Lecture 24 - Density of states

What's Important:
- density of states in phase space

Text: Reif

Counting quantum states

Some time back, we said that we needed to introduce a "density of states" factor in order to convert a sum over discrete states into an integral over continuum states:

$$\Sigma_r \exp(-\beta\varepsilon_r) \rightarrow \int d^3q\, d^3p \exp(-\beta\varepsilon).$$

Similarly, we have now evaluated the number distributions for photons, BE and FD systems, as a function of ε_r and N. But what is N for a box of photons?

We now address these issues with a digression into quantum mechanics. The "old" quantum theory will be used, based upon de Broglie's idea that a particle has wave characteristics by virtue of its momentum:

$\lambda = h / p$ (verified by neutron scattering)

Suppose that we place a number of particles with their associated waves in a cubic box with perfectly reflecting walls. If there are interactions among the particles, then we have to solve for a coupled set of dynamical equations for all N particles at once. If the particles are non-interacting, then we just need to find the behavior of a single as it samples phase space. The behavior of the whole system is just a sum over the single particle properties.

The motion of the particle in each direction is independent. Consider what happens with the de Broglie wavelength in a given direction under the usual quantization condition

The general relation between the wavelength λ and the box size L is

$\lambda = 2L / n$ $n = 1, 2, 3, ...$

where n is called the quantum number of the state. This means that the allowed values of the particle's momentum p are:

$$p = h / \lambda = h / [2L / n] = nh / 2L.$$

Because the directions are orthogonal, the solutions add independently in three dimensions. The corresponding kinetic energy is then

$$E = p^2 / 2m = (h^2 / 8mL^2)\,(n_x^2 + n_y^2 + n_z^2) \qquad n_i = 1, 2, 3, ...$$

Now, as we have set up this problem, each n runs from 1 to ∞: clearly, $n = 0$ is not a wave ($\lambda = \infty$) and $n < 0$ makes no sense in our context.

To find the number of states within a given phase space volume, we examine the behavior of E. Let's fix the energy to have a maximal value E_{max} (like the Fermi energy, for example). Corresponding to E_{max} there is a maximal momentum p_{max} given by

$$E_{max} = p_{max}^2 / 2m.$$

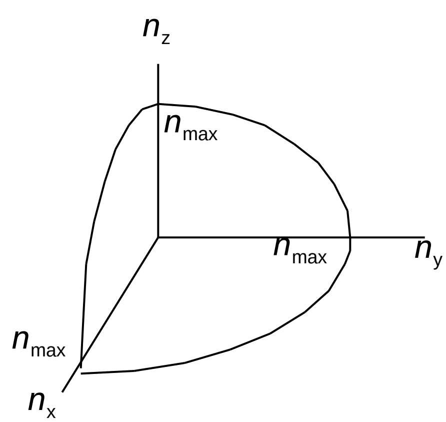
The maximal value of n is then

$$n_{max} = 2Lp_{max} / h.$$

The allowed states of the system correspond to any combination of n_x, n_y, or n_z which satisfies

$$n_x^2 + n_y^2 + n_z^2 \leq n_{max}^2 \qquad (\text{so } E \leq E_{max}),$$

as a consequence of which no individual n_x, n_y, or n_z is greater than n_{max}.



Each value of (n_x, n_y, n_z) inside the box corresponds to one unique state. Thus, the number of states N with $E \leq E_{max}$ is just the volume of the octant with positive n_i, or

$$N(E \leq E_{max}) = \frac{1}{8} \cdot \frac{4\pi}{3} n_{max}^3$$

where the factor of 1/8 arises from the volume of the octant. We can work backwards from n's to physical quantities as follows

$$N = \frac{1}{8} \cdot \frac{4\pi}{3} n_{max}^3 = \frac{1}{8} \cdot \frac{4\pi}{3} \left(\frac{2Lp_{max}}{h} \right)^3$$

$$= \left(\frac{2^3 L^3}{8} \right) \left(\frac{4\pi}{3} p_{max}^3 \right) \frac{1}{h^3}$$

The first piece on the right-hand side is the volume of physical space, and the second is the volume of momentum space. Thus, the density of states must be

$$density = \frac{N}{L^3(4\pi p_{max}^3/3)} = \frac{1}{h^3}$$

Knowing the density of states in phase space, we can replace the sum over discrete states by an integral over continuum states

$$\sum_q \sum_p \to \frac{1}{h^3}\int d^3q\, d^3p$$

Now, if the particles are non-interacting, then $\int d^3q = V$, the volume, and we can write

$$d^3n \to \frac{V}{h^3} d^3p$$

Note: Reif performs this calculation differently by imposing periodic boundary conditions on the wavefunctions for plane waves. The final result is the same, although the intermediate steps are different.