Condensed Matter Physics I

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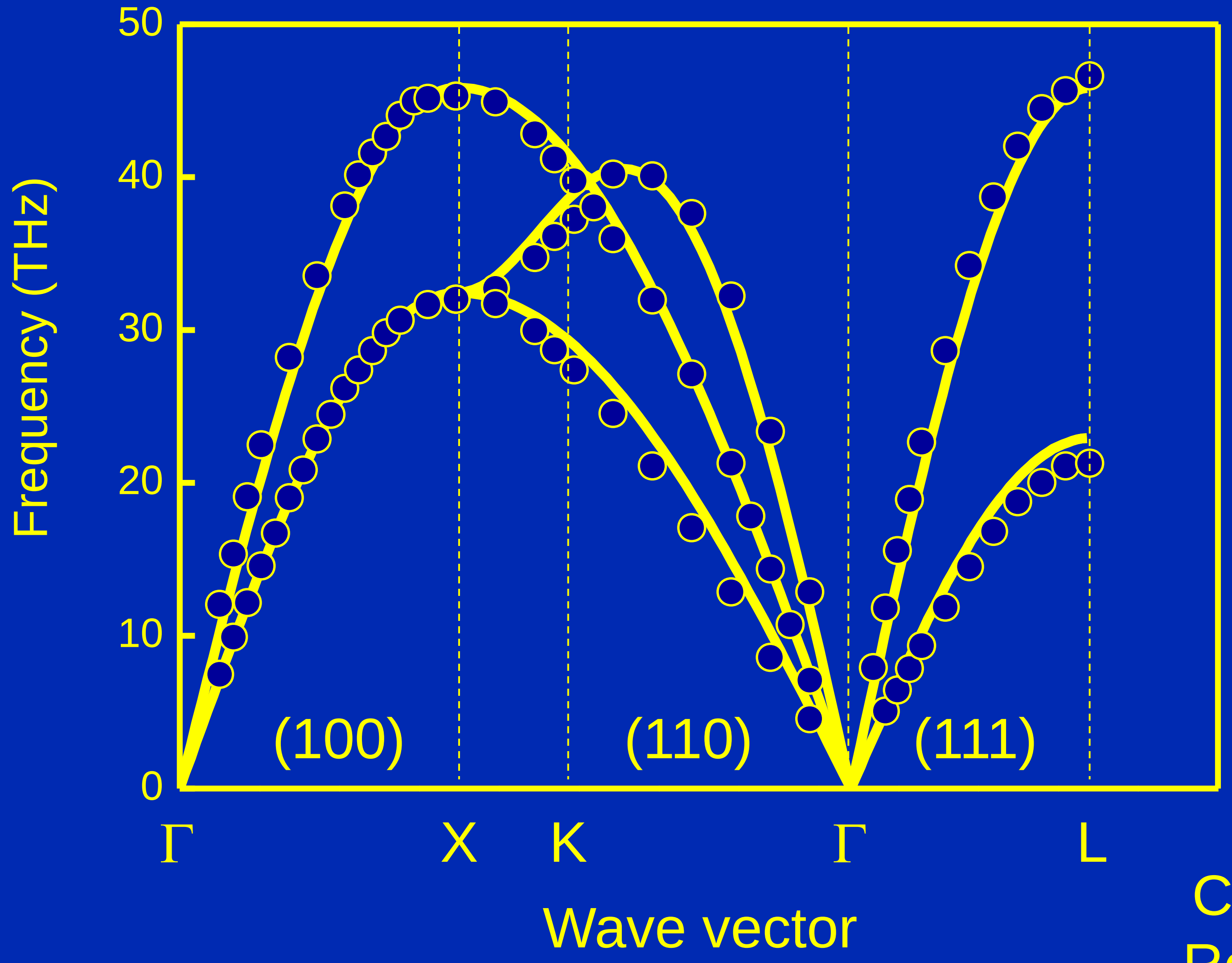
Previously

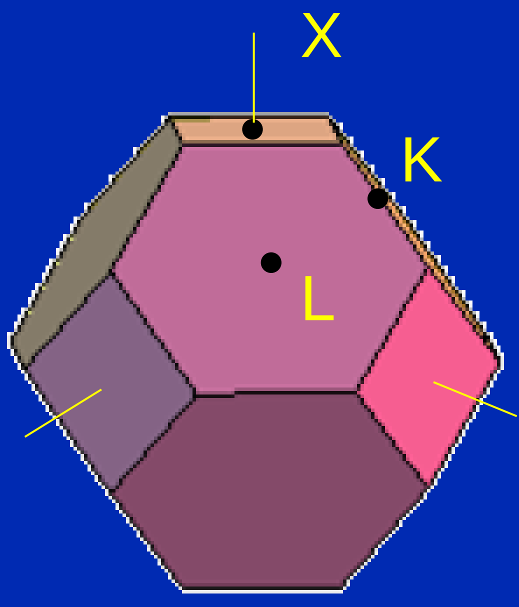
PHONONS

- Quantized lattice vibrations
- #modes: 3s; Optical & acoustical; Transversal & longitudinal
- Eigenmodes
- Relevant **k** vectors in first BZ
- Thermal occupation: Planck
- Dispersion $\omega(\mathbf{k})$
- ‘Momentum’ $\hbar\mathbf{k}$
- Group velocity; Sound velocity
- Measuring of phonons;

  inelastic spectroscopy

Phonon dispersion in copper





Γ at (0,0,0)

Cu: FCC (1 at/cell)
Recipr. Space BCC

Today

- Phonons & physical properties (Ch.4 & 5 Kittel)

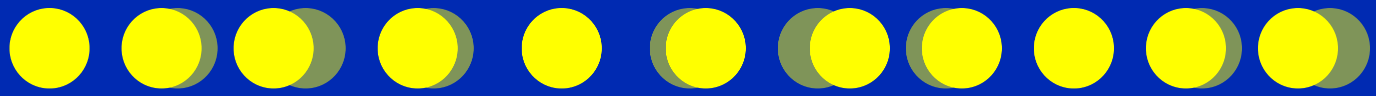
Phonons & Physical properties

- Propagation of sound
- Optical properties (infrared)
- Lattice expansion
- Heat capacity
- Thermal conductivity

Today: Thermal properties

- Thermal expansion (classical)
- Lattice specific heat
    - Density of States
        - Debye model
        - Einstein model
- Thermal conductivity
    - Phonon scattering, mean free path

Harmonic crystal: No thermal expansion



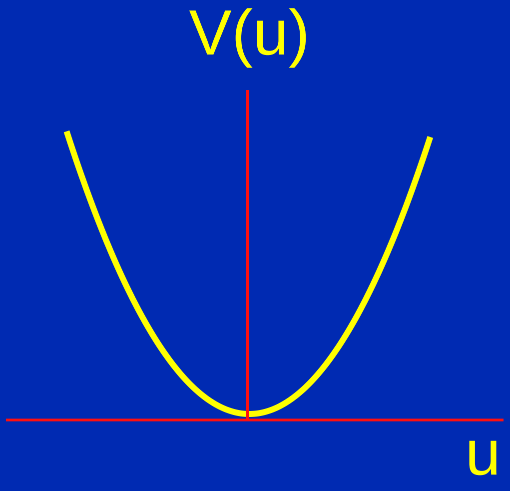
$$r_j = ja + u_j$$

Harmonic

$$V(u_j) = \alpha \cdot u_j^{\,2}$$

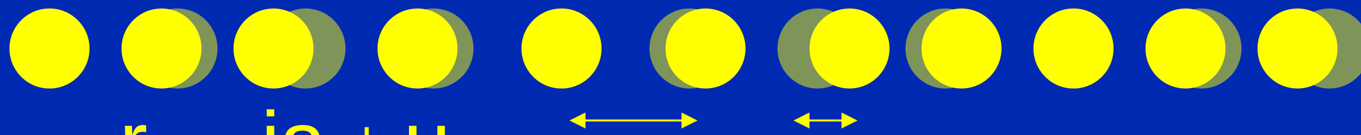
$$a(T) = a + \langle u_j \rangle_T = a$$

$$\langle u_j \rangle_T = \frac{\int du \cdot u\, e^{-V(u_j)/k_B T}}{\int du \cdot e^{-V(u_j)/k_B T}} = 0$$



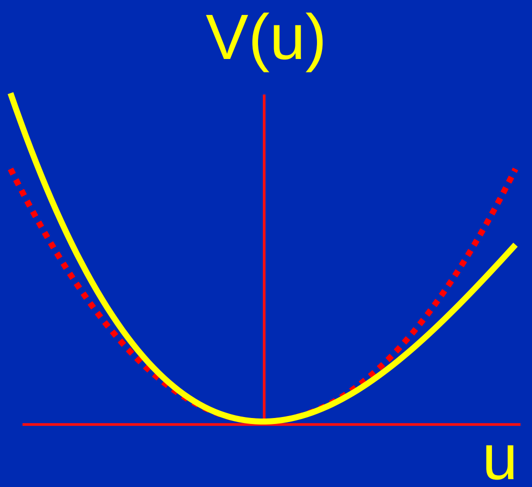
No lattice expansion !!

Anharmonicity: Thermal expansion (classical)



$$r_j = ja + u_j$$

Weak anharmonicity



$$V(u_j) = \alpha \cdot u_j^{\,2} - \gamma \cdot u_j^{\,3}$$

$$\langle u_j \rangle_T = \frac{\int du \cdot u\, e^{-V(u_j)/k_B T}}{\int du \cdot e^{-V(u_j)/k_B T}} \approx \frac{3/4\,(k_B T)^{3/2} \sqrt{\pi}\, \gamma\, \alpha^{-5/2}}{\sqrt{k_B T}\sqrt{\pi}\, \alpha^{-1/2}}$$

$$a(T) = a_0 + \langle u_j \rangle_T = a_0 + \frac{3\gamma}{4\alpha^2} k_B T$$

Lattice expansion is caused by anharmonicity !

Specific heat

Heat capacity: $C_v = \left.\frac{\partial U}{\partial T}\right|_V$

Summation over modes k and branches p:

$$U = \sum_{k,p} U_{k,p} = \sum_{k,p} \langle n_{k,p} \rangle \hbar\omega_{k,p} = \sum_{k,p} \frac{\hbar\omega_{k,p}}{e^{\hbar\omega_{k,p}/k_B T} - 1}$$

Number of modes in range $\omega \to \omega + d\omega$: $d\omega \, D_p(\omega)$

D(ω): Density of states

$$\sum_k \quad \to \quad \int d\omega \, D_p(\omega)$$

$$U = \sum_p \int d\omega D_p(\omega) \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

Lattice heat capacity

$$\sum_{k} \rightarrow \int d\omega\, D_p(\omega)$$

$$U = \sum_p \sum_k U_{k,p} = \sum_p \sum_k \langle n_{k,p} \rangle \hbar\omega_{k,p} = \sum_p \int d\omega\, D_p(\omega) \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

$$\Rightarrow \quad C_{lattice} = \frac{\partial U}{\partial T} = k_B \sum_p \int d\omega\, D_p(\omega) \frac{x^2 e^x}{\left(e^x - 1\right)^2}$$

All lattice properties in $D(\omega)$:

<u>Density of states:</u> # modes per unit frequency

Density of states in 1D

1D crystal, N atoms, length L=Na

Vibrational mode: $u_k(j,t) = u_k e^{-i(\omega t - kaj)}$

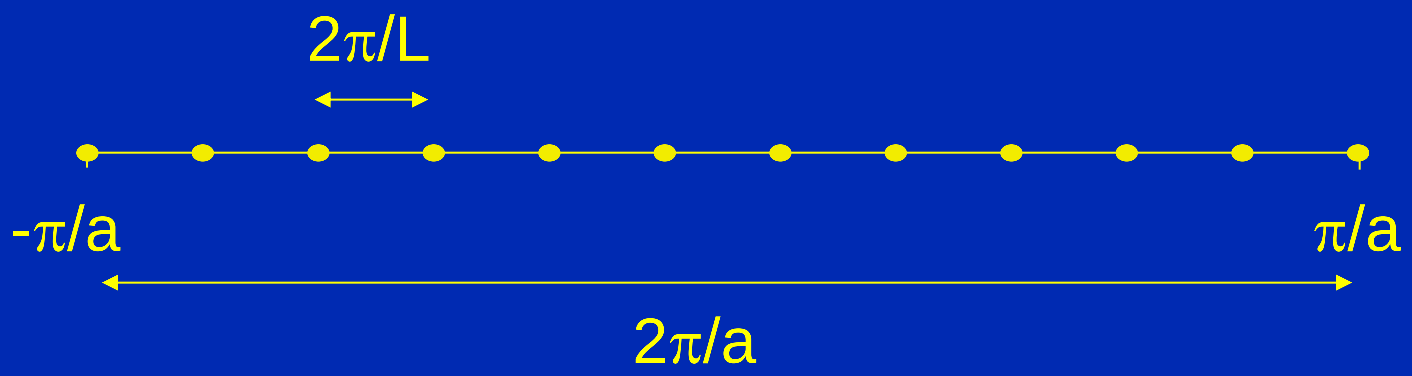
Periodicity over L=Na: $u_k \cdot e^{ikaj} = u_k \cdot e^{ika(j+N)}$

$$\Longrightarrow \quad e^{ikaN} = 1 \qquad kaN = 2\pi s \qquad k = \frac{2\pi s}{Na} = \frac{2\pi}{L} s$$

$$-\frac{\pi}{a} < k \le \frac{\pi}{a} \quad \Rightarrow \quad s = -\frac{N-1}{2}, \ldots, \frac{N-1}{2}, \frac{N}{2}$$

i.e. <u>N modes in the first BZ</u>

Density of states in 1D

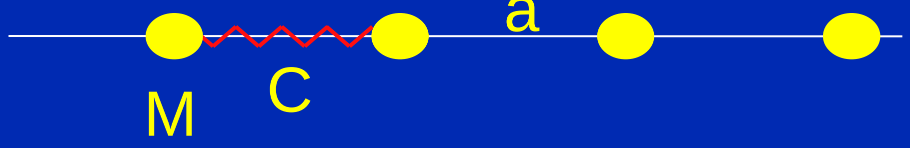


modes/unit length = N / (2π/a) = L/ 2π

In interval dk: $$D(k)dk = \frac{N}{2\pi / a} dk = \frac{L}{2\pi} dk$$

$$\boxed{D(\omega)d\omega = \frac{L}{2\pi} \frac{dk}{d\omega} d\omega}$$

Density of states (1D)



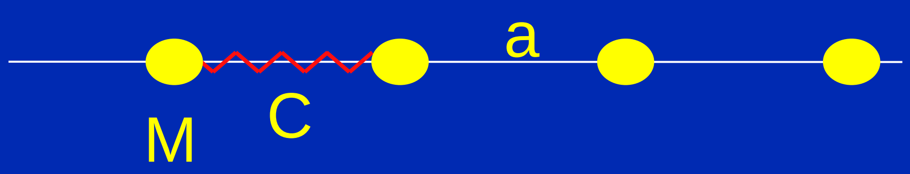
$$D(\omega)d\omega = \frac{L}{2\pi}\frac{dk}{d\omega}d\omega$$

1D, 1 at./cell: $\omega(k) = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right| \quad \Rightarrow \quad \omega(k) = \omega_m \left|\sin(ka/2)\right|$

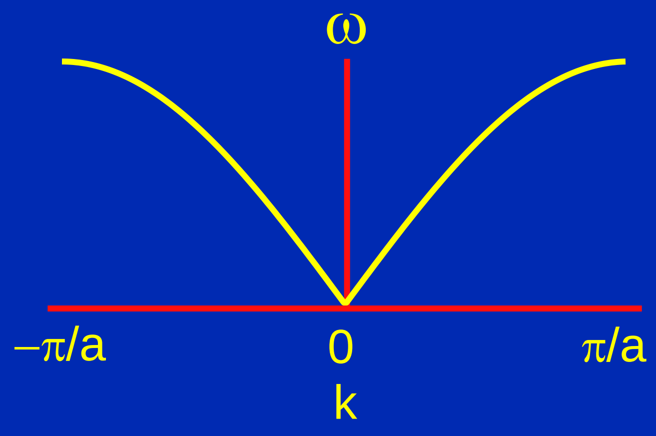
$$\left[\frac{\partial\omega(k)}{\partial k}\right]^{-1} = \frac{2}{a}\frac{1}{\omega_m\left|\cos(ka/2)\right|} = \frac{2}{a}\frac{1}{\sqrt{\omega_m^2 - \omega^2}}$$

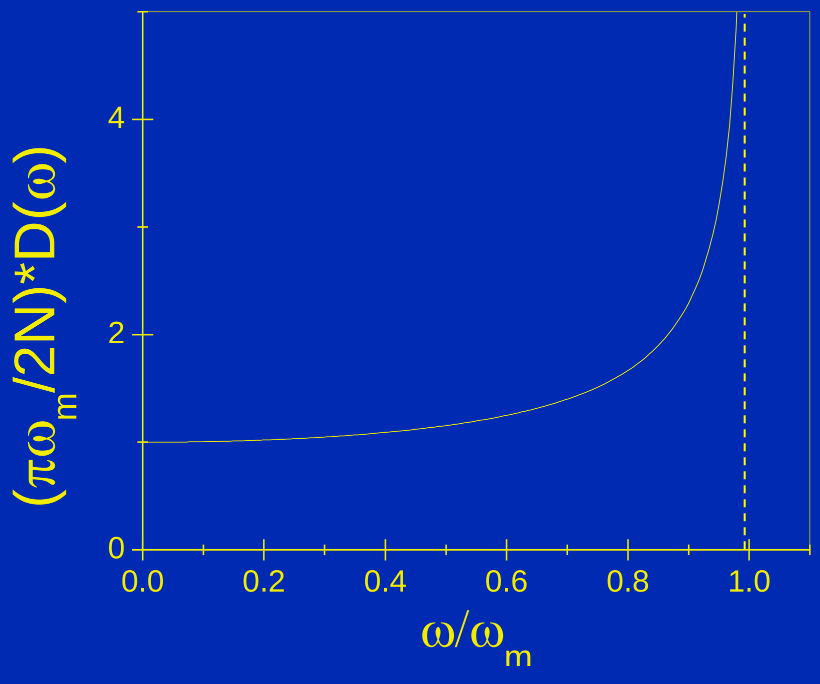
$$\Rightarrow \quad D(\omega) = 2\frac{N}{\pi}\frac{1}{\sqrt{1-\omega^2}}$$

Density of states (1D)



$$D(\omega) = 2\frac{N}{\pi}\frac{1}{\sqrt{\omega_m^2 - \omega^2}}$$





Density of states in 3D

3D crystal, N^3 atoms, cube length L

Periodic boundary conditions: $e^{i\left(k_x x+k_y y+k_z z\right)} = e^{i\left(k_x(x+L)+k_y(y+L)+k_z(z+L)\right)}$

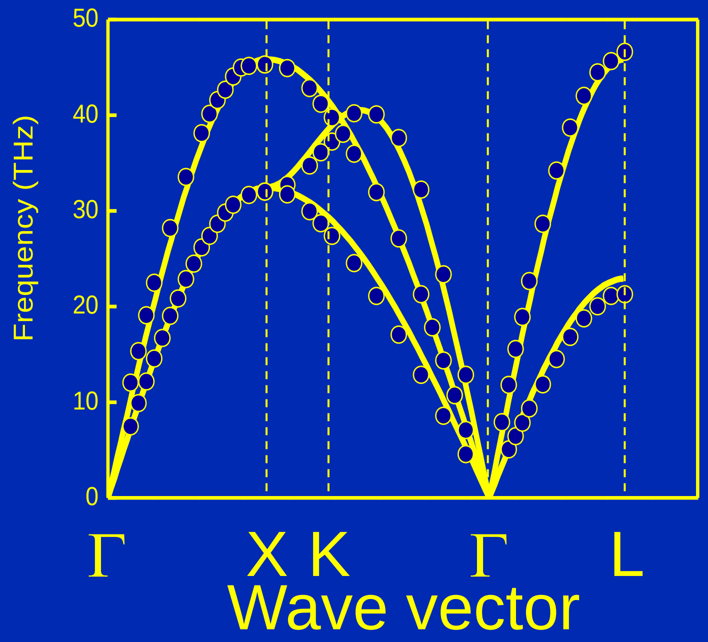
$$\Rightarrow \quad k_x, k_y, k_z = s \cdot \frac{2\pi}{L}; \qquad s = -\frac{N-1}{2}, \ldots, \frac{N-1}{2}, \frac{N}{2}$$

One value of k per volume $\left(\frac{2\pi}{L}\right)^3$

Total # k values in sphere with radius k: $N(k) = \frac{V_k}{\left(2\pi/L\right)^3} = \frac{4\pi k^3/3}{\left(2\pi\right)^3/V}$

$$D(k) = \frac{dN(k)}{dk} = \frac{Vk^2}{2\pi^2} \qquad \boxed{D(\omega) = \frac{Vk^2}{2\pi^2}\frac{dk}{d\omega}}$$

Density of states in 3D



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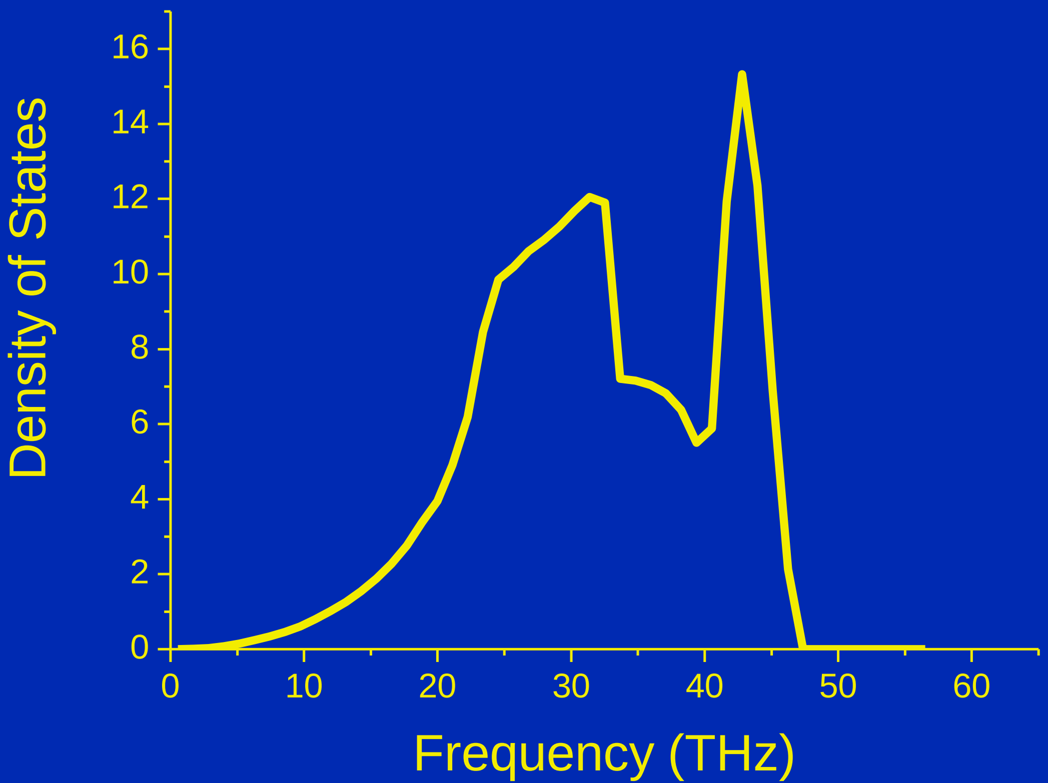


Density of States

	$D(k)$	$D(\omega)$
1D	$\frac{L}{2\pi}$	$\frac{L}{2\pi}\frac{dk}{d\omega}$
2D	$\frac{A}{2\pi^2}k$	$\frac{A}{2\pi^2}k\frac{dk}{d\omega}$
3D	$\frac{V}{2\pi^2}k^2$	$\frac{V}{2\pi^2}k^2\frac{dk}{d\omega}$

Back to lattice heat capacity

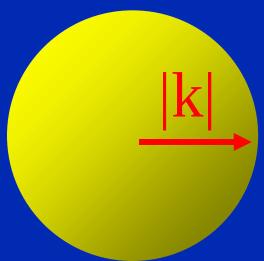
$$C_{lattice} = \frac{\partial U}{\partial T} = k_B \sum_p \int d\omega D_p(\omega) \frac{x^2 e^x}{\left(e^x - 1\right)^2}$$

DOS in general complicated function
Simplifications:

- Debye model (take sound velocity constant)
- Einstein model (take phonon frequency constant)

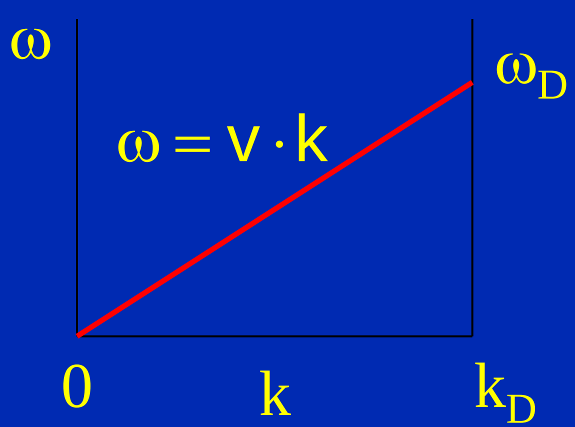
Debije model for DOS $\omega = v \cdot k$

Number of modes with |k'| < |k| for each polarization (branch):



$$N\left(|\vec{k}|\right) = \frac{V_{cell}}{(2\pi)^3}\frac{4\pi}{3}|\vec{k}|^3$$

Number of modes: $N(k_D) = N_{atom}$



$$\Rightarrow k_D = \left(\frac{6\pi^2 N_{atom}}{V_{cell}}\right)^{1/3}$$

$$\Rightarrow N(\omega < \omega_D) = \frac{V_{cell}}{(2\pi)^3}\frac{4\pi}{3}\left(\frac{\omega}{v}\right)^3$$

Debije model

Debije Frequency: $$\omega_D = v\left(\frac{6\pi^2 N_{atom}}{V}\right)^{1/3}$$

Debije Temperature: $$\theta = \frac{\hbar\omega_D}{k_B} = \frac{\hbar v}{k_B}\left(\frac{6\pi^2 N_{atom}}{V}\right)^{1/3}$$

Density of states: $$D(\omega) = \frac{dN(\omega)}{d\omega} = V\,\frac{\omega^2}{2\pi^2 v^3}$$

Total energy stored in phonons:

$$U = \sum_k \frac{\hbar\omega_k}{e^{\hbar\omega_k/k_BT} - 1} = 3\int_0^{\omega_D} \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} D(\omega)d\omega$$

Debije specific heat

Total energy :

$$U = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3}{\exp(\hbar\omega / k_B T) - 1} d\omega$$

Specific heat:

$$C_{lat} = \frac{dU}{dT} = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3 \exp(\hbar\omega / k_B T)}{(\exp(\hbar\omega / k_B T) - 1)^2} \frac{\hbar\omega}{k_B T^2} d\omega$$

$$C_{lat} = \frac{dU}{dT} = 9 N_{atom} \left(\frac{T}{\theta}\right)^3 \cdot \int_0^{\theta / T} \frac{x^4 e^x}{(e^x - 1)^2} dx \qquad x = \frac{\hbar\omega}{k_B T}$$

Debije T^3 law

Low temperature limit: $\theta / T \to \infty$

$$\int_0^\infty \frac{x^4 e^x}{(e^x - 1)^2} dx = \frac{\pi^4}{15}$$

$$C_{lat} = \frac{12\pi^4}{5} N_{atom} k_B \left(\frac{T}{\theta} \right)^3$$

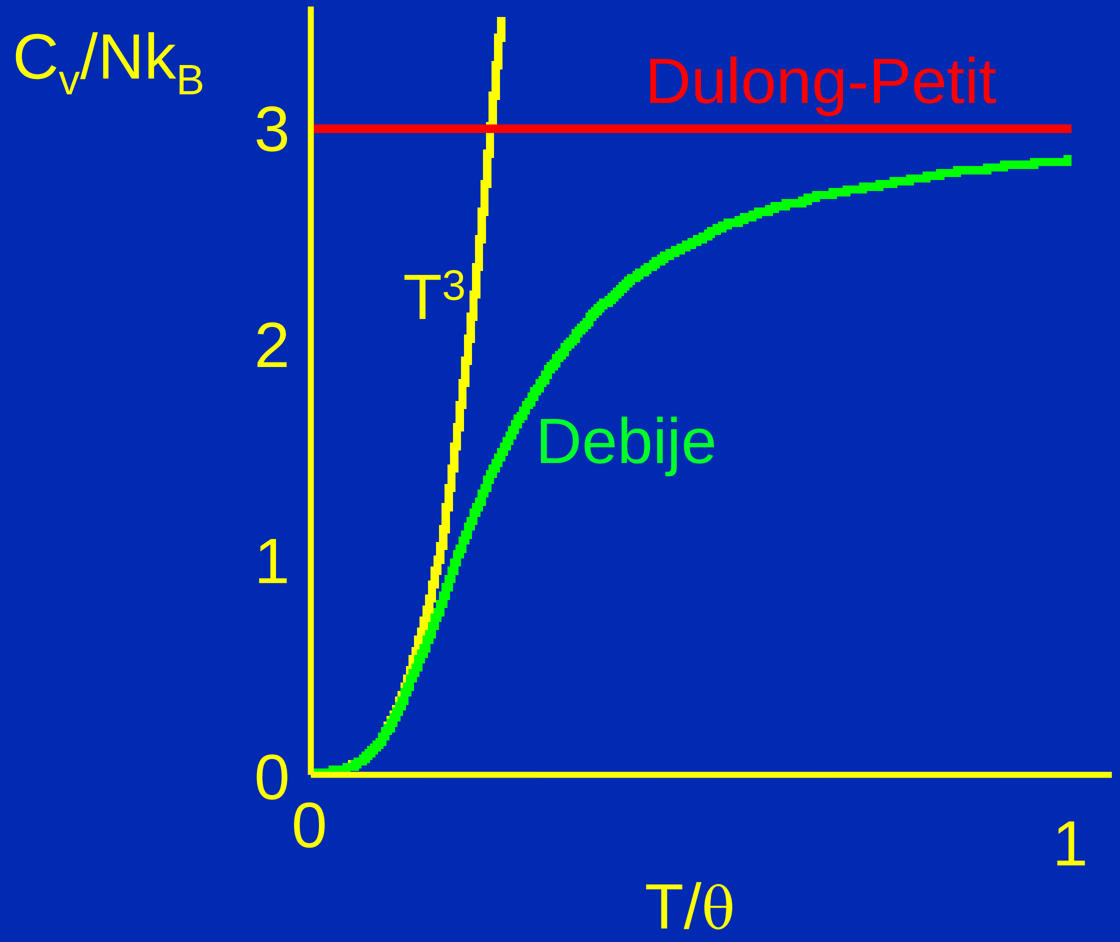
High temperature limit: $\theta / T \to 0$

$$\int_0^{\theta / T} \frac{x^4 e^x}{(e^x - 1)^2} dx \approx \frac{1}{3} \left(\frac{\theta}{T} \right)^3$$

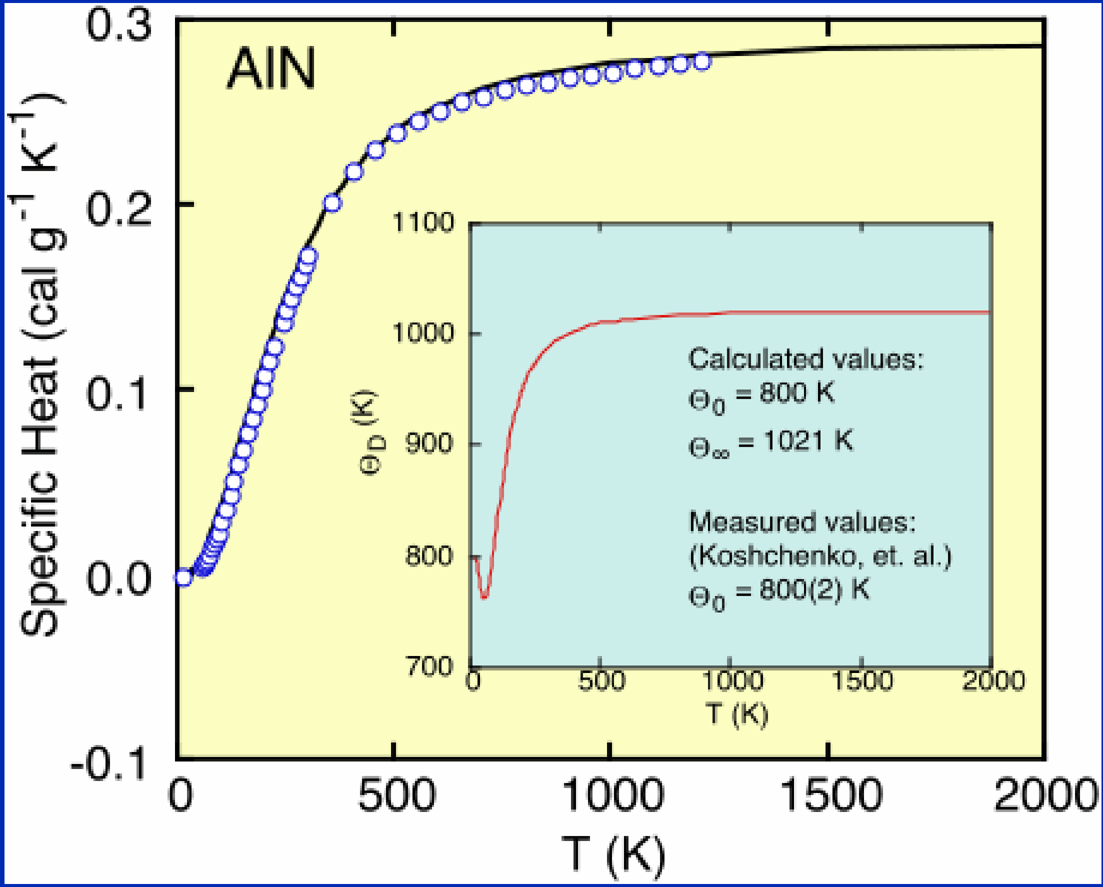
$$C_{lat} = 3N_{atom} k_B$$

(Dulong-Petit, $U=3N \cdot k_B T$)

Specific heat



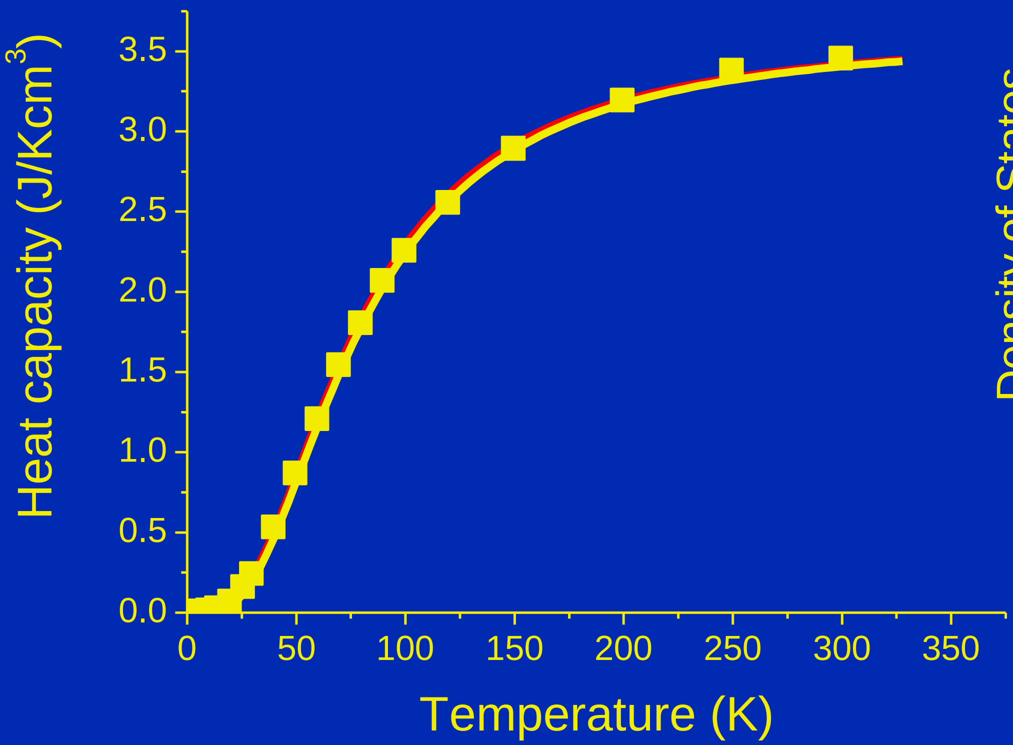
Specific heat AlN

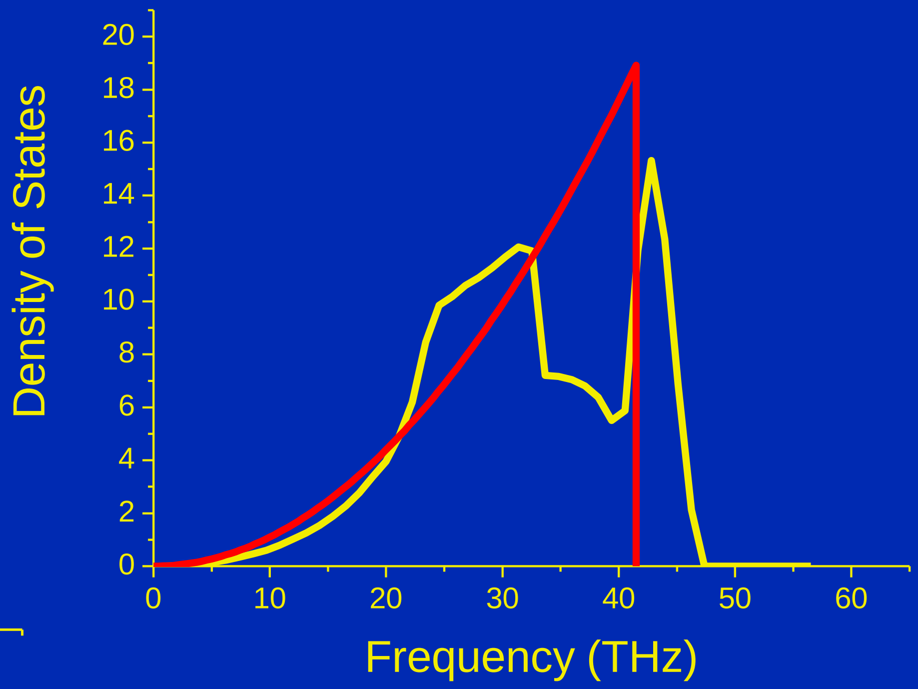


Specific heat Aluminum Nitride (Koshchenko et al., 1985)

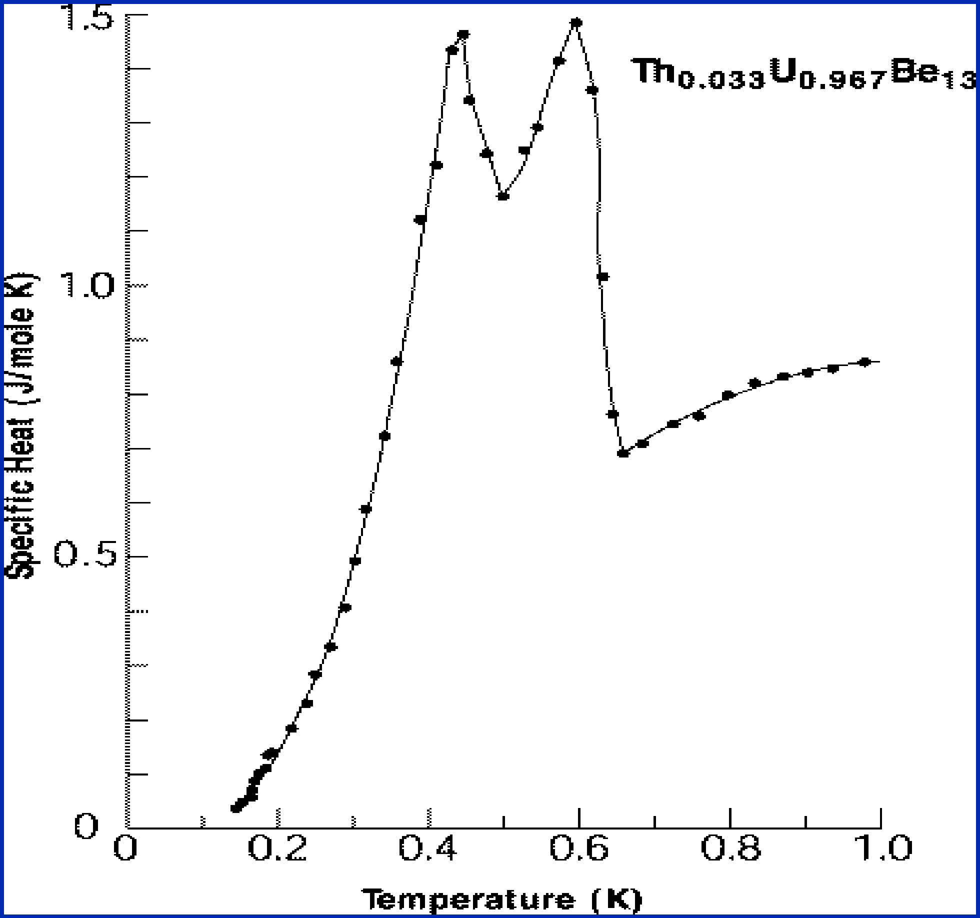
Specific heat Cu

Copper again





Specific heat $Th_xU_{1-x}Be_{13}$



Heavy fermion system, 2 S.C. transitions (Z. Fisk et al., 2000)

Einstein model

Simpler model, approximation for optical phonons

$$D(\omega) = N_{atoms}\,\delta(\omega - \omega_e)$$

$$U = 3N_{atoms}\langle n(\omega_e)\rangle \hbar\omega_e = \frac{3N_{atoms}\hbar\omega_e}{e^{\hbar\omega_e/k_B T} - 1}$$

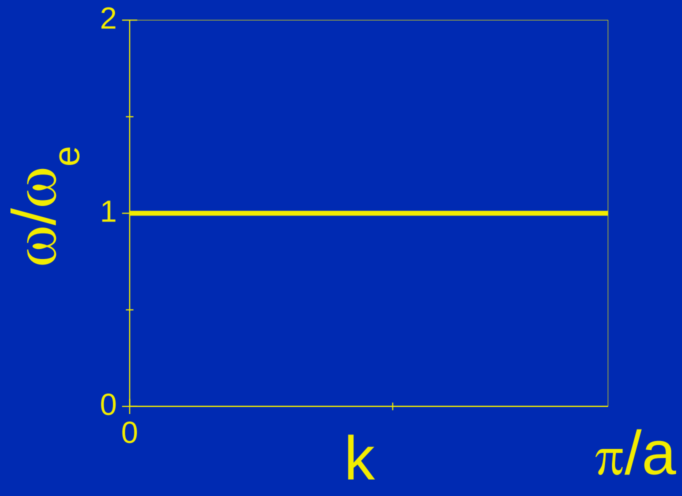
$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = 3N_{atoms}k_B\left(\frac{\hbar\omega_e}{k_B T}\right)^2 \frac{e^{\hbar\omega_e/k_B T}}{\left(e^{\hbar\omega_e/k_B T} - 1\right)^2}$$

<u>Limits</u>

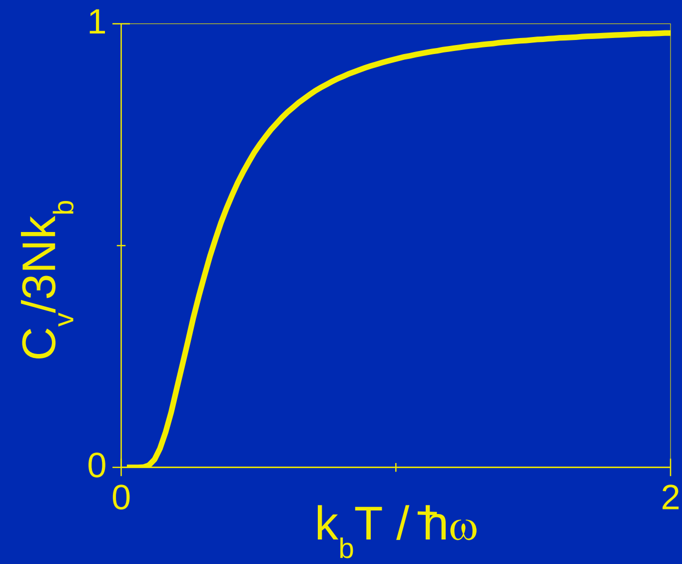
$$T \to 0: \quad C_v \propto x^2 e^{-x} = 0$$

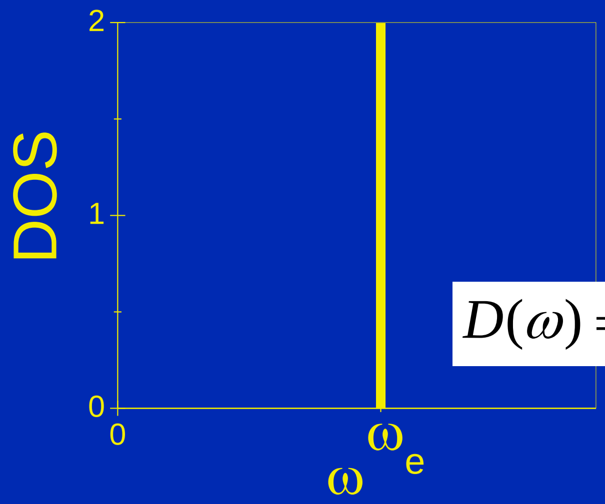
$$T \to \infty: \quad C_v = 3N_{atoms}k_B$$

Einstein model, C_V



$$C_V = 3N_{atoms}k_B\left(\frac{\hbar\omega_e}{k_BT}\right)^2\frac{e^{\hbar\omega_e/k_BT}}{\left(e^{\hbar\omega_e/k_BT}-1\right)^2}$$





$$D(\omega) = N_{atoms}\delta(\omega-\omega_e)$$