23. Harmonic crystal:

$$E = \sum_{k,s} \left(n_{k,s} + \tfrac{1}{2}\right)\hbar\omega_s(k)$$

$$n_s(k) = \frac{1}{e^{\beta\hbar\omega_s(k)} - 1}$$

$$u = u^{eq} + \frac{1}{V}\sum_{k,s} \tfrac{1}{2}\hbar\omega_s(k) + \frac{1}{V}\sum_{k,s} \frac{\hbar\omega_s(k)}{e^{\beta\hbar\omega_s(k)} - 1}$$

?cas.

$$c_v = \frac{1}{V}\sum_{k,s} \frac{\partial}{\partial T} \frac{\hbar\omega_s(k)}{e^{\beta\hbar\omega_s(k)} - 1}$$

High T: $\dfrac{\hbar\omega_s(k)}{e^{\beta\hbar\omega_s(k)} - 1} \approx \dfrac{1}{\beta} = k_B T$, Dulong & Petit (T indep.)

Low T: $$c_v = \frac{\partial}{\partial T} \sum_k \int \frac{d^3k}{(2\pi)^3} \frac{\hbar c_s(\hat{k}) k}{e^{\beta\hbar c_s(\hat{k}) k} - 1}$$

$$= \frac{\partial}{\partial T} \frac{(k_B T)^4}{(\hbar c)^3} \frac{3}{2\pi^2} \underbrace{\int_0^\infty \frac{x^3 dx}{e^x - 1}}_{\frac{\pi^4}{15}}$$

$$\frac{1}{c^3} = \frac{1}{3}\sum_s \int \frac{d\Omega}{4\pi} \frac{1}{c_s(\hat{k})^3}$$

$$c_v \approx \frac{2\pi^2}{5} k_B \left(\frac{k_B T}{\hbar c}\right)^3$$

$$\boxed{C_V = \frac{1}{V}\sum_{k,s} \frac{\partial}{\partial T}\frac{\hbar\omega_s(k)}{e^{\beta\hbar\omega_s(k)}-1}}$$

$$\frac{1}{e^x-1} = \frac{1}{x+\frac{x^2}{2}+\cdots}$$

$$= \frac{1}{x}\left[\frac{1}{1+\frac{x}{2}+\cdots}\right]$$

$$= \frac{1}{x}\left[1-\frac{x}{2}\cdots + \mathcal{O}(x^2)\right] \qquad x = \frac{\hbar\omega}{k_B T}$$

$$= \frac{k_B T}{\hbar\omega} + \mathcal{O}\left(\frac{\hbar\omega}{k_B T}\right)$$

$$C_V = \frac{1}{V}\sum_{k,s} \frac{k_B\hbar\omega}{\hbar\omega} + \mathcal{O}\left(\frac{\hbar\omega}{k_B T^2}\right)\hbar\omega$$

$$= \frac{1}{V}\sum_{k,s} k_B\left(1 + \underset{-\frac{1}{12}}{\uparrow}\left(\frac{\hbar\omega_s(k)}{k_B T}\right)^2\right)$$

$$= 3n\, k_B$$

$$C_V = \frac{\partial}{\partial T} \sum_s \int \frac{d^3k}{(2\pi)^3} \frac{\hbar \omega_s(k)}{e^{\beta\hbar\omega_s} - 1}$$

$$\text{low } T \approx \frac{\partial}{\partial T} \sum_s \int \frac{d^3k}{(2\pi)^3} \underbrace{\frac{\hbar c_s(\hat{k})k}{e^{\beta\hbar c_s(\hat{k})k} - 1}}_{\frac{k_B T}{(\beta\hbar c_s(k))^3} \frac{x}{e^x - 1}}$$

$$x = \beta\hbar c_s(\hat{k})k$$

$$\frac{1}{c^3} = \frac{1}{3} \sum_s \int \frac{d\Omega}{4\pi} \frac{1}{c_s(\hat{k})^3}$$

$$c_V = \frac{\partial}{\partial T} \frac{(k_B T)^4}{(\hbar c)^3} \underbrace{\int \frac{x^3 dx}{e^x - 1}}_{\pi^4/15} \cdot \underbrace{\frac{4\pi \cdot 3}{(2\pi)^3}}_{\frac{3}{2\pi^2}}$$

$$= \underbrace{4}\, k_B \left(\frac{k_B T}{\hbar c}\right)^3 \cdot \underbrace{\frac{3}{2\pi^2} \frac{\pi^4}{15}}$$

$$= \frac{2\pi^2}{5} k_B \left(\frac{k_B T}{\hbar c}\right)^3$$

Debye: $\omega = ck$

$$\int \frac{d^3k}{(2\pi)^3} = n = \frac{4\pi}{3} \frac{k_D^3}{(2\pi)^3} = \frac{k_D^3}{6\pi^2}$$

$$\frac{1}{V}\sum_k = \int \frac{d^3k}{(2\pi)^3}$$

$$\omega_D = k_D c$$

$$k_B \Theta_D = \hbar\omega_D = \hbar c k_D$$

$$\Theta_D = \hbar c k_D / k_B$$

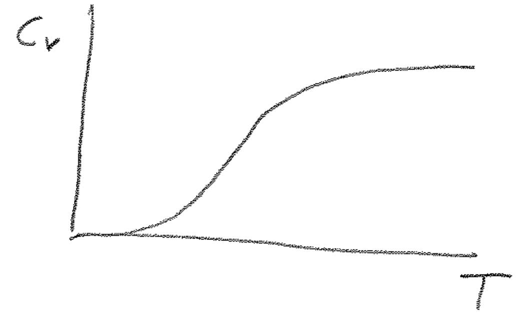
$$x = \hbar c k / k_B T$$

$$\text{max} = \hbar c k_D / k_B T = \Theta_D / T$$

$$C_V = \frac{6}{\pi^2} k_B \left(\frac{k_B T}{\hbar c}\right)^3 \int_0^{\Theta_D/T} \frac{x^4\,dx}{e^x - 1}$$

$$= \frac{6}{\pi^2} k_B \left(\frac{T}{\Theta_D}\right)^3 k_D^3 \int_0^{\Theta_D/T} \frac{x^4\,dx}{e^x - 1}$$

$$= 36 n k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D/T} \frac{x^4\,dx}{e^x - 1} \quad (\text{Typo } 36 \leftarrow 9)$$



Low T $= \underbrace{\frac{36\pi^4}{15}}_{\frac{12\pi^4}{5}} n k_B \left(\frac{T}{\Theta_D}\right)^3$

Einstein:

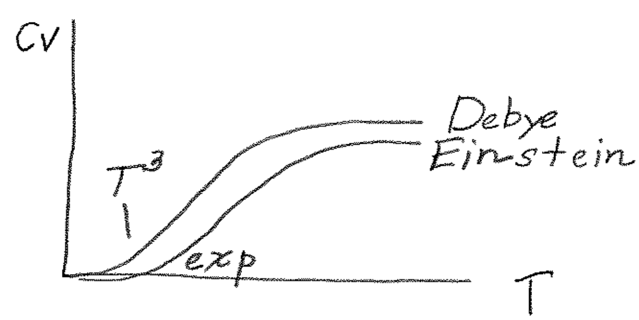
$$c_V = \frac{\partial}{\partial T} \sum_s \int \frac{d^3k}{(2\pi)^3} \frac{\hbar\omega_E}{e^{\beta\hbar\omega_E} - 1}$$

$$= \frac{\partial}{\partial T} \; p \; n \; \frac{\hbar\omega_E}{e^{\beta\hbar\omega_E} - 1}$$

p = number optical branches

$$= -\frac{p n \hbar\omega_E}{(e^{\beta\hbar\omega_E} - 1)^2} \, e^{\beta\hbar\omega_E} \left(-\frac{\hbar\omega_E}{k_B T^2} \right)$$

$$= p n k_B \frac{(\hbar\omega_E / k_B T)^2 e^{\beta\hbar\omega_E}}{(e^{\beta\hbar\omega_E / k_B T} - 1)^2}$$



Lattice & Electronic: cross-over few K

Density of States

$$\frac{1}{V}\sum_{ks} Q(\omega_s(k))$$

$$= \sum_s \int \frac{d^3k}{(2\pi)^3} Q(\omega_s(k))$$

$$= \int d\omega \, g(\omega) \, Q(\omega)$$

$$g(\omega) = \sum_s \int \frac{d^3k}{(2\pi)^3} \, \delta(\omega - \omega_c(k))$$

$$g_D(\omega) = 3 \int_{k<k_D} \frac{d^3k}{(2\pi)^3} \delta(\omega - ck)$$

$$= \frac{3}{2\pi^2} \int_0^{k_D} k^2 dk \, \delta(\omega - ck)$$

$$= \begin{cases} \dfrac{3}{2\pi^2} \dfrac{\omega^2}{c^3} & \omega < \omega_D = k_D c \\ 0 & \omega > \omega_D \end{cases}$$

$$g_E(\omega) = \int \frac{d^3k}{(2\pi)^3} \, \delta(\omega - \omega_E) = n \, \delta(\omega - \omega_E)$$

Analog Blackbody

# normal modes	$3p$ each k $\omega = \omega_s(k)$	2 each k $\omega = ck$
wave-vector	B. Z.	all k
Thermal	$\sum_s \int \frac{d^3k}{(2\pi)^3} \frac{\hbar\omega_s(k)}{e^{\beta\hbar\omega_s(k)}-1}$	$2\int \frac{d^3k}{(2\pi)^3} \frac{\hbar c k}{e^{\beta\hbar\omega}-1}$