Density of States for a Particle in a Box—C.E. Mungan, Spring 2002

Derive the density of states $g(E)$ for a particle in an M-dimensional box. A one-dimensional box is a string of length L. The standing-wave condition is $n\lambda / 2 = L$ for the n-th mode (i.e., $n = 1$ for the fundamental, $n = 2$ for the second harmonic, and so on). But the de Broglie relation gives the momentum, $p = h / !$. For a three-dimensional box of volume L^3, the momentum components thus become $p_x = n_1 h / 2L$, $p_y = n_2 h / 2L$, and $p_z = n_3 h / 2L$ where (n_1, n_2, n_3) is a triplet of positive integers. Thus the energy, which is purely kinetic, is $E = p^2 / 2m = (n_1^2 + n_2^2 + n_3^2) h^2 / 8mL^2$ for nonrelativistic particles. In M dimensions, we generalize this to

$$E = \frac{h^2}{8mL^2} \sum_{i=1}^{M} n_i^2 \tag{1}$$

where there is one mode for each set of values $(n_1, n_2, \ldots, n_M)$ or, in other words, one mode in each M-dimensional hypercube of unit volume. Now let us renumber the modes in order of increasing energy by the single label n, where $n^2 \equiv \sum n_i^2$. [Note that some modes will in general be degenerate. For example, modes (1,0,0) and (0,1,0) and (0,0,1) have the same energy and are all labeled with $n = 1$.] We therefore rewrite Eq. (1) as

$$E = \frac{h^2}{8mL^2} n^2 . \tag{2}$$

Consider the set of N modes which have energy less than or equal to the energy of mode n. For example, in three dimensions these modes fill the positive octant of a sphere of radius n. Generalizing to M dimensions, these modes occupy the positive part of a hypersphere of radius n. The volume of an M-dimensional hypersphere equals $\upsilon_M n^M$, where υ_M is a geometrical constant (eg. $\upsilon_3 = 4\pi / 3$). The value of this constant is calculated in the document http://usna.edu/Users/physics/mungan/_files/documents/Scholarship/HypersphereVolume.pdf. To get just the positive part of the hypersphere, divide by 2^M (eg. one-quarter of a circle is in the positive quadrant). Therefore

$$N = \upsilon_M \left(\frac{n}{2} \right)^M \quad \Rightarrow \quad dN = \frac{M}{2^M} \upsilon_M n^{M-2} n dn , \tag{3}$$

where dN is the number of modes having energy between E and $E + dE$. Differentiating Eq. (2) gives

$$dE = \frac{h^2}{8mL^2} 2n dn . \tag{4}$$

Solve Eq. (2) for n and substitute it into n^{M-2} in Eq. (3). Also solve Eq. (4) for ndn and substitute it into Eq. (3). The result gives the density of states,

$$g(E) \equiv \frac{dN}{dE} = \frac{M\upsilon_M}{2}(2m)^{M/2}\frac{V_M}{h^M}E^{(M-2)/2} \tag{5}$$

where $V_M \equiv L^M$ is the volume of an M-dimensional hypercube (eg.$V_1 = L$ is the length, $V_2 = A$ is the area, and $V_3 = V$ is the volume of the box). Here is a table of the first few values.

M	$g(E)$
1	$\frac{\sqrt{2m}L}{h} \cdot \frac{1}{\sqrt{E}}$
2	$\frac{2\pi mA}{h^2}$
3	$\frac{2\pi(2m)^{3/2}V}{h^3}\sqrt{E}$

Notice that for a 1D box, the spacing between levels increases as you go up in energy, in accord with Tipler Fig. 27.2. On the other hand, for a 3D box the levels get closer together as you go up in energy; the above result agrees with Tipler Eq. (27.28). The significance of these values is that at absolute zero, the average energy of a set of fermions will be less than half of the Fermi energy in 1D, equal to the Fermi energy in 2D, and greater than the Fermi energy for $M \geq 3$.