Density of States

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0.1 Density of States

It is often useful to know the density of states (DOS) as function of energy. To begin, how is the DOS defined?

First, we define $N(\epsilon)$ as the total number of states with energy less than or equal to ϵ. Then, the density of states is,

$$D(\epsilon) = \frac{\mathrm{d}N}{\mathrm{d}\epsilon} \tag{0.1}$$

In other words,

$$N(\epsilon) = \int_0^{\epsilon} D(\epsilon')\,\mathrm{d}\epsilon' \tag{0.2}$$

0.2 Particle in a Box

The energy eigenstates of a particle in a cubical box of length L with no potential ($V = 0$) are,

$$\psi(x, y, z) = \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L} z\right) \tag{0.3}$$

where,

$$\epsilon = \frac{\pi^2 \hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2); \quad n_x, n_y, n_z \in \mathbb{N} \tag{0.4}$$

The states are equal spaced in three-dimensions in “n-space,” but how do we relate this to energy? If we define the variable,

$$n = \sqrt{n_x^2 + n_y^2 + n_z^2} \tag{0.5}$$

then,

$$\epsilon = \frac{\pi^2 \hbar^2}{2mL^2} n^2 \tag{0.6}$$

Now, we must find $N(n)$. Notice that the contour of n is a sphere in “n-space.” However, $n_x, n_y, n_z > 0$, so $N(n)$ must be the volume of a octant of radius n.

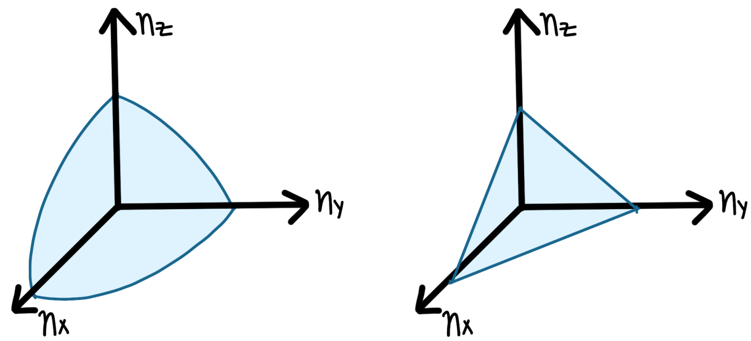

Figure 1: (a) contour for $n = \sqrt{n_x^2 + n_y^2 + n_z^2}$, (b) contour for $n = n_x + n_y + n_z$

Therefore, the number of states up to n is given by,

$$N(n) = \frac{1}{8}\left(\frac{4}{3}\pi n^3\right) = \frac{\pi}{6}n^3 \tag{0.7}$$

The density of states as a function of n,

$$D(n) = \frac{\mathrm{d}N}{\mathrm{d}n} = \frac{\pi}{2}n^2 \tag{0.8}$$

Finally,

$$D(n)\,\mathrm{d}n = D(\epsilon)\,\mathrm{d}\epsilon \tag{0.9}$$

$$D(\epsilon) = D(n)\left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right) = \left(\frac{\pi}{2}n^2\right)\left(\frac{mL^2}{\pi^2\hbar^2 n}\right) = \frac{mL^2}{2\pi\hbar^2}n \tag{0.10}$$

Where n is a function of ϵ,

$$D(\epsilon) = \frac{mL^2}{2\pi\hbar^2}\sqrt{\frac{2mL^2\epsilon}{\pi^2\hbar^2}} \tag{0.11}$$

$$\boxed{D(\epsilon) = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2}} \tag{0.12}$$

This method generalizes to 1 and 2-dimensions.

0.3 Harmonic Oscillator

Suppose now that we are trying to find the DOS of a harmonic oscillator with energy (ignoring the zero-point energy),

$$\epsilon = (n_x + n_y + n_z)\hbar\omega \tag{0.13}$$

Now, the energy is no longer a function of n as we have defined it in the previous section (eq. 0.5). We must now define n to be,

$$n = n_x + n_y + n_z \tag{0.14}$$

$$\epsilon = n\hbar\omega \tag{0.15}$$

Again, we can find $N(n)$; but now, notice that the contour of n is no longer a sphere, but a plane (Fig. 1). Thus,

$$N(n) = \frac{1}{3}A \cdot h = \frac{1}{3}\left(\frac{1}{2}n^2\right) \cdot n = \frac{n^3}{6} \tag{0.16}$$

As before, we can manipulate this into the DOS in energy,

$$D(n) = \frac{\mathrm{d}N}{\mathrm{d}n} = \frac{n^2}{2} \tag{0.17}$$

$$D(\epsilon) = D(n)\left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right) = \left(\frac{n^2}{2}\right)\left(\frac{1}{\hbar\omega}\right) \tag{0.18}$$

$$\boxed{D(\epsilon) = \frac{\epsilon^2}{2(\hbar\omega)^3}} \tag{0.19}$$