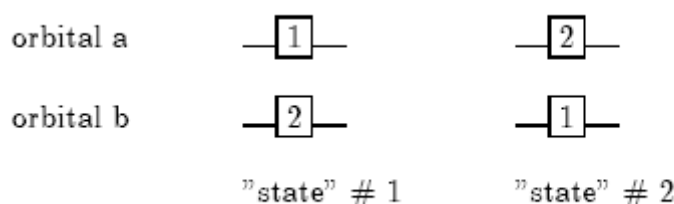


## CHAPTER 6: DEGENERATE SYSTEMS OF NON-INTERACTING PARTICLES

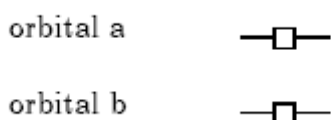
### 6a: Identical particles (see also Ch 4,5,6 of 2<sup>nd</sup> year Notes)

The Gibbs Paradox: semiclassical theory says that allowing two gases of the same type of particle to mix will increase entropy. But this is contrary to observation. The standard resolution is to make the following postulate, which has been confirmed wherever it can be tested: **“there is no element of Nature corresponding to multiple states which differ only by the identity (labelling) of particles of the same species”**

More colloquially, particles with the same properties are not individuals. This has consequences for many-particle quantum states. For example, consider the following two “states” (in which 1 represents an electron labelled “1” and 2 represents another electron labelled “2”)



These are really not two different states, but correspond to only one physical state which can be pictured as



This is the only state with one particle on each orbital. That is, there is no element of reality corresponding to the assignment of labels to the two electrons.

Another way of saying this is that, if we insist on labelling the particles, then any measured property must remain the same when the labels are swapped. Consider the case where there are two particles, one in orbital  $a$  and the other in orbital  $b$ . (We can allow orbitals  $a$  and  $b$  to be same, but for the moment think of them as different orbitals.) Then swapping the labels for the particles is the same as swapping the labels of the orbitals. Now, the expectation of any physical quantity for the two particles in a two-particle state for example, can be determined from the two-body wavefunction  $\Psi_{ab}(r_1, r_2)$ . Thus, since the swapping of labels must have no physical consequences, this must have the property

$$\Psi_{ba}(r_1, r_2) \propto \Psi_{ab}(r_1, r_2).$$

The proportionality allows for a different global factor  $\exp(i\phi)$ , since a global phase has no physical consequences. It is found that all the elementary particles (and some combined ones) fall into two categories, Fermions and Bosons. It can further be argued that in 3-dimensional space, swapping the labels twice must be the same as doing nothing. Thus whatever phase factor appears when swapping the particles must give unity when squared. From this we get two cases:

#### 1. FERMIONS.

For these particles,  $\phi = \pi$  so  $\exp(i\phi) = -1$ . Thus the many-body wavefunction changes sign upon exchanging the labels: e.g. for a two-fermion state

$$\Psi_{ba}(r_1, r_2) = -\Psi_{ab}(r_1, r_2) \quad (6a.1)$$

It follows that two Fermions cannot occupy the same single-particle orbital “a”, since this would give

$$\Psi_{aa}(r_1, r_2) = -\Psi_{aa}(r_1, r_2)$$

so that  $\Psi_{aa}$  must be zero, meaning there is no such state. This leads to the

**Pauli Principle:** two or more identical fermions cannot occupy the same orbital.

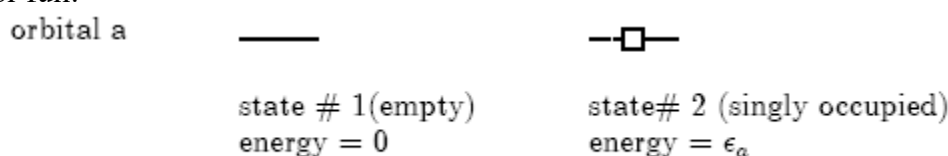
(6a.2)

*Some examples of Fermions:* All elementary particles (as opposed to quanta of fields) are spin-1/2 Fermions – electrons, neutrinos, and quarks. Compound particles an ODD number of elementary Fermions are also Fermions.

**Exercise:** Explain why, by considering the wavefunction.

Examples of a compound Fermion are a neutron, a proton (= a H-nucleus = a  $H^+$  ion), a  $^3He$ -nucleus (= a  $^3He^{++}$  ion) and a  $^3He$  atom.

For Fermions the allowed configurations of an orbital “a” (e.g. hydrogen  $1s\uparrow$  orbital) is just empty or full:



## 2. BOSONS

These are the second category of elementary particles known to date. Here the phase angle is  $\phi = 0$ , so that the wavefunction is unchanged by label reversal:

$$\Psi_{ba}(r_1, r_2) = +\Psi_{ab}(r_1, r_2) \quad (6a.3)$$

There is now no contradiction when  $a = b$ , so for these species, two particles (and in fact any number) of the same species can crowd into the same orbital (or mode as it often called).

*Some examples of Bosons:* Quanta of fundamental fields (Higgs boson, gluons, photons) behave like bosonic particles in a low-energy limit. Compound particles comprising an EVEN number of Fermions, plus ANY number of Bosons, are Bosons.

**Exercise:** Explain why, by considering the wavefunction.

Examples of a compound Boson are a  $\pi$ -meson, a H atom, a  $^4He$ -nucleus (= an alpha particle = a  $^4He^{++}$  ion) or a  $^4He$  atom. The allowed states for a Bosonic orbital or mode are as follows (the expressions for the energy ignore the inter-particle interaction energy, which may or may not be a good approximation):



## 3. ANYONS

There are even some situations where compound particles can have a nontrivial phase factor: e.g. the relation

$$\Psi_{ba}(r_1, r_2) = \exp(i2\pi/3)\Psi_{ab}(r_1, r_2) \quad (6a.4)$$

holds for effective particles consisting of 1/3 of an electron bound to a magnetic flux vortex. These concepts are useful in describing the Fractional Quantum Hall Effect occurring in two-dimensional electron gas layers formed in semiconductors under the influence of a very strong magnetic field at low temperature. The physics of this situation depends in an essential way on the Coulomb interaction between the electrons, a very different regime from the ideal

gases we will be considering, and one that we will not explore further. For those interested, mind-boggling qualitative discussion is given in the following articles:

- ‘Electrons in flatland’, S. Kivelson, D. H. Lee and S. C. Zhang, Scientific American, March 1996 p. 86.
- ‘When the electron falls apart’, P.W. Anderson, Physics Today, March 1997, p. 42.
- K. I. Bolotin et al., “Observation of the fractional quantum Hall effect in graphene”, Nature 62, 196 (2009).

## 6b The concept of degeneracy (for further discussion see 2nd year Notes Sec.6a)

For a system of  $N$  particles with volume  $V$  we can define a volume per particle  $V_1 = V/N$ . If we require the particles to have *non-overlapping orbitals* then we have to imagine each particle has a wavefunction that is basically confined within a little sphere of volume  $V_1$ . If we assume a uniform wavefunction in the sphere as an extreme case, the standard deviation in  $x$  (or  $y$  or  $z$ ) is

$$\sigma_1(x) = \alpha \left( \frac{3V}{4\pi N} \right)^{1/3}. \quad (6b.1)$$

**Exercise:** Show this.

Now, consider that a particle of mass  $m$  in a gas at temperature  $T$  has a typical thermal energy  $\frac{1}{2}k_B T$  per kinetic degree of freedom (this is a consequence of the **equipartition theorem**). That is,  $\frac{1}{2}k_B T = \langle p^2 / 2m \rangle \Rightarrow \sigma(p) = \sqrt{mk_B T}$  where this relates to the momentum in any direction, and we have used the fact that the mean momentum is zero. But by the uncertainty principle,  $\sigma(x)\sigma(p) \geq \hbar/2$ . Thus we find a minimum standard-deviation in position due to the fluctuations in momentum of

$$\sigma_{th}(x) = \frac{\hbar}{2\sqrt{mk_B T}} \quad (6b.2)$$

This quantity is, apart from a numerical factor of order unity, the so-called **thermal de Broglie wavelength**,  $\lambda_{th} = \hbar/p_{RMS} = \hbar/\sqrt{2\pi mk_B T}$ . (Recall de Broglie’s relation  $\lambda = \hbar/p$ .)

Thus we have two cases:

### **Non-degenerate case**

If  $\sigma_{th}(x) < \sigma_1(x)$  then a wavefunction/orbital with the required thermal energy can fit inside the volume allowed for each particle. That is, the orbitals for the different particles can be non-overlapping. Thus we may ignore the indistinguishability of the particles, as we can distinguish each particle by its position in practice. Thus we may treat each (non-interacting) particle as a separate system (if there are no forces between them) and simple “Maxwell-Boltzmann” statistics results in the limit  $\sigma_{th}(x) \ll \sigma_1(x)$ . Note that in this limit the partition function for a single particle is necessarily large, since  $Z_1 = (V/\lambda_{th}^3) \gg (V_1/\lambda_{th}^3) \gg 1$ , and that for the whole gas,  $Z = (Z_1)^N$  is larger still. See 2<sup>nd</sup> year Notes, Chapter 4.

### **Degenerate case.**

If  $\sigma_{th}(x) \geq \sigma_1(x)$  then a wavefunction/orbital with the required thermal energy *cannot* fit inside the volume allowed for each particle. That is, the orbitals for the different particles must be overlapping. In this case, the system is said to be **degenerate**, and the indistinguishability of the particles becomes important. We cannot then treat the particles as independent. For example, for Fermions, no two particles can occupy the same orbital, so at

most Fermions can reach equality (roughly) in the above inequality. For Bosons, if one particle occupies an orbital “ $a$ ” then other particles are *more* likely to do so. In the absence of forces between the particles we can still treat the system analytically by considering each orbital “ $a$ ” of energy  $\epsilon_a$  as a system. (This is true whether we are in the degenerate or non-degenerate limit.) The Grand ensemble then gives the average occupancy of each orbital  $a$ . (for more detail see the earlier Sec 4b of this course).

$$\bar{N}_a = \frac{1}{\exp(\beta(\epsilon_a - \mu)) \pm 1} \quad (+\text{for Fermions, } - \text{ for Bosons}) \quad (6b.4)$$

### 6c. Independent Fermions

This is important, particularly for electrons in metals and in stellar matter. See 2<sup>nd</sup> year notes and Condensed Matter Notes. We will not give further detail on this in the present Chapter.

### 6d. Independent Bosons: Bose-Einstein Condensation

These remarks will apply only to “real” bosons whose total number is conserved, as opposed to “fake” bosons (e.g. photons, phonons, magnons, excitons, and polaritons) whose number is not conserved.

*Groundstate* of  $N$  noninteracting bosons has them all in some single-particle state of energy  $\epsilon_0$ . Thus total energy of groundstate is  $N\epsilon_0$ . (This is not possible for Fermions because of the Pauli exclusion principle). This groundstate is very peculiar: consider for example bosons in a rigid box of dimensions  $L \times L \times L$ . The  $N$ -particle wavefunction is

$$\Psi(\mathbf{r}_1 \cdots \mathbf{r}_N) = \prod_{i=1}^N \left[ \left( \frac{2}{L} \right)^{\frac{3}{2}} \sin\left(\frac{\pi x_i}{L}\right) \sin\left(\frac{\pi y_i}{L}\right) \sin\left(\frac{\pi z_i}{L}\right) \right],$$

just a product of normalized single-particle wavefunctions. Note it's already symmetric under interchange of particle labels and so is a valid boson wavefunction. The total particle number density is thus

$$\rho(\mathbf{r}) = \frac{N}{L^3} \cdot 8 \sin^2\left(\frac{\pi x}{L}\right) \sin^2\left(\frac{\pi y}{L}\right) \sin^2\left(\frac{\pi z}{L}\right)$$

This macroscopic density is not even approximately uniform, but rises to a broad maximum at the centre of the box. By looking at macroscopic density, we see a reflection of a microscopic single particle wavefunction, so it is sometimes called a “Macroscopic Wavefunction”. (Fermions by contrast, give an almost uniform density with oscillations only within a Fermi wavelength of the edge of the box). Other odd properties involve the excited states: this is related to superfluid properties etc. of  $^4\text{He}$ , and macroscopic interference properties of trapped atomic gases.

*Finite temperature.* The macroscopic occupation of the groundstate, and associated odd properties, can sometimes persist up to a finite temperature, called the “Bose-Einstein condensation temperature”  $T_C$ . That is, a macroscopic fraction of the particles can still occupy the groundstate at finite temperature, while all other single-particle states have occupations  $O(1)$  (fractional occupations of  $O(1/N)$ ). This phenomenon is termed “**Bose condensation**” or “**Bose-Einstein Condensation**” (“**BEC**”), and it has been the subject of an enormous amount of research, especially since it was first achieved experimentally in 1995.

Let us measure all single particle energies relative to the single particle groundstate energy  $\epsilon_0$  (i.e. set  $\epsilon_0=0$ ). In the Grand Canonical Ensemble, the total *mean* particle number  $\bar{N}$  fixed.

(Note that  $\tilde{N}$  is just a fudge for  $\bar{N}$  which is a pain to make in MS-Word. Note also that it is common to treat this as if it is a fixed particle number,  $N$ . Indeed we will do so later in this chapter. This issue will be covered more in Problem Sheet 2.) This is the sum of mean occupations of the modes:

$$\bar{N} = \bar{n}_0 + \sum_{\vec{k} \neq 0} \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1} \quad (6d.1)$$

$$\bar{n}_0 = \frac{1}{e^{-\beta\mu} - 1} = \frac{\xi}{1 - \xi} \quad (6d.2)$$

where  $\xi = \exp(\beta\mu)$  is the fugacity. Here the ground state energy has been defined to be zero, which means that all energies levels are relative to that (in an additive sense). At given values of  $\tilde{N}$  and  $T$  (the usual parameters given for the Grand ensemble), the tricky problem is to find the chemical potential  $\mu$ . If  $\mu$  is just below the zero energy, i.e.  $\beta\mu = O(-1/\tilde{N})$ , then  $\bar{n}_0 = O(\tilde{N})$  and so we have BEC.

## 6e. Continuum theory of BEC

We assume (and justify later) that the only state (if any) with macroscopic occupation is the groundstate. In “continuum theory” we then replace the sum in (6d.1) by an integral:

$$\bar{N} = \bar{n}_0 + \int_0^\infty \frac{D(\varepsilon)d\varepsilon}{\exp(\beta[\varepsilon - \mu]) - 1} = \bar{n}_0 + \bar{N}_{\text{excited}}(\mu, T) \quad (6e.1)$$

where  $D(\varepsilon)$  is the density of states such that the number of orbitals between energy  $\varepsilon - d\varepsilon/2$  and  $\varepsilon + d\varepsilon/2$  is  $D(\varepsilon)d\varepsilon$ , in the limit of small  $d\varepsilon$ . (Density of states is discussed in Condensed matter notes). This integral represents the number of particles in excited orbitals at assumed values of  $\mu$  and  $T$ .

As stated above, in order to have macroscopic occupation of the ground orbital i.e.  $\bar{n}_0 = O(\tilde{N})$  we require  $\beta\mu = O(-1/\tilde{N})$ , or equivalently  $\xi = 1 - O(1/\tilde{N})$ . Thus we are led to examine the behaviour of the integral in (6e.1) for the case  $\mu = 0$  (i.e.  $\xi = 1$ ) since this is typically a good enough approximation for the integral (obviously not for  $\bar{n}_0$  itself, which would be infinite if we took  $\mu = 0$  for  $\mu = 0$  it becomes

$$\bar{N}_{\text{excited}}(\mu=0, T) = \int_0^\infty \frac{D(E)}{\exp(\beta E) - 1} dE \quad (6e.2)$$

This integral is “dangerous” in that it is potentially divergent at the lower limit where the denominator goes to zero. *Near the lower integration limit* we can approximate the integrand as follows

$$\bar{N}_{\text{excited}}(\mu = 0, T) \approx n_f + \int_0 \frac{D(E)dE}{(1 + \beta E + \dots) - 1} = n_f + k_B T \int_0 \frac{D(E)dE}{E} \quad (6e.3)$$

Here  $n_f$  is the contribution from the total integral where  $\beta E$  is not small. (This is always finite because There is no problem with convergence at the upper limit. The integral is convergent there because of the exponentially growing inverse Boltzmann factor in the denominator: the  $D(E)$  on the numerator never rises as fast as exponentially for realistic confinement potentials.) There are thus two basic cases to consider

**Case (i): the integral in (6e.3) is convergent  $\Rightarrow$  BEC occurs.** This happens when  $D(E)$  falls rapidly enough to zero as  $E$  goes to 0, so that there are *few excited states available near to the ground energy*. Then we expect we might be forced to have a large occupation of the ground orbital at low temperature. Indeed if  $\bar{N}_{\text{excited}}(\mu=0, T)$  is finite, then for a *large* total number of particles satisfying  $\tilde{N} > \bar{N}_{\text{excited}}(\mu=0, T)$  we are forced to put a large number of particles  $\bar{n}_0 = \tilde{N} - \bar{N}_{\text{excited}}(\mu=0, T)$  into the ground orbital – see Eq (6e.1). [We certainly could not have  $\mu$  significantly below 0 in this case because  $\bar{N}_{\text{excited}}(\mu, T)$  is an *increasing* function of  $\mu$  so this

would make  $\tilde{N}_{\text{excited}}$  smaller: then  $\tilde{n}_0$  would have to be even more macroscopic, but that is impossible unless  $\mu$  is just below zero<sup>-</sup>, by Eq.(6d.2).]

Another way of looking at this case is to note that  $\tilde{N}_{\text{excited}}(\mu, T)$  from Eq. (6d.1) is an increasing function of both  $\mu$  and  $T$  so, for given values of  $\tilde{N}$  and  $T$ , the problem of finding  $\mu$  and hence determining  $\tilde{n}_0$  from (6d.2) can be represented graphically as follows.

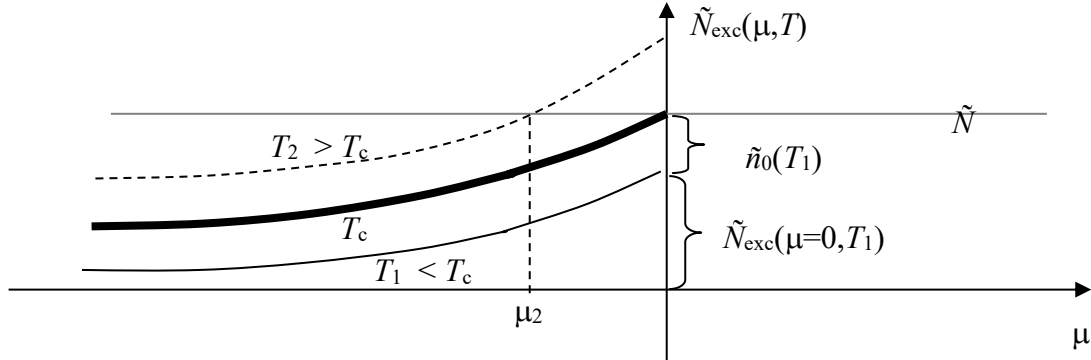


Fig. 6e1: choosing  $\mu$  in Bose condensing systems via Eq. (6e.1) (continuum theory).

Note that for each value of  $\tilde{N}$  (or  $\mu$ ) there is a **critical temperature  $T_c$  for BEC** satisfying

$$\tilde{N}_{\text{excited}}(\mu = 0, T_c) \equiv \int_0^\infty \frac{D(E)dE}{\exp(E/(k_B T_c)) - 1} = \tilde{N} \quad (6e.4)$$

For  $T < T_c$  we have BEC: for  $T > T_c$  there is no condensate.

**Case 2: the integral (6e.3) is divergent  $\Rightarrow$  No BEC.** This will happen when  $D(E)$  does not vanish fast enough as  $E$  goes to zero. Then there are relatively many excited orbitals *near* to the ground energy, and so perhaps we can accommodate essentially all the particles in low-lying excited orbitals, without being forced to put a substantial fraction of them into the ground orbital. This is indeed the case and we can illustrate it graphically as follows.

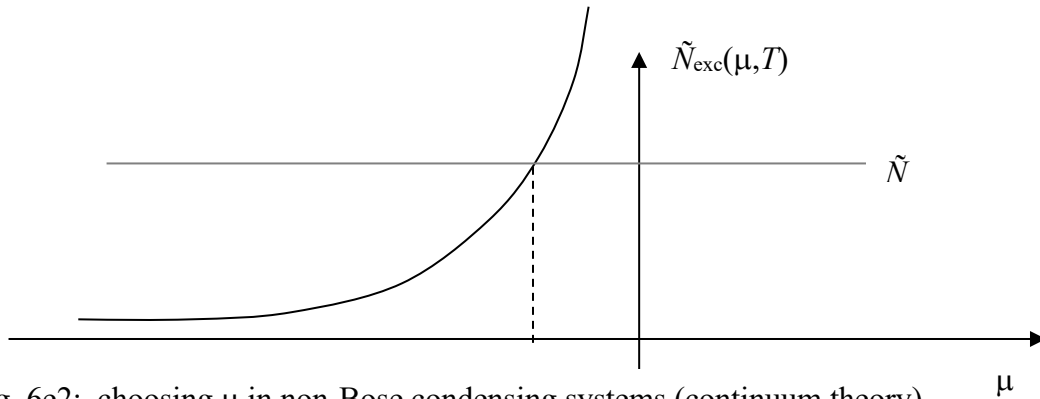


Fig. 6e2: choosing  $\mu$  in non-Bose condensing systems (continuum theory).

Note that at any  $N$  and  $T > 0$ , because  $\tilde{N}_{\text{excited}}(\mu, T) \rightarrow \infty$  as  $\mu \rightarrow 0^-$  there is always a finite negative  $\mu$  satisfying Eq. (6e.1) with small  $\tilde{n}_0$ , and then (consistently)  $\tilde{n}_0$  is not macroscopic, according to Eq. (6d.2) – no BEC.

## 6f: BEC for power-law density of states (continuum theory)

In all the cases we will be examining, the density of states varies as a power of  $\varepsilon$  so that

$$D(\varepsilon) = c\varepsilon^p \quad (6f.4)$$

(see Condensed Matter notes for some examples) and then

$$\begin{aligned}\int_0^\infty \frac{D(\varepsilon)d\varepsilon}{\exp(\beta[\varepsilon-\mu])-1} &= \int_0^\infty \frac{D(\varepsilon)d\varepsilon}{\xi^{-1}\exp(\beta\varepsilon)-1} = \int_0^\infty \frac{c\varepsilon^p d\varepsilon}{\xi^{-1}\exp(\beta\varepsilon)-1} \text{ [now set, } \beta\varepsilon = x\text{]} \\ &= \int_0^\infty \frac{c(\beta^{-1}x)^p d(\beta^{-1}x)}{\xi^{-1}\exp x-1} = c(k_B T)^{p+1} \int_0^\infty \frac{x^p dx}{\xi^{-1}\exp x-1}.\end{aligned}$$

where  $\xi = \exp(\beta\mu)$  is the fugacity, which will have to approach 1<sup>+</sup> (corresponding to  $\mu = 0$ ) in order to achieve Bose Condensation. We can then rewrite the continuum-theory condition (6e.4) for the BEC critical temperature as

$$c(k_B T_c)^{p+1} \int_0^\infty \frac{x^p dx}{\exp x-1} = \bar{N}$$

so that the critical temperature is given by

$$k_B T_c = \left( \frac{\bar{N}}{c G_p} \right)^{\frac{1}{p+1}} \quad (6f.5)$$

Here  $G_p$  is a pure number given in terms of standard special functions by

$$\begin{aligned}G_p &= \int_0^\infty \frac{x^p dx}{\exp x-1} = \int_0^\infty \frac{x^p e^{-x} dx}{1-e^{-x}} = \int_0^\infty dx x^p e^{-x} \sum_{n=0}^\infty e^{-nx} = \sum_{n=0}^\infty \int_0^\infty dx x^p e^{-(n+1)x} \\ &= \sum_{n=0}^\infty \int_0^\infty dx x^p e^{-(n+1)x} = \sum_{n=0}^\infty \frac{1}{(n+1)^{p+1}} \int_0^\infty dy y^p e^{-y} = \Gamma(p+1) \sum_{n=1}^\infty \frac{1}{n^{p+1}} \\ &= \Gamma(p+1) \zeta(p+1)\end{aligned}$$

Some sample values of  $G_p$  determined by Maple software are

$$\begin{aligned}G_{1/2} &= \int_0^\infty \frac{x^{1/2}}{\exp(x)-1} dx = \Gamma\left(\frac{3}{2}\right) \zeta\left(\frac{3}{2}\right) = 2.3151573_7 \\ G_1 &= \int_0^\infty \frac{x}{\exp(x)-1} dx = \frac{1}{6} \pi^2 = 1.64493406_7 \\ G_{3/2} &= \int_0^\infty \frac{x^{3/2}}{\exp(x)-1} dx = 1.7832931_9 \\ G_2 &= \int_0^\infty \frac{x^2}{\exp(x)-1} dx = 2.40411380_6\end{aligned}$$

Note that these cases all correspond to a convergent integral for  $\tilde{N}_{\text{excited}}(\mu=0, T)$  and hence to Bose condensation. On the other hand, **if  $D(E)$  goes as  $E^p$  with  $p \leq 0$ ,  $G_p$  is infinite (divergent) and we don't get BEC. (i.e. the transition temperature  $T_c$  is zero.)**

The details are a little different according to the method used to confine the Bose particles.

## 6g: BEC for Box confinement in continuum theory

We first look at the case of **Box confinement** in which the particles move to fill up a **fixed volume**  $V$ , and the particle number-density  $\rho = \tilde{N}/V$  can be controlled by adding particles. (Note that here we are eliding the distinction between mean number and fixed number, as alluded to earlier.)

For box confinement the density of states has been studied in previous physics courses (see e.g. Condensed Matter course or the books by Kittel or Ashcroft and Mermin). The density of states for box-confinement in  $d$  dimensions has the form

$$D(\varepsilon) = a_d L^d \varepsilon^p,$$

$$p = \begin{cases} 1/2, d = 3 \\ 0, d = 2 \\ -1/2, d = 1 \end{cases}$$

and  $a_d$  is a constant depending on the # of space dimensions  $d$

In particular  $a_3 = (4\pi^2)^{-1} (2m/\hbar^2)^{3/2}$  so that the density of states in 3D box confinement is

$$D(E) = \frac{V}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} E^{1/2} \quad (3D \text{ box}) \quad (6g.1)$$

Thus  $p = 1/2$  in our formulae gives the 3D Bose condensation temperature from Eq. (6f.5) as

$$k_B T_c = \left( \frac{N}{cG_{1/2}} \right)^{\frac{1}{1+1/2}} = \left[ \frac{1}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \right]^{-2/3} \left( \frac{N}{V} \right)^{2/3} \left( \frac{1}{2.315} \right)^{2/3} = \left( \frac{\hbar^2}{2m} \right) \left( \frac{4\pi^2}{2.315} \right)^{2/3} \rho^{2/3} \quad (6g.2)$$

Thus the BEC transition temperature gets higher as the density is raised, for box confinement. See also Ch. 7 of Kittel & Kroemer “Thermal Physics”.

**For 2D and 1D box confinement, the continuum model predicts No BEC: see problem sheet 2.**

### 6h: Semiclassical density of states for a particle confined by an external potential

Most of the modern experiments on BEC have the Bose-condensing particles confined in a *harmonic well* which is different from box-confinement in that the volume occupied by the particles grows as the temperature is raised: this is because the “walls are soft” for this type of confinement. In the continuum theory of BEC the analysis is straightforward but requires us to compute the Density of States for non-box confinement. See also V. Bagnato, D. E. Pritchard and D. Kleppner, Phys. Rev. A **35**,4354 (1987)

The density of states at energy  $E$  for confinement in **three dimensions** by a potential  $U(|\mathbf{r}|)$

The semiclassical (continuum) assumption is that the number of allowed quantum states corresponding to a region  $d^3\mathbf{r}$ ,  $d^3\mathbf{p}$  of classical phase space is (see Sec 4k of 2<sup>nd</sup> year Notes)

$$g(\mathbf{r}, \mathbf{p}) d^3\mathbf{r} d^3\mathbf{p} = \frac{1}{h^3} d^3\mathbf{r} d^3\mathbf{p}$$

i.e. the density of allowed states in classical phase space is  $h^{-3}$ .

Now the energy is  $E = p^2/(2m) + U(r)$ , where  $p=|\mathbf{p}|$  and  $r=|\mathbf{r}|$ . This means that (unlike the box confinement case), the maximum allowed  $p$ , for a given maximum  $E$ , depends on  $r$ . Specifically the maximum is  $p(r) \equiv (2m[E - U(r)])^{1/2}$ . Thus the number of allowed states with the particle, up to energy  $E$ , is an integral over phase space:

$$N(E) = \int_{V(E)} d^3\mathbf{r} \int_{p < p(r)} d^3\mathbf{p} h^{-3}$$

Here  $V(E)$  is the volume in real space for which  $U(r) < E$ , so that  $p(r)$  is real. Now the  $p$ -integral is simple to perform: it is just the volume (in  $p$ -space) of a sphere of radius  $p(r)$ :

$$\int_{p < p(r)} d^3\mathbf{p} h^{-3} = h^{-3} \frac{4\pi}{3} [p(r)]^3 = h^{-3} \frac{4\pi}{3} (2m[E - U(r)])^{3/2}$$

The total number of states with energy up to  $E$  is thus

$$N(E) = \int_{V(E)} h^{-3} \frac{4\pi}{3} (2m)^{3/2} (E - U(r))^{3/2} d^3\mathbf{r}$$



The density of states for 3D confinement is then

$$D(E) \equiv \frac{dN(E)}{dE} = \int_{V(E)} h^{-3} \frac{4\pi}{3} (2m)^{3/2} \frac{3}{2} (E - U(r))^{1/2} d^3\mathbf{r}$$

$$= \frac{2\pi}{h^3} (2m)^{3/2} \int_{V(E)} (E - U(r))^{1/2} d^3\mathbf{r} \quad (6h.1)$$

Note that we have neglected the boundary term that arises from the change in the limits of the integral as a function of  $E$  because at this boundary the integrand goes to zero anyway. Thus there is no contribution from this extra term.

**Exercise:** check that (6h.1) gives the box-confinement density of states for 3D when we set  $U(r) = 0$  and assume always the same volume – i.e.  $V(E) = V$ , independently of  $E$ .

The density of states at energy  $E$  for confinement in **two dimensions** by a potential  $U(r)$

Following the same style of derivation as in the 3D case, the number of states with the particle in an infinitesimal area  $d^2\mathbf{r}$  at position  $\mathbf{r}$ , and with energy up to  $E$ , and hence momentum up to  $p(r) = [2m(E - U(r))]^{1/2}$  is:

$$n = h^{-2} \pi [p(r)]^2 d^2\mathbf{r} \quad (\text{proportional to area of circle in } p \text{ space})$$

$$= h^{-2} \pi 2m(E - U(r)) d^2\mathbf{r} \quad \text{provided } E - U(r) > 0, \text{ and zero if } E - U(r) < 0.$$

Then the total number of states with energy up to  $E$  is

$$N(E) = h^{-2} \pi 2m \int_{A(E)} (E - U(r)) d^2\mathbf{r}$$

where  $A(E)$  is the area in 2D-space where  $E - U(r) > 0$ . Thus the density of states, again ignoring the boundary term from the same argument as above, is

$$D(E) = dN(E)/dE = h^{-2} \pi 2m \int_{A(E)} 1 d^2\mathbf{r} = h^{-2} 2\pi m A(E) \quad (6h.2)$$

### Example: a 2D harmonic potential

Here  $U(r) = \frac{1}{2} K r^2$  so  $A(E)$  is a circle with radius  $(2E/K)^{1/2}$ , having area  $\pi(2E/K)$ . Thus from (6h.2) the density of states is

$$D(E) = h^{-2} \pi 2m (2E/K) = bE, \quad \text{where } b = \text{a constant independent of } E.$$

Then the relevant integral for Bose condensation (see 6e.3) is

$$\int_0^{\frac{D(E)}{E}} \frac{D(E)}{E} dE = \int_0^{\frac{bE}{E}} \frac{bE}{E} dE \quad (\text{convergent})$$

Since this is convergent, a **2D harmonically confined gas can Bose-condense**. (In contrast to the 2D **box** confinement case above, where there is no BEC)

The density of states at energy  $E$  for confinement in **one dimension** by a potential  $U(r)$

The result is 
$$D(E) = (2h)^{-1} (2m)^{1/2} \int_{-U^{-1}(E)}^{U^{-1}(E)} (E - U(r))^{-1/2} dr \quad (6h.3)$$

**Exercise:** You will prove this on Sheet 2.

### Example: 1D harmonic potential.

By contrast with the 2D case, this theory predicts **no BEC in a harmonically confined 1D gas**: see **Sheet 2** and also V. Bagnato and D. Kleppner, Phys. Rev. A **44**, 7439 (1991).

Actual BEC experiments (discussed more below) do not necessarily operate in the limit of an effectively infinite number of particles. Rather, they use a large but finite number of particles. In this case the situation is more subtle and one does indeed see a rather rapid rise in the ground orbital occupation as the temperature is lowered below a critical value. Many people would regard this as BEC provided that the ground orbital occupation  $n_0$  is a significant fraction of the total particle number  $N$ , at a temperature  $T \gg \hbar\omega/k_B$  where classical Boltzmann (distinguishable-particle) physics would not give a large value of  $n_0$ . See W. Ketterle and N. J. van Druten, Phys. Rev. A **54**, 656 (1996).

## 6i: Bose Einstein condensation prior to atomic BECs.

For many years, until the mid-1990s, the examples cited for Bose Einstein Condensation were (a) Superfluidity of Liquid He4 and (b) superconductivity.

### (a) Liquid He4

Bose particle: neutral He<sup>4</sup> atom, a composite Boson consisting of 2 electrons, 2 protons and 2 neutrons.

Observed condensation temperature is:  $T_c = 2.19K$ . This is in approximate agreement with the above simple theory (6g.2), which gives 3.13K at the known density of liquid He.

Manifestations of the condensation:

- flow of fluid without resistance below a critical velocity (relative to the stirrer or the sides of the container).
- macroscopic tunneling of the fluid out of a beaker into the bottom of a lower outer container (manifestation of a macroscopic wavefunction).
- quantized vortices: persistent flow around a column of zero density, with velocity constrained by  $\oint_C m\mathbf{v} \cdot d\mathbf{r} = hn$ ,  $C$  is any path around a single vortex and  $n$  is an integer, the order of that vortex.

### (b) Superconductivity

Bose particle: a *Cooper pair* of two electrons bound by an attractive phonon-mediated effective force (at least for conventional “low- $T_C$ ” superconductors.)

The condensation temperature varies with the superconductor, but is below 30K for conventional superconductors.

Manifestations of the condensation:

- \* flow of current without resistance
- \* Meissner effect (complete exclusion of external magnetic fields)

The problem with the above examples is that the Bose particles in these cases are not even approximately independent; at the known particle separation, the forces between particles are quite strong (liquid He<sup>4</sup> is a *liquid*!). The interpretation of the condensation phenomena in terms of the theory for non-interacting particles given above is mainly wishful thinking. Good theories of liquid He4 and conventional (low- $T_C$ ) superconductors do now exist. (However, the theory of high- $T_C$  superconductors remains controversial.) These theories show that indeed the inter-particle forces are important, and many-body effects are not negligible. Thus the interpretation as simple Bose condensation of independent Bosons is doomed.

## 6j: Bose condensation of atomic gases

In the 1980s it became possible to cool and trap dilute gases of neutral atoms using lasers in conjunction with magnetic fields. In the 1990s the additional technique of *evaporative cooling* was developed. This finally made it possible to cool gases at relatively low densities (much less dense than air, in fact) below the BEC critical temperature. The low densities mean that the interatomic forces remain weak, and the simple theory of non-interacting bosons accurately predicts  $T_C$ . This temperature is typically very low – below a micro-Kelvin, and the temperatures achieved by this process are the lowest temperatures ever achieved in an earth laboratory, down to a few nanoKelvin!

The first Bosonic atom to be trapped and Bose condensed was  $^{87}\text{Rb}$ , a composite system containing an odd number of electrons and an odd number of nucleons, making a bound combination of an even number of Fermions as required for Bosonic behaviour. This was first achieved by the group of Eric Cornell at the University of Colorado (M. H. Anderson *et al.*, Science **198** (1995)). After cooling below 170 nK, the thermal de Broglie wavelength was comparable to the interparticle spacing (about  $10^{-4}\text{m}$ ), which was large enough for inter-atomic van der Waals forces to be considered weak.

Gaseous BEC has now been achieved in a great many atomic, and even some molecular, species. It has been studied in great detail experimentally, and sophisticated theories far beyond those presented here have been developed, including finite number effects, the dynamics of cooling and condensation itself, and the effects of interactions. On this last point, it is important to note is that although the simple BEC theory of non-interacting particles describes atomic BEC much better than it does liquid Helium, for example, it is necessary to include interactions to get right some pretty basic things like the shape of the macroscopic ground-state wavefunction. In a harmonic trap, atoms with a repulsive interactions condense into a ground-state wavefunction that is larger than the ground-state of non-interacting particles. (Hopefully it is obvious why.)

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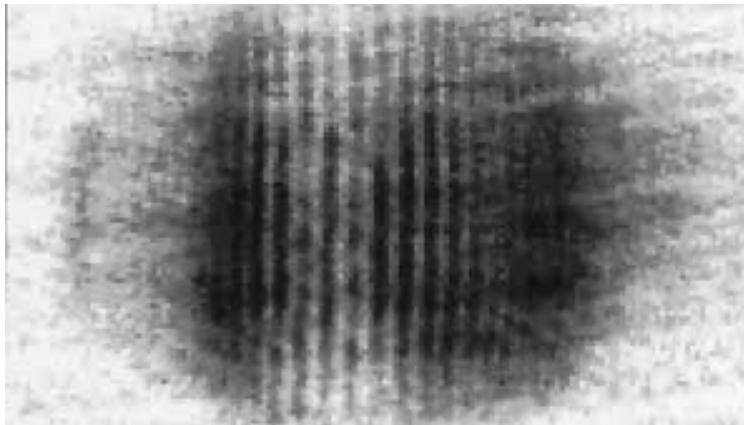
Aside: This ground-state is well described by the solution to the Gross-Pitaevskii equation (GPE): [[https://en.wikipedia.org/wiki/Gross-Pitaevskii\\_equation](https://en.wikipedia.org/wiki/Gross-Pitaevskii_equation)]

$$\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + V(\mathbf{r}) + \frac{4\pi\hbar^2 a_s}{m} |\psi(\mathbf{r})|^2 \right) \psi(\mathbf{r}) = \mu \psi(\mathbf{r}),$$

with the smallest value of  $\mu$ . Here  $\mu$  is the chemical potential (the energy per atom), which makes sense as this equation is just the time-independent Schrödinger's equation except for the term involving  $a_s$ . This parameter has the dimensions of length and is called the “scattering length”. It describes the interactions between atoms, and can be either positive (repulsive interactions) or negative (attractive interactions). The form of this term, however makes the GPE fundamentally different from Schrödinger's equation because it is nonlinear. (The linearity of Schrödinger evolution is one of the absolutely core features of QM). This is because the GPE is only an approximation. It is in fact a particular case of the Hartree-Fock approximation, which is a type of mean-field theory. Mean-field theories will be considered in Chapter 9.

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Gaseous BEC allows control and imaging of the macroscopic wavefunction to a fantastic degree. For example, it has enabled the demonstration of interference fringes, similar to that seen between two coherent optical sources (such as lasers), from two BECs, as shown opposite: [M. R. Andrews *et al.*, Science 275, 637-641 (1997).



### 6k: Bosons without number conservation

The analysis of Bose condensation given above used the grand ensemble, and assumed that the expected number of particles  $\tilde{N}$  was fixed (“number conservation”). There are, however, many entities commonly regarded as particles, whose number is not conserved. These zero-mass bosons are the “fake Bosons” such as photons and phonons. These entities should be regarded as quanta of energy of an excitation mode of some underlying physical system, and they are Bosons in the sense that any number of these quanta of excitation energy can be found in one mode. (Actually, this last statement is also only an approximation – if a mode has too much energy then nonlinear dynamics may come into play, and the energy levels in the mode will cease to be evenly spaced, even approximately. But this is really no different from the fact that “real” bosons can interact too, which changes the energy eigenstates depending on how many there are, as described by the GPE in the Aside above.)

**Example: Phonons.** These are quantised excitations of the vibrational modes of a crystal lattice, each lattice mode being effectively a separate mechanical oscillator. A given mode labelled by wavenumber  $\mathbf{k}$  and polarisation  $\lambda$  (a discrete index) can have any number  $n(\mathbf{k},\lambda)$  of phonons, with energy  $(n(\mathbf{k},\lambda) + \frac{1}{2})\hbar\omega(\mathbf{k},\lambda)$ . Although energy must be conserved overall, this does not mean that the number of phonons is conserved. For example one phonon in a mode of frequency  $2\omega$  can be replaced by 2 phonons in a mode of frequency  $\omega$ , with conservation of energy.

Consider first the simplest case of a single one-dimensional harmonic oscillator. The Hamiltonian is  $H = \frac{p^2}{2m} + \frac{1}{2}Kx^2$

Classically,  $E = \frac{1}{2}kT + \frac{1}{2}kT = kT$  (equipartition)

Quantally, levels have energy  $(n + \frac{1}{2})\hbar\omega$ .

Partition function:  $Z = \sum_{n=0}^{\infty} e^{-\beta(n+\frac{1}{2})\hbar\omega} = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}$

Energy :  $E = -\frac{\partial}{\partial\beta} \ln Z = \hbar\omega \left( \frac{1}{2} + \bar{n} \right) = \frac{1}{2}\hbar\omega \coth \frac{\beta\hbar\omega}{2}$  where  $\bar{n} = \frac{1}{e^{\beta\hbar\omega}-1}$

Specific heat (see chapter 7):

$$C_v = \frac{\partial}{\partial T} \frac{1}{2} \hbar \omega \coth \frac{\beta \hbar \omega}{2} = k \left( \frac{\hbar \omega}{kT} \right)^2 \frac{e^{\hbar \omega / kT}}{(e^{\hbar \omega / kT} - 1)^2}$$

(a) High  $T$ ,  $C_v \approx k_B$   $\therefore$  as for classical case.

(b) Low  $T$ ,  $C_v \sim k \left( \frac{\hbar \omega}{kT} \right)^2 e^{-\hbar \omega / kT} \rightarrow 0$  very fast as  $T \rightarrow 0$ .

This model, applied to a single ion in a crystal, assumed to vibrate independently of the others, was a triumph for quantum theory in that it explained qualitatively the vanishing specific heat of crystals as  $T \rightarrow 0$ . (Einstein model). See Reif "FSTP" p. 252 or 2<sup>nd</sup> year Notes.

Note on interpretation. The average energy was

$$E = \left( \bar{n} + \frac{1}{2} \right) \hbar \omega, \quad \bar{n} = \frac{1}{e^{\beta \hbar \omega} - 1}$$

This looks like a Bose-Einstein distribution with  $\mu=0$ . We can say when the oscillator is in  $n^{\text{th}}$  quantum state it contains  $n$  quanta, each of energy  $\hbar \omega$ . Regarded as particles, these quanta are bosons in that: (i) they're indistinguishable; (ii) any number can be in same "state" of energy  $\hbar \omega$ . (3) their expected number goes as a Bose distribution with  $\mu = 0$ .

However, these Bosons differ from material Bosons (like  $\text{He}^4$  atoms) in that their number is not conserved. So there's no corresponding Lagrange multiplier ( $\Rightarrow \mu=0$ ). Also there is no Bose condensation here. As you take the temperature down to zero, all the physical systems go to their groundstate, i.e. to a state with no Boson excitations. The Bosons simply go away as  $T$  goes to 0, rather than there being a large number in one particular mode (the lowest frequency one).

**Example: Photons in a box.** From purely classical E&M Theory,  $E$  and  $B$  fields in a conducting box are linear combinations of discrete modes

$$\mathbf{E}_{jkl}^\lambda(\mathbf{r}) e^{i\omega_{jkl}t}, \quad \mathbf{B}_{jkl}^\lambda(\mathbf{r}) e^{i\omega_{jkl}t}$$

where  $jkl$  define the wave-vector and  $p$  the polarization. In a box normalization, these modes vary sinusoidally with  $\mathbf{r}$ , and only discrete wavelengths and frequencies are allowed. This is of course quantization of a sort, and arises mathematically from imposing boundary conditions, same reason an electron wavefunction gets quantized. So although there is no quantum mechanics here, mode counting is basically same as for electrons in box.

Classically the energy is  $U = \int d^3\mathbf{r} \left( \frac{\epsilon |\mathbf{E}|^2}{2} + \frac{|\mathbf{B}|^2}{2\mu} \right)$  and this can take any value, as the amplitudes  $E$  and  $B$  can take any value. In quantum mechanics, however the energy is quantized in such a way that each mode can only have energy  $\hbar \omega_{jkl} (n_{jkl} + 1/2)$ , where  $n_{jkl}$  is an integer. [Primitive QED: Planck's hypothesis].

So each mode ( $jkl$ ) behaves like a separate harmonic oscillator. The quanta of energy of these oscillators are photons. The modes ( $jkl$ ) are separate entities, something like "single-particle levels" that energy can be distributed among. We should not say "that photons can be distributed among" because there is no conservation law for photons.

By previous work for the harmonic oscillator, the average # of photons in the  $jkl$  mode is

$$\bar{n}_{jkl} = \frac{1}{e^{\beta \hbar \omega_{jkl}} - 1}, \quad \bar{U}_{jkl} = \hbar \omega_{jkl} \left( \bar{n}_{jkl} + \frac{1}{2} \right)$$

So the photons are bosons (with  $\mu=0$  corresponding to the fact that their number isn't conserved). *Dropping the unimportant  $+1/2$  in the photon energy term*, the total energy in some small region  $d\omega$  of frequencies is thus

$$D(\omega) \hbar \omega \frac{1}{e^{\beta \hbar \omega} - 1} d\omega$$

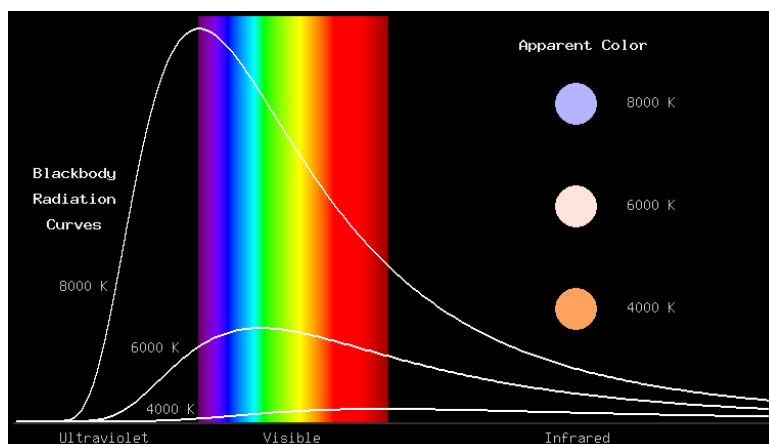
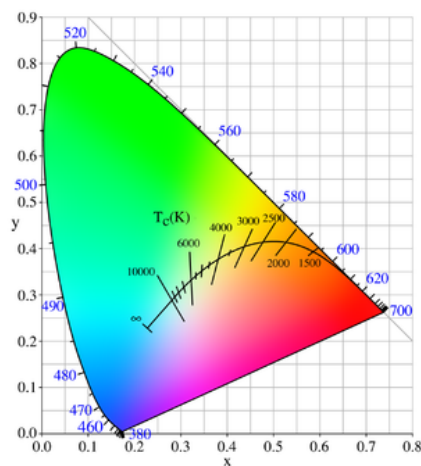
where  $D(\omega)$  is the density of states such that the number of modes in the range  $[\omega, \omega+d\omega]$  is  $D(\omega)d\omega$ . It is not difficult to show [see e.g. 4<sup>th</sup> year QED notes chapter 5] that

$$D(\omega)d\omega = \frac{V}{\pi^2} \frac{\omega^2}{c^3} d\omega$$

Note: this includes the two polarisations. Thus the total (photon energy/volume/unit frequency) at  $\omega$  is

$$P(\omega, T) = \frac{\hbar \omega^3}{\pi^2 c^3} \frac{1}{e^{\beta \hbar \omega} - 1} \text{ Planck distribution for "black-body radiation"}$$

This function has its maximum at  $\hbar \omega \approx 2.9 kT$ , so the colour of the black-body radiation changes towards the blue as the temperature is raised.



Left: [https://en.wikipedia.org/wiki/Black-body\\_radiation](https://en.wikipedia.org/wiki/Black-body_radiation)

Right: Dr. Bob's stuff, <http://scisyn.com/umuc/astro/ASTR100Notes/black-body.html>

**Exercise:** Show that the total (i.e. integrated over  $\omega$ ) photon energy at temp  $T$ , is  $\propto T^4$  (Stefan-Boltzmann Law).