Density of States

In our earlier article "Infinite potential well," we calculated possible values of momentum of a particle in a box. In this article, we will obtain a formula for the number of possible states, given the range of momentum.

First, we will consider 2 dimensional case, then generalize it to 3 dimensional ones. Remember that we had following formulas:

$$p_x = \frac{n_x h}{2L}, \qquad p_y = \frac{n_x h}{2L} \tag{1}$$

where n_x and n_ys are positive integers.

Then, how many states are there between $p_{x0} < p_x < p_{x0} + \Delta p_x$ and $p_{y0} < p_y < p_{y0} + \Delta p_y$? To this end, we have to consider (1). We can re-express this formula as:

$$n_x = \frac{2p_x L}{h}, \qquad n_x = \frac{2p_x L}{h} \tag{2}$$

Then, we can say that we want to know how many states there are between $n_{x0} < n_x < n_{x0} + \Delta n_x$ and $n_{y0} < n_y < n_{y0} + \Delta n_y$. However, as n_x and n_ys are positive integers, the total number of state is given by $\Delta n_x \Delta n_y$ if Δn_x and Δn_y are sufficiently big compared to 1. See, Fig.1. The number of possible states are denoted by dots. Their spacings are 1 as they are positive integers. You also see that there are 30 states, which agree with $\Delta n_x = 5$ and $\Delta n_y = 6$

Given this, how many states are there for the total momentum (i.e. $\sqrt{p_x^2 + p_y^2}$) between p and $p + dp$? First, we translate this into ns as follows using (2):

$$n = \frac{2pL}{h}, \qquad dn = \frac{2Ldp}{h} \tag{3}$$

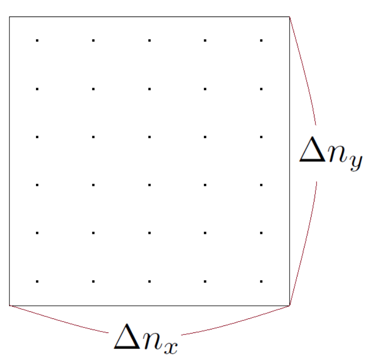

Figure 1: $\Delta n_x \Delta n_y = 5 \times 6 = 30$ states

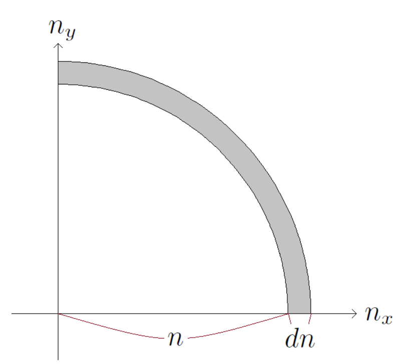

Figure 2: $(\pi n/2)dn$ states

We also have:

$$n^2 < n_x^2 + n_y^2 < (n + dn)^2 \tag{4}$$

This is drawn on Fig.2. Remembering our earlier argument explained no Fig.1, we conclude that the shaded area in Fig.2 gives the number of states. Interpreting it as a "bent rectangle" with width $(\pi n/2)$ (i.e. the length of the arc) and height dn, the number of states is given as follows:

$$\frac{\pi n}{2} dn \tag{5}$$

This is true for very small dn. Plugging (3), we conclude that between p and $p + dp$, there are

$$\frac{2\pi L^2}{h^2} p dp \tag{6}$$

states.

We can repeat this process for 3 dimensional case as well. The number of states is then given by $\Delta n_x \Delta n_y \Delta n_z$ and between n and $n + dn$, there are

$$\frac{4\pi n^2}{8} dn \tag{7}$$

since the surface area of sphere is $4\pi n^2$ and n_x, n_y, n_zs being positive implies we are considering one-eighth of the sphere, and we can consider the concerned region as a "bent rectangular box" with base $(4\pi n^2)/8$ and height dn.

Using (3), we conclude, between momentum p and $p + dp$, there are

$$\frac{(4\pi p^2 dp)}{h^3} L^3 \tag{8}$$

number of states. Using the fact that the volume of the box V is given by L^3, we can re-express the above formula as

$$\frac{(4\pi p^2 dp)}{h^3} V \tag{9}$$

We have derived this formula assuming that the particle is in a box with the shape a cube, but it is worth remarking that the above formula is valid for any shape of box. Actually, there is a still better way to express the above formula. Expressing $4\pi p^2 dp = d^3 p$, which is the familiar volume element for p (Here, we release the previous condition that p_x, p_y, p_z must be positive. They are now allowed to be negative.[1]) and $V = \int d^3 x$, (9) can be re-expressed as

$$\frac{d^3 p \, d^3 x}{h^3} = \left(\frac{dp_x dx}{h}\right)\left(\frac{dp_y dy}{h}\right)\left(\frac{dp_z dz}{h}\right) \tag{10}$$

In conclusion, the small cell $\Delta p_x \Delta x = \Delta p_y \Delta y = \Delta p_z \Delta z = h$ is one unit.

Summary

- The density of state is given by $\dfrac{d^3 p \, d^3 x}{h^3}$.

[1] If you think carefully, p_x and p_y in (1) are just the absolute values of real p_x and p_y. We set n_x and n_y to be positive.