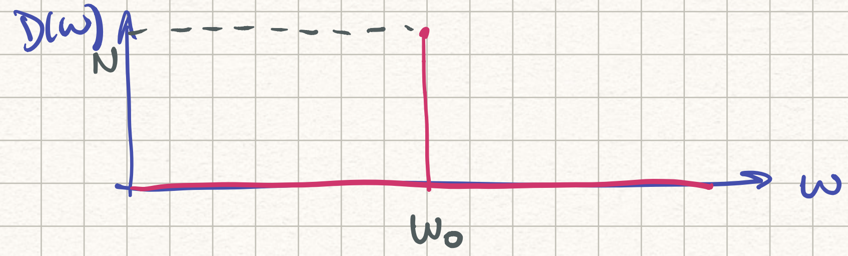
Einstein model of the density of states

Consider N oscillators with the same frequency ω_0, 1D case.

$$D(\omega) = N\,\delta(\omega-\omega_0)$$

δ - is the Dirac δ-function centered at ω_0



The thermal energy of the system

$$U = \int d\omega\, D(\omega)\,\langle n(\omega)\rangle\,\hbar\omega$$

$$= \int d\omega\, N\,\delta(\omega-\omega_0)\,\frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}$$

$$\boxed{U = N\hbar\omega_0\,\frac{1}{e^{\hbar\omega_0/k_BT}-1}}$$

The heat capacity $C_V = \frac{\partial U}{\partial T}$

$$\boxed{C_V = \left(\frac{\partial U}{\partial T}\right) = N k_B \left(\frac{\hbar\omega_0}{k_BT}\right)^2 \frac{e^{\hbar\omega_0/k_BT}}{\left(e^{\hbar\omega_0/k_BT}-1\right)^2}}$$

Obtained in 1907 (Einstein); contribution from N identical oscillators to the heat capacity

In 3D: $$C_V = \left(\frac{\partial U}{\partial T}\right) = 3N k_B \left(\frac{\hbar\omega_0}{k_BT}\right)^2 \frac{e^{h\omega_0/k_BT}}{\left(e^{\hbar\omega_0/k_BT}-1\right)^2}$$

Check that $T \to \infty$, $\boxed{C_V = 3Nk_B}$ classical value of the heat capacity

Dulong - Petit value

$$C_V = 3Nk_B \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T}-1)^2}$$

$$\theta_E = \frac{\hbar\omega_0}{k_B}$$

General result for $D(\omega)$

we want to find a general expression for $D(\omega)$
# of states per unit frequency range
given that we have a dispersion relation $\omega(\vec{k})$

→ The number of allowed $\vec{k}$-values for which the phonon frequency lies between ω, $\omega + d\omega$ is given by

$$D(\omega)\, d\omega = \frac{V}{(2\pi)^3} \int_{\text{shell}} d^3k$$

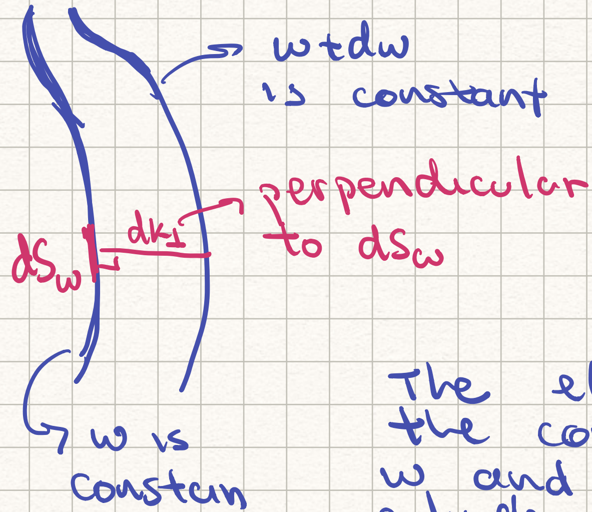
The integration is done over the volume of the shell in $\vec{k}$-space bounded by two surfaces on which the frequency of phonons is constant

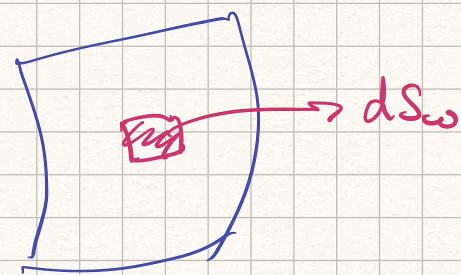
→ one has frequency ω

→ other has frequency $\omega + d\omega$

The problem is to evaluate the volume of the shell.

Let dS_ω denote an element of area on the surface in $\vec{k}$-space at which is freq. is ω





The element of volume between the constant frequency surfaces ω and $\omega+d\omega$ is a right cylinder of base dS_ω and height $dk_\perp$

$$\int_{shell} d^3k = \int dS_\omega \, dk_\perp$$

$dk_\perp$ is the perpendicular distance between the two surfaces, and it may vary from one point to another

The gradient of ω, given $\vec{\nabla}_k \omega$, is also $\perp$ to the surface where ω is constant

$$\vec{\nabla}_k = (\partial_{k_x}, \partial_{k_y}, \partial_{k_z})$$

$|\vec{\nabla}_k \omega| \, dk_\perp = d\omega$ is the difference in frequency between the two surfaces corected by $dk_\perp$

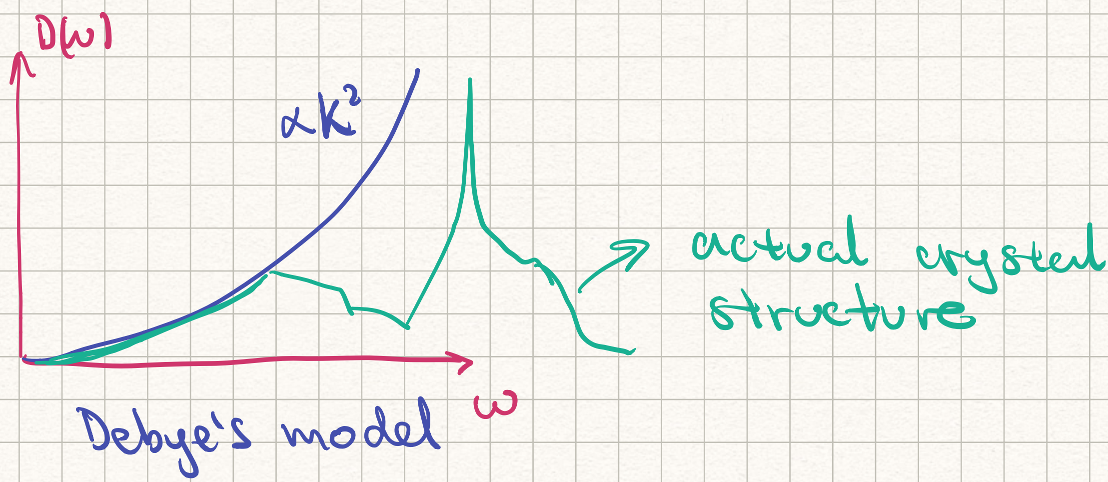
$$dS_\omega \, dk_\perp = dS_\omega \frac{d\omega}{|\vec{\nabla}_k \omega|} = dS_\omega \frac{d\omega}{|\vec{v}_g|}$$

$|\vec{v}_g| = |\vec{\nabla}_k \omega|$ is the magnitude of the group velocity of phonons

$$D(\omega)\, d\omega = \frac{V}{(2\pi)^3} \int_{shell} d^3k$$

$$= \frac{V}{(2\pi)^3} \int \frac{dS_\omega}{v_g} d\omega$$

$$\boxed{D(\omega) = \frac{V}{(2\pi)^3} \int \frac{dS_\omega}{v_g}}$$



Free electron Fermi Gas

Energy levels : 1D

An electron confined in a length L in 1D.

The Schrödinger Eq.

$$H \psi_n = E_n \psi_n$$

The Hamitonian $H = \frac{p^2}{2m}$ $\quad p = -i\hbar \partial_x$

$$\frac{p^2}{2m} = \frac{(-i\hbar\partial_x)^2}{2m} = -\frac{\hbar^2 \partial_x^2}{2m}$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n}{\partial x^2} = E_n \psi_n$$

we know that the solution to this equation

$$\psi_n(x) = A_n \sin(kx) + B_n \cos(kx)$$

Because the electron is confined to a lenght L

$$\psi_n(0) = \psi_n(x=L) = 0$$

$$\psi_n(x) = A_n \sin(kx) \qquad kL = n\pi \qquad n \in \mathbb{Z}$$

$$k = \frac{n\pi}{L}$$

$$= A_n \sin\left(\frac{n\pi x}{L}\right)$$

Replacing in S.E. : $E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$

we want to accommodate N electrons

- Pauli exclusion principle
  - → No two electrons can have all their quantum numbers equal.
- The Q.N. that play a role are
  - n: principal quantum number : Associated to E_n
  - m_s: magnetic q. number : Associated to the spin

Electrons can have $m_s = \pm 1/2$; $\{\uparrow, \downarrow\}$ "spin"

Example: we have 8 electrons

n	m_s	Occupation (how many e^-)
1	↑	1
1	↓	1
2	↑	1
2	↓	1
3	↑	1

3	$\downarrow$	1
4	$\uparrow$	1
4	$\downarrow$	1
5	$\uparrow$	0
5	$\downarrow$	0

n_F : Fermi level

Topmost filled energy level of the system

→ we start filling at the bottom ($n=1$).

→ all e^- are accommodated

In this case $n_F = 4$

If N in an even number $\Rightarrow n_F = N/2$: This cond. determines n_F

E_F: Fermi energy

Energy of the topmost filled level in the ground state of the N electron system

$$E_F = \frac{\hbar^2}{2m}\left(\frac{n_F \pi}{L}\right)^2 = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2L}\right)^2$$

Effect of temperature

→ The ground state is defined a $T=0$

when we increase the temperature

↳ e^- gain kinetic energy

The probability of having an energy level ϵ occupied is given by the Fermi-Dirac distribution

$$f(\epsilon) = \frac{1}{\exp\left[(\epsilon-\mu)/k_B T\right] + 1}$$

μ: chemical potential = energy that we need to add/remove a particle

μ depends on T, and when $T=0$, $\mu = E_F$.

The high energy tail of the distribution for which $\epsilon - \mu \gg k_B T$, is dominated by

$$f(\epsilon) \approx e^{-(\epsilon-\mu)/k_B T}$$

which is the Maxwell-Boltzman distribution, describing classical particles (no spin).