constructed out of ω, $k_B T$ and
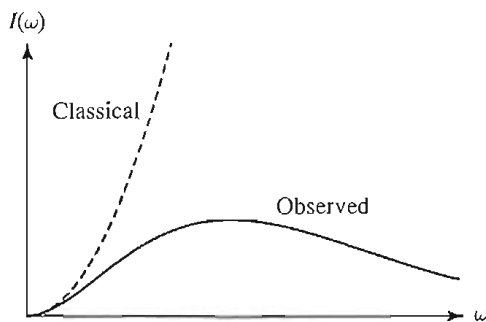
Fig. 1.1 The ultraviolet catastrophe. The classical prediction for the intensity of radiation coming from a blackbody disagrees with experimental observation at large frequencies.

c. We will set $c = 1$ from now on, since it can be restored by dimensional analysis (see Appendix A).

The classical spectrum implies that the amount of radiation emitted per unit frequency should increase with frequency, a result called the **ultraviolet catastrophe**. Experimentally, the distribution looks more like a Maxwell–Boltzmann distribution, peaked at some finite ω, as shown in Figure 1.1. Clearly the equipartition theorem does not work for blackbody radiation.

The incompatibility of observations with the classical prediction led Planck to postulate that the energy of each electromagnetic mode in the cavity is quantized in units of frequency:[1]

$$E_n = \hbar\omega_n = \frac{2\pi}{L}\hbar|\vec{n}| = |\vec{p}_n|, \tag{1.3}$$

where h is the Planck constant and $\hbar \equiv \frac{h}{2\pi}$. Albert Einstein later interpreted this as implying that light is made up of particles (later called **photons**, by the chemist Gilbert Lewis). Note that if the excitations are particles, then they are massless:

$$m_n^2 = E_n^2 - |\vec{p}_n|^2 = 0. \tag{1.4}$$

If Planck and Einstein are right, then light is really a collection of massless photons. As we will see, there are a number of simple and direct experimental consequences of this hypothesis: quantizing light resolves the blackbody paradox; light having energy leads to the photoelectric effect; and light having momentum leads to Compton scattering. Most importantly for us, the energy hypothesis was the key insight that led to the development of quantum field theory.

With Planck's energy hypothesis, the thermal distribution is easy to compute. Each mode of frequency ω_n can be excited an integer number j times, giving energy $jE_n = j(\hbar\omega_n)$

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[1] Planck was not particularly worried about the ultraviolet catastrophe, since there was no strong argument why the equipartition theorem should hold universally; instead, he was trying to explain the observed spectrum. He first came up with a mathematical curve that fit data, generalizing previous work of Wilhelm Wien and Lord Rayleigh, then wrote down a toy model that generated this curve. The interpretation of his model as referring to photons and the proper statistical mechanics derivation of the blackbody spectrum did not come until years later.

in that mode. The probability of finding that much energy in the mode is the same as the probability of finding energy in *anything*, proportional to the Boltzmann weight $\exp(-energy/k_BT)$. Thus, the expectation value of energy in each mode is

$$\langle E_n \rangle = \frac{\sum_{j=0}^{\infty}(jE_n)e^{-jE_n\beta}}{\sum_{j=0}^{\infty}e^{-jE_n\beta}} = \frac{-\frac{d}{d\beta}\frac{1}{1-e^{-\hbar\omega_n\beta}}}{\frac{1}{1-e^{-\hbar\omega_n\beta}}} = \frac{\hbar\omega_n}{e^{\hbar\omega_n\beta}-1}, \tag{1.5}$$

where $\beta = 1/k_BT$. (This simple derivation is due to Peter Debye. The more modern one, using ensembles and statistical mechanics, was first given by Satyendra Nath Bose in 1924.)

Now let us take the continuum limit, $L \to \infty$. In this limit, the sums turn into integrals and the average total energy up to frequency ω in the blackbody is

$$E(\omega) = \int^{\omega} d^3\vec{n}\frac{\hbar\omega_n}{e^{\hbar\omega_n\beta}-1} = \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi \int_0^{\omega} d|\vec{n}|\frac{|\vec{n}|^2\hbar\omega_n}{e^{\hbar\omega_n\beta}-1}$$

$$= 4\pi\hbar\frac{L^3}{8\pi^3}\int_0^{\omega} d\omega'\frac{\omega'^3}{e^{\hbar\omega'\beta}-1}. \tag{1.6}$$

Thus, the intensity of light as a function of frequency is (adding a factor of 2 for the two polarizations of light)

$$I(\omega) = \frac{1}{V}\frac{dE(\omega)}{d\omega} = \frac{\hbar}{\pi^2}\frac{\omega^3}{e^{\hbar\omega\beta}-1}. \tag{1.7}$$

It is this functional form that Planck showed in 1900 correctly matches experiment.

What does this have to do with quantum field theory? In order for this derivation, which used equilibrium statistical mechanics, to make sense, light has to be able to equilibrate. For example, if we heat up a box with monochromatic light, eventually all frequencies must be excited. However, if different frequencies are different particles, equilibration must involve one kind of particle turning into another kind of particle. So, particles must be created and destroyed. Quantum field theory tells us how that happens.

1.2 Einstein coefficients

A straightforward way to quantify the creation of light is through the coefficient of spontaneous emission. This is the rate at which an excited atom emits light. Even by 1900, this phenomenon had been observed in chemical reactions, and as a form of radioactivity, but at that time it was only understood statistically. In 1916, Einstein came up with a simple proof of the relation between emission and absorption based on the existence of thermal equilibrium. In addition to being relevant to chemical phenomenology, his relation made explicit why a first principles quantum theory of fields was needed.

Einstein's argument is as follows. Suppose we have a cavity full of atoms with energy levels E_1 and E_2. Assume there are n_1 of the E_1 atoms and n_2 of the E_2 atoms and let $\hbar\omega = E_2 - E_1$. The probability for an E_2 atom to emit a photon of frequency ω and transition to state E_1 is called the **coefficient for spontaneous emission** A. The probability for

a photon of frequency ω to induce a transition from 2 to 1 is proportional to the **coefficient of stimulated emission** B and to the number of photons of frequency ω in the cavity, that is, the intensity $I(\omega)$. These contribute to a change in n_2 of the form

$$dn_2 = -\left[A + BI(\omega)\right] n_2. \tag{1.8}$$

The probability for a photon to induce a transition from 1 to 2 is called the **coefficient of absorption** B'. Absorption decreases n_1 and increases n_2 by $B'I(\omega)n_1$. Since the total number of atoms is conserved in this two-state system, $dn_1 + dn_2 = 0$. Therefore,

$$dn_2 = -dn_1 = -\left[A + BI(\omega)\right] n_2 + B'I(\omega)n_1. \tag{1.9}$$

Even though we computed $I(\omega)$ above for the equilibrium blackbody situation, these equations should hold for any $I(\omega)$. For example, $I(\omega)$ could be the intensity of a laser beam we shine at some atoms in the lab.

At this point, Einstein assumes the gas is in equilibrium. In equilibrium, the number densities are constant, $dn_1 = dn_2 = 0$, and determined by Boltzmann distributions:

$$n_1 = Ne^{-\beta E_1}, \qquad n_2 = Ne^{-\beta E_2}, \tag{1.10}$$

where N is some normalization factor. Then

$$\left[B'e^{-\beta E_1} - Be^{-\beta E_2}\right] I(\omega) = Ae^{-\beta E_2} \tag{1.11}$$

and so

$$I(\omega) = \frac{A}{B'e^{\hbar\beta\omega} - B}. \tag{1.12}$$

However, we already know that in equilibrium

$$I(\omega) = \frac{\hbar}{\pi^2} \frac{\omega^3}{e^{\hbar\beta\omega} - 1} \tag{1.13}$$

from Eq. (1.7). Since equilibrium must be satisfied at any temperature, i.e. for any β, we must have

$$B' = B \tag{1.14}$$

and

$$\frac{A}{B} = \frac{\hbar}{\pi^2}\omega^3. \tag{1.15}$$

These are simple but profound results. The first, $B = B'$, says that the coefficient of absorption must be the same as the coefficient for stimulated emission. The coefficients B and B' can be computed in quantum mechanics (not quantum field theory!) using time-dependent perturbation theory with an external electromagnetic field. Then Eq. (1.15) determines A. Thus, all the Einstein coefficients A, B and B' can be computed without using quantum field theory.

You might have noticed something odd in the derivation of Eqs. (1.14) and (1.15). We, and Einstein, needed to use an equilibrium result about the blackbody spectrum to derive

the A/B relation. Does spontaneous emission from an atom have anything to do with equilibrium of a gas? It does not seem that way, since an atom radiates at the same rate no matter what is around it. The calculation of A/B from first principles was not performed until 10 years after Einstein's calculation; it had to wait until the invention of quantum field theory.

1.3 Quantum field theory

The basic idea behind the calculation of the spontaneous emission coefficient in quantum field theory is to treat photons of each energy as separate particles, and then to study the system with multi-particle quantum mechanics. The following treatment comes from a paper of Paul Dirac from 1927 [Dirac, 1927], which introduced the idea of second quantization. This paper is often credited for initiating quantum field theory.

Start by looking at just a single-frequency (energy) mode of a photon, say of energy Δ. This mode can be excited n times. Each excitation adds energy Δ to the system. So, the energy eigenstates have energies $\Delta, 2\Delta, 3\Delta, \ldots$. There is a quantum mechanical system with this property that you may remember from your quantum mechanics course: the simple harmonic oscillator (reviewed in Section 2.2.1 and Problem 2.7).

The easiest way to study a quantum harmonic oscillator is with creation and annihilation operators, $a^\dagger$ and a. These satisfy

$$[a, a^\dagger] = 1. \tag{1.16}$$

There is also the number operator $\hat{N} = a^\dagger a$, which counts modes:

$$\hat{N}|n\rangle = n|n\rangle. \tag{1.17}$$

Then,

$$\hat{N}a^\dagger|n\rangle = a^\dagger a a^\dagger|n\rangle = a^\dagger|n\rangle + a^\dagger a^\dagger a|n\rangle = (n+1)a^\dagger|n\rangle. \tag{1.18}$$

Thus, $a^\dagger|n\rangle = C\,|n+1\rangle$ for some constant C, which can be chosen real. We can determine C from the normalization $\langle n|n\rangle = 1$:

$$C^2 = \langle n+1|C^2|n+1\rangle = \langle n|aa^\dagger|n\rangle = \langle n|\big(a^\dagger a + 1\big)|n\rangle = n+1, \tag{1.19}$$

so $C = \sqrt{n+1}$. Similarly, $a|n\rangle = C'|n-1\rangle$ and

$$C'^2 = \langle n-1|C'^2|n-1\rangle = \langle n|a^\dagger a\,|n\rangle = n, \tag{1.20}$$

so $C' = \sqrt{n}$. The result is that

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \qquad a|n\rangle = \sqrt{n}|n-1\rangle. \tag{1.21}$$

While these normalization factors are simple to derive, they have important implications.

Now, you may recall from quantum mechanics that transition rates can be computed using Fermi's golden rule. Fermi's golden rule says that the transition rate between two states is proportional to the matrix element squared:

$$\Gamma \sim |\mathcal{M}|^2 \delta(E_f - E_i), \qquad (1.22)$$

where the δ-function serves to enforce energy conservation. (We will derive a similar formula for the transition rate in quantum field theory in Chapter 5. For now, we just want to use quantum mechanics.) The matrix element $\mathcal{M}$ in this formula is the projection of the initial and final states on the interaction Hamiltonian:

$$\mathcal{M} = \langle f|H_{\text{int}}|i\rangle. \qquad (1.23)$$

In this case, we do not need to know exactly what the interaction Hamiltonian H_{int} is. All we need to know is that H_{int} must have some creation operator or annihilation operator to create the photon. H_{int} also must be Hermitian. Thus it must look like[2]

$$H_{\text{int}} = H_I^\dagger a^\dagger + H_I a, \qquad (1.24)$$

with H_I having non-zero matrix elements between initial and final atomic states.

For the $2 \to 1$ transition, the initial state is an excited atom we call atom_2 with n_ω photons of frequency $\omega = \Delta/\hbar$:

$$|i\rangle = |\text{atom}_2; n_\omega\rangle. \qquad (1.25)$$

The final state is a lower energy atom we call atom_1 with $n_\omega + 1$ photons of energy Δ:

$$\langle f| = \langle \text{atom}_1; n_\omega + 1|. \qquad (1.26)$$

So,

$$
\begin{aligned}
\mathcal{M}_{2\to1} &= \langle \text{atom}_1; n_\omega + 1|(H_I^\dagger a^\dagger + H_I a)|\text{atom}_2; n_\omega\rangle \\
&= \langle \text{atom}_1|H_I^\dagger|\text{atom}_2\rangle\langle n_\omega + 1|a^\dagger|n_\omega\rangle + \langle \text{atom}_1|H_I|\text{atom}_2\rangle\langle n_\omega + 1|a|n_\omega\rangle \\
&= \mathcal{M}_0^\dagger\langle n_\omega + 1|n_\omega + 1\rangle\sqrt{n_\omega + 1} + 0 \\
&= \mathcal{M}_0^\dagger\sqrt{n_\omega + 1}
\end{aligned}
\qquad (1.27)
$$

where $\mathcal{M}_0^\dagger = \langle \text{atom}_1|H_I^\dagger|\text{atom}_2\rangle$. Thus,

$$|\mathcal{M}_{2\to1}|^2 = |\mathcal{M}_0|^2(n_\omega + 1). \qquad (1.28)$$

If instead we are exciting an atom, then the initial state has an unexcited atom and n_ω photons:

$$|i\rangle = |\text{atom}_1; n_\omega\rangle \qquad (1.29)$$

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[2] Dirac derived H_I from the canonical introduction of the vector potential into the Hamiltonian: $H = \frac{1}{2m}\vec{p}^2 \to \frac{1}{2m}(\vec{p} + e\vec{A})^2$. This leads to $H_{\text{int}} \sim \frac{e}{m}\vec{A} \cdot \vec{p}$ representing the photon interacting with the atom's electric dipole moment. In our coarse approximation, the photon field $\vec{A}$ is represented by a and so H_I must be related to the momentum operator $\vec{p}$. Fortunately, all that is needed to derive the Einstein relations is that H_I is something with non-zero matrix elements between different atomic states; thus, we can be vague about its precise definition. For more details consult [Dirac, 1927] or [Dirac, 1930, Sections 61–64].

and the final state has an excited atom and $n_\omega - 1$ photons:

$$\langle f| = \langle \text{atom}_2; n_\omega - 1|. \tag{1.30}$$

This leads to

$$\begin{aligned}
\mathcal{M}_{1\to 2} &= \langle \text{atom}_2; n_\omega - 1|H_I^\dagger a^\dagger + H_I a|\text{atom}_1; n_\omega\rangle \\
&= \langle \text{atom}_2|H_I|\text{atom}_1\rangle\langle n_\omega - 1|a|n_\omega\rangle \\
&= \mathcal{M}_0\sqrt{n_\omega}
\end{aligned} \tag{1.31}$$

and therefore,

$$dn_2 = -dn_1 = -|\mathcal{M}_{2\to 1}|^2 n_2 + |\mathcal{M}_{1\to 2}|^2 n_1 = -|\mathcal{M}_0|^2(n_\omega + 1)n_2 + |\mathcal{M}_0|^2(n_\omega)n_1. \tag{1.32}$$

This is pretty close to Einstein's equation, Eq. (1.9):

$$dn_2 = -dn_1 = -[A + BI(\omega)]\,n_2 + B'I(\omega)n_1. \tag{1.33}$$

To get them to match exactly, we just need to relate the number of photon modes of frequency ω to the intensity $I(\omega)$. Since the energies are quantized by $\Delta = \hbar\omega = \hbar\frac{2\pi}{L}|\vec{n}|$, the total energy is

$$E(\omega) = \int^\omega d^3\vec{n}(\hbar\omega)n_\omega = (4\pi)\hbar L^3 \int_0^\omega \frac{d\omega}{(2\pi)^3}\omega^3 n_\omega. \tag{1.34}$$

We should multiply this by 2 for the two polarizations of light. (Dirac actually missed this factor in his 1927 paper, since polarization was not understood at the time.) Including the factor of 2, the intensity is

$$I(\omega) = \frac{1}{L^3}\frac{dE}{d\omega} = \frac{\hbar\omega^3}{\pi^2}n_\omega. \tag{1.35}$$

This equation is a standard statistical mechanical relation, independent of what n_ω actually is; its derivation required no mention of temperature or of equilibrium, just a phase space integral.

So now we have

$$dn_2 = -dn_1 = -|\mathcal{M}_0|^2\left[1 + \frac{\pi^2}{\hbar\omega^3}I(\omega)\right]n_2 + |\mathcal{M}_0|^2\left[\frac{\pi^2}{\hbar\omega^3}I(\omega)\right]n_1 \tag{1.36}$$

and can read off Einstein's relations,

$$B' = B, \qquad \frac{A}{B} = \frac{\hbar}{\pi^2}\omega^3, \tag{1.37}$$

without ever having to assume thermal equilibrium. This beautiful derivation was one of the first ever results in quantum field theory.