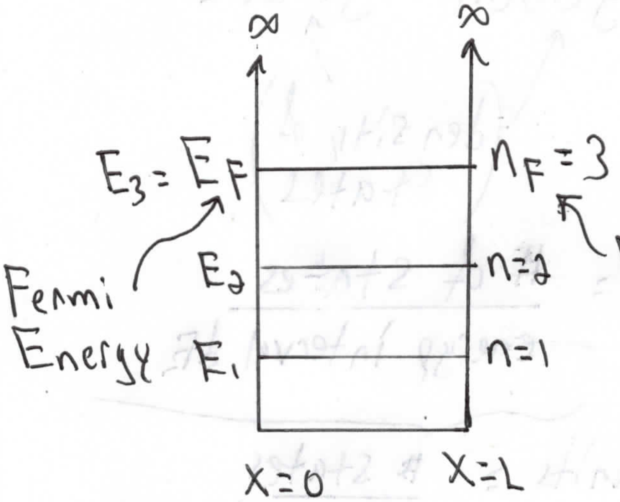
Density of States

Particle in a Box (infinite square well)



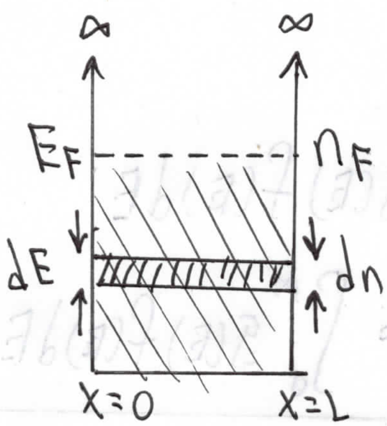
Discrete Case

There are

$N = 3 \times 2 = 6$ states

(energy levels) (2 spins each)

Note: $E_n = \left(\frac{\hbar^2 \pi^2}{2 m L^2}\right) n^2 \Longrightarrow$ as $L \to \infty$, $\underbrace{\Delta E_n \to 0}_{\text{density of states increases as } L \text{ increases}}$



Continuous case

for Solids, we have Avagadro's # of energy levels

$N_A \sim 10^{23}$ levels

How many states are in the interval dn or dE?

To answer this, let's define a density of states

Discrete: Number of states $= N = \sum_{n=1}^{3} dn = \underbrace{2+2+2 = 6}_{\text{example above}}$

Krane's notation $\rightarrow$ (degeneracy of each state n)

Continuous:

$$dN = \begin{pmatrix}\text{Number of states} \\ \text{in interval } dn \text{ or } dE\end{pmatrix} = g(n)\,dn = g(E)\,dE$$

(density of states)

$$g(n) = \frac{\#\text{ of states}}{\text{unit interval } dn} \qquad g(E) = \frac{\#\text{ of states}}{\text{energy interval } dE}$$

units = # of states   units = $\frac{\#\text{ states}}{\text{Joules (Energy)}}$

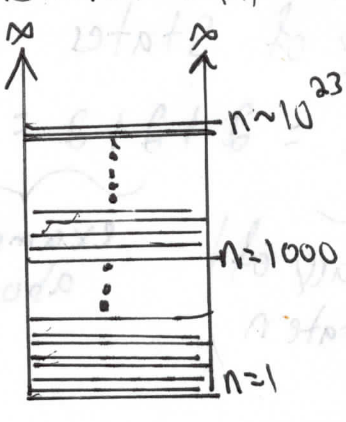
There is a probability $f(E)$ that a state may be occupied

Discrete: $N = \sum_n dn\, f(E_n)$

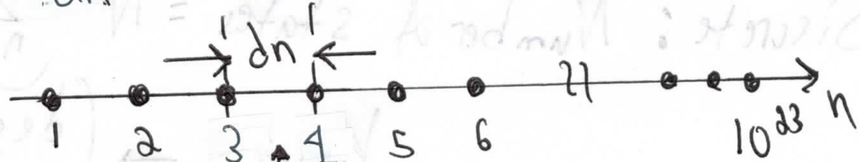
Continuous: $dN = g(n)f(n)\,dn = g(E)f(E)\,dE$

$$N = \int_0^\infty g(n)f(n)\,dn = \int_0^\infty g(E)f(E)\,dE$$

1-Dimensional Example! Infinite square well in 1-dimension



We can plot all n states along an n-axis



notice, there is only 1 state in interval dn

What is the density of states $g(E)$?

$$g(E)\,dE = g(n)\,dn$$

$$g(n) = \frac{1 \text{ state}}{\text{interval } dn} \times \underset{\uparrow}{2} = 2$$

degeneracy factor for spin up & down states

Then, $g(E) = g(n)\dfrac{dn}{dE} = 2\dfrac{dn}{dE}$

For an infinite square well, $E_n = \left(\dfrac{\hbar^2\pi^2}{2mL^2}\right)n^2 = E_1 n^2$

Then, $dE = d\left(E_1 n^2\right) = 2E_1 n\,dn$

$$\Rightarrow \frac{dn}{dE} = \frac{1}{2E_1 n}$$

$$E = E_1 n^2 \Rightarrow n = \sqrt{\frac{E}{E_1}}$$

Then, $\dfrac{dn}{dE} = \dfrac{1}{2E_1 n} = \dfrac{1}{2E_1}\sqrt{\dfrac{E_1}{E}} = \dfrac{1}{2\sqrt{E_1 E}}$

This gives: $g(E) = 2\dfrac{dn}{dE} = \dfrac{1}{\sqrt{E_1 E}} = \left(\dfrac{L\sqrt{2m}}{\hbar\pi}\right)\dfrac{1}{\sqrt{E}}$

$$\left(\begin{array}{c}\#\text{ of states}\\ \text{in interval } dE\end{array}\right) = dN = g(E)f(E)\,dE$$

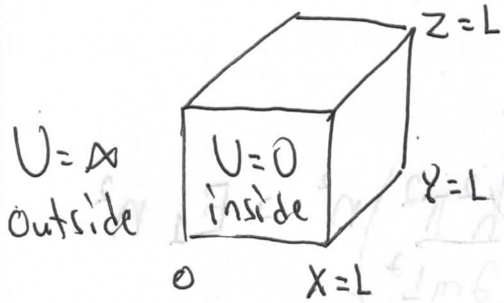
$$= \left(\frac{L\sqrt{2m}}{\hbar\pi}\right)\frac{1}{\sqrt{E}}f(E)\,dE \quad \Big\}\ \text{1-dimension}$$

Since $g(E) \to \infty$ as $L \to \infty$, textbooks like to define a density of states per unit Length

$$g_L(E) = \frac{g(E)}{L} = \left(\frac{\sqrt{2m}}{\hbar\pi}\right)\frac{1}{\sqrt{E}}\, f(E)\, dE$$

3-dimensional Example: Particle in a Box

$U = 0$ inside, $U = \infty$ outside box

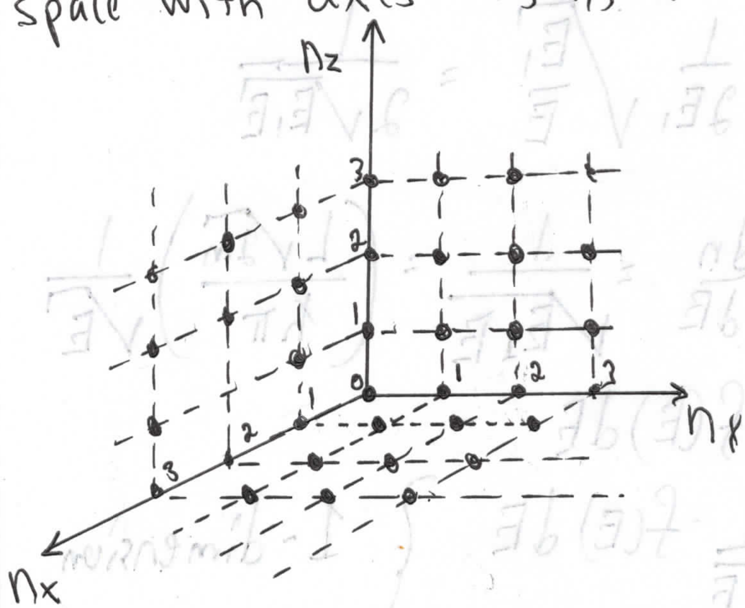


$U=\infty$ outside } Particle in a box

The allowed energies are similar to that for a 1-dimensional problem:

$$E_{n_x n_y n_z} = \left(\frac{\hbar^2\pi^2}{2mL^2}\right)\left(n_x^2 + n_y^2 + n_z^2\right)$$

Each state can be defined as a point in 3-dimensional space with axes n_x, n_y, n_z

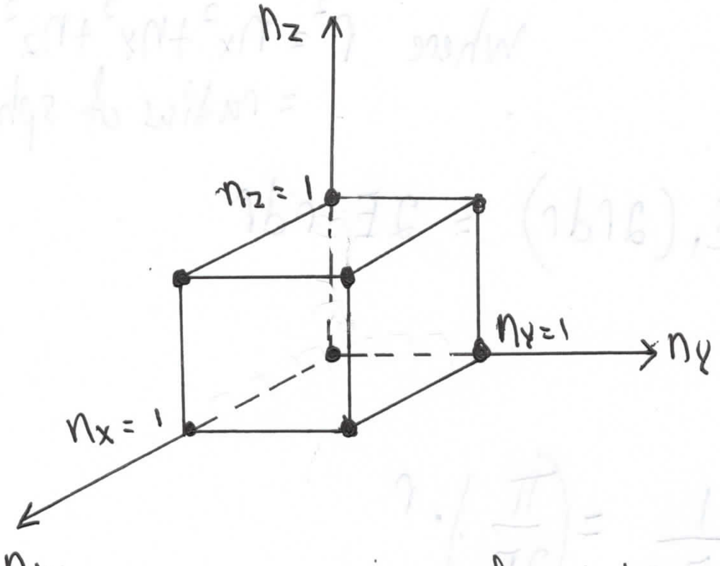


Only positive values of n_x, n_y, n_z are allowed:

$n_x \geq 0,\ n_y \geq 0,\ n_z \geq 0$

Thus, only the 1st quadrant in space is filled with allowed states.

Let's examine the states where $n_x = 1, 0$, $n_y = 1, 0$, $n_z = 1, 0$



Note that there is only 1 state in this cube (the corners are shared by 8 other cubes)

Thus, $g(n) = \dfrac{\#\text{ of states}}{\text{unit volume } dn_x\, dn_y\, dn_z} = 1 \text{ state} \times 2 = 2$ (spin up & down states)

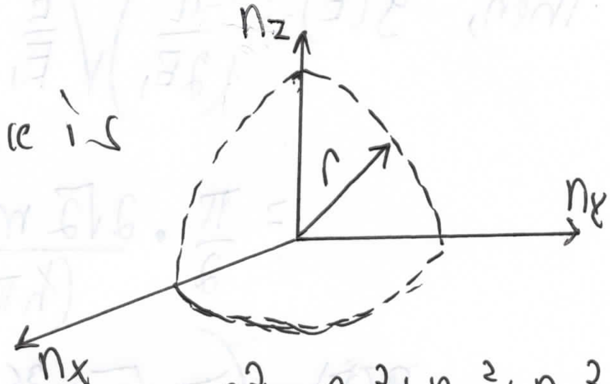
$$g(E)\,dE = g(n)\,\underbrace{dV_n}_{\text{Volume in } n\text{-space}} = 2 \cdot dn_x\, dn_y\, dn_z$$

A spherical volume in n-space is

$$V_n = \frac{4}{3}\pi r^3$$

$$dV_n = d\left(\frac{4}{3}\pi r^3\right) = \frac{4}{3}\pi\left(3r^2 dr\right)$$

$$dV_n = 4\pi r^2 dr$$



$r^2 = n_x^2 + n_y^2 + n_z^2$

r = radius of a sphere

$$\Rightarrow g(E)\,dE = 2 \cdot \left(4\pi r^2 dr\right) \cdot \frac{1}{8}$$

n_x, n_y, n_z only allowed in 1^{st} quadrant of sphere = $\frac{1}{8}$th of the volume of the sphere

$$g(E)\,dE = \pi r^2 dr$$

$$\Rightarrow g(E) = \pi r^2 \frac{dr}{dE}$$

n_x, n_y, n_z must not be negative

Since $E = \underbrace{\left(\frac{\hbar^2\pi^2}{2mL^2}\right)}_{E_1}(n_x^2+n_y^2+n_z^2) = E_1 r^2$

where $r^2 = n_x^2+n_y^2+n_z^2$
= radius of sphere

$$dE = d(E_1 r^2) = E_1(2r\,dr) = 2E_1 r\,dr$$

$$\Rightarrow \frac{dr}{dE} = \frac{1}{2E_1 r}$$

$$\Rightarrow g(E) = \pi r^2 \frac{dr}{dE} = \pi r^2 \cdot \frac{1}{2E_1 r} = \left(\frac{\pi}{2E_1}\right)\cdot r$$

But, $E = E_1 r^2 \Rightarrow r = \sqrt{\frac{E}{E_1}}$

Then, $g(E) = \left(\frac{\pi}{2E_1}\right)\sqrt{\frac{E}{E_1}} = \left(\frac{\pi}{2E_1^{3/2}}\right)\sqrt{E} = \frac{\pi}{2}\left(\frac{2mL^2}{\hbar^2\pi^2}\right)^{3/2}\sqrt{E}$

$$= \frac{\pi}{2}\cdot\frac{2\sqrt{2}\,m^{3/2}L^3}{(\hbar\pi)^3}\cdot\sqrt{E}$$

$$g(E) = \left(\frac{\pi\sqrt{2}\,m^{3/2}V}{(\hbar\pi)^3}\right)\sqrt{E}$$

where $V = L^3$ = volume in x,y,z-space

$\left(\begin{matrix}\text{\# of states}\\ \text{in interval } dE\end{matrix}\right) = dN = g(E)f(E)dE$

$$= \left(\frac{\pi\sqrt{2}\,m^{3/2}V}{(\hbar\pi)^3}\right)\sqrt{E}\,f(E)\,dE \Big\}\ \text{3-dimensions}$$

$\left(\begin{matrix}\text{density of states}\\ \text{per unit volume}\end{matrix}\right) = g_V(E) = \left(\frac{\pi\sqrt{2}\,m^{3/2}}{(\hbar\pi)^3}\right)\sqrt{E}$ ← Krane's notation