

# Density of States

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# BE, FD, and MB Distribution

$$\langle n_k \rangle = \frac{1}{e^{\beta(\epsilon_k - \mu)} + \alpha},$$

- $\alpha = -1$ : Bose-Einstein Distribution
- $\alpha = +1$ : Fermi-Dirac Distribution
- $\alpha = 0$ : Maxwell-Boltzmann Distribution

For quantum gases,

$$\langle n_k \rangle = \frac{1}{e^{\beta(\epsilon_k - \mu)} \pm 1},$$

where  $-$  for bosons and  $+$  for fermions.

# Number of Particles and Energy

Then, the number of total particles and energy are then

$$N = \sum_k \langle n_k \rangle = \int_0^\infty \frac{g(E)dE}{e^{\beta(E-\mu)} \pm 1},$$
$$E = \sum_k \langle n_k \rangle E_k = \int_0^\infty \frac{Eg(E)dE}{e^{\beta(E-\mu)} \pm 1},$$

where  $g(E)$  is the density of states. And, defining the fugacity  $z = e^{\beta\mu}$ ,

$$N = \sum_k \langle n_k \rangle = \int_0^\infty \frac{g(E)dE}{z^{-1}e^{\beta E} \pm 1},$$
$$E = \sum_k \langle n_k \rangle E_k = \int_0^\infty \frac{Eg(E)dE}{z^{-1}e^{\beta E} \pm 1}.$$

# Density of States (Free Particles)

Consider particles in a box with  $V = L \times L \times L$ .

$$\Psi(x, y, z) = \left(\frac{2}{L}\right)^{3/2} \sin(k_x x) \sin(k_y y) \sin(k_z z),$$
$$E_n = \frac{\hbar^2 k^2}{2m}, \quad k_x = \frac{n_x \pi}{L}, \quad k_y = \frac{n_y \pi}{L}, \quad k_z = \frac{n_z \pi}{L},$$

where  $n_x$ ,  $n_y$ , and  $n_z$  are integer. Thus,

$$k^2 = \frac{\pi^2}{L^2} (n_x^2 + n_y^2 + n_z^2) = \frac{\pi^2}{L^2} r^2.$$

where  $r^2 = n_x^2 + n_y^2 + n_z^2 = \left(\frac{kL}{\pi}\right)^2$ .

# Density of States (Free Particles)

The total number of states  $G(k)$  with  $k$ -vectors of magnitude between 0 and  $k$  is one-eighth ( $1/8$ ) of the volume of the sphere of radius  $r$ ,

$$G(k) = \frac{1}{8} \times \frac{4}{3} \pi r^3 = \frac{1}{8} \times \frac{4}{3} \pi \left( \frac{kL}{\pi} \right)^3 .$$

And, the density of states is

$$g(k)dk = \frac{dG(k)}{dk} dk = \frac{1}{8} \times 4\pi k^2 \left( \frac{L}{\pi} \right)^3 dk = \frac{V k^2}{2\pi^2} dk .$$

# Density of States (Electron)

Electrons in solids (metals) are fermions and are not fixed in number. The density of states in  $k$ -space is the same as

$$g(k)dk = \frac{Vk^2}{2\pi^2}dk.$$

For the density of state in energy space,

$$\begin{aligned}\epsilon &= \frac{\hbar^2 k^2}{2m}, & d\epsilon &= \frac{\hbar^2}{2m}(2k)dk, \\ g(\epsilon)d\epsilon &= 2 \times \frac{Vk^2}{2\pi^2} \frac{m}{\hbar^2 k} d\epsilon = 2 \times \frac{V}{2\pi^2} \frac{m}{\hbar^2} k d\epsilon \\ &= 2 \times \frac{V}{2\pi^2} \frac{m}{\hbar^2} \frac{\sqrt{2m\epsilon}}{\hbar} d\epsilon = 2 \times \frac{mV}{2\pi^2 \hbar^3} \sqrt{2m\epsilon} d\epsilon,\end{aligned}$$

where 2 is for two different spins.

# Density of States (Photon)

The density of states in  $k$ -space is (we can derive it from Maxwell equations)

$$g(k)dk = \frac{Vk^2}{2\pi^2} dk.$$

In order to obtain the density of state for photons in energy space,

$$\begin{aligned}\epsilon &= \hbar\omega = \hbar ck, & d\epsilon &= \hbar c dk, \\ g(\epsilon)d\epsilon &= 2 \times \frac{V[\epsilon/(c\hbar)]^2}{2\pi^2} \frac{1}{c\hbar} d\epsilon = 2 \times \frac{V\epsilon^2}{2\pi^2(c\hbar)^3} d\epsilon,\end{aligned}$$

where 2 is for two different polarizations. And, for the density of state in frequency space,

$$\begin{aligned}\omega &= ck, & d\omega &= c dk, \\ g(\omega)d\omega &= 2 \times \frac{V\omega^2}{2\pi^2 c^3} d\omega.\end{aligned}$$

# Density of States (Phonon)

Phonons are quantized thermal waves in a solid. They are bosons and are not fixed in number. The density of states in  $k$ -space is

$$g(k)dk = \frac{Vk^2}{2\pi^2} dk.$$

For the density of state in frequency space,

$$\epsilon = \hbar\omega, \quad \omega = vk, \quad d\omega = vdk,$$
$$g(\omega)d\omega = 3 \times \frac{V\omega^2}{2\pi^2v^3} d\omega,$$

where 3 is for two different polarizations (2 transverse and 1 longitudinal).