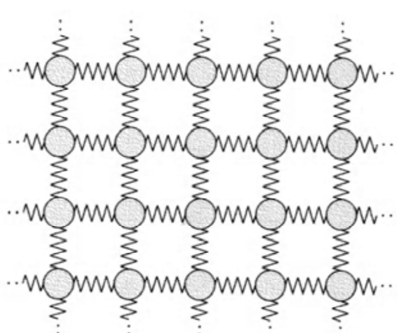
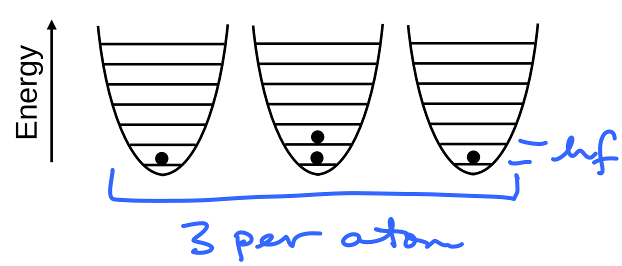
ANNOUNCEMENTS

- midterm #2
  - remark requests to Prof. Walker
    will remark all questions!
- make-up laboratory
  - contact Prof. Wetterfield by midnight
- class – 1 Dec. → cancelled

Review

- Einstein model of a solid
  - In 3-D, can vibrate in three independent directions





  - Each oscillator can have multiple energy units

$\varepsilon = hf$ size of energy unit

Einstein Solid

- In Tutorial #9, predicted heat capacity as

$$C_V = 3Nk\frac{(\varepsilon/kT)^2 e^{\varepsilon/kT}}{(e^{\varepsilon/kT}-1)^2}$$

$U = \varepsilon q$

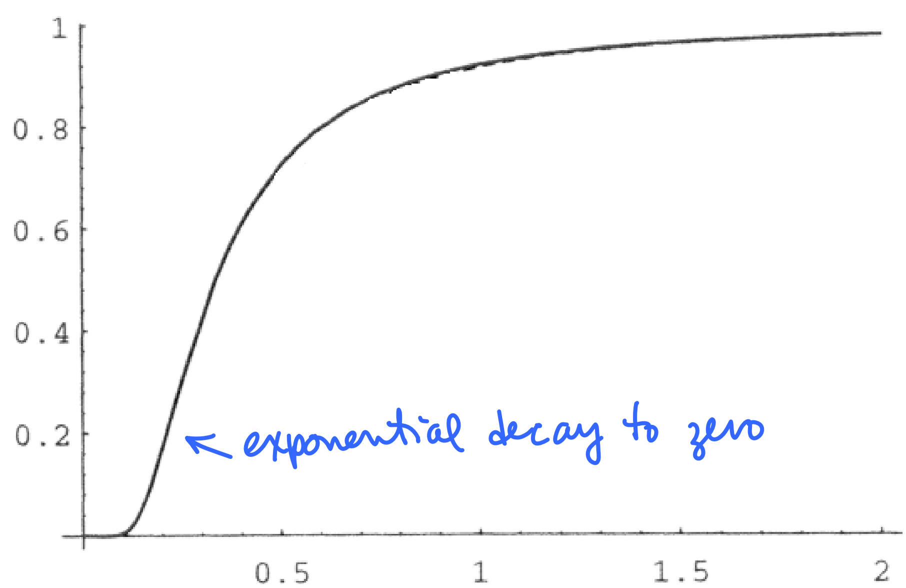
  ε is size of the unit of energy for identical oscillators and we're taking N as number of atoms in this case!

- Considering usual limits
  - $kT >> \varepsilon$: C_V approaches equipartition value $3Nk$
  - Below $kT \approx \varepsilon$: decreases approaching zero as T→0 K

Heat Capacity of Einstein Solid

$\frac{C_V}{3Nk}$

↑ no. of atoms



$\frac{kT}{\varepsilon}$

expt. $C_V \propto T^3$ at low T

Limitation of Einstein Model

- Einstein model assumes that all vibrations are independent
- However, one atom in crystal cannot vibrate without affecting others nearby
  - Number affected depends on frequency of vibration mode
  - Different frequencies - units of energy vary in size
  - Variation means that C_V approaches zero less dramatically

Modelling Mechanical Oscillations

- Using modes of oscillation model for blackbody EM field
- Description of lattice vibrations
  - Moving from photons to phonons (both bosons)
  - Can describe number of energy units per mode using Planck distribution

mode index $|\vec{n}|$ (n_x, n_y, n_z)

$$\bar{n}_{Pl} = \frac{1}{e^{\varepsilon/kT} - 1} \qquad \varepsilon = hf = \frac{hc_s n}{2L}$$

$\varepsilon \rightarrow$ energy unit for vibration mode, f

$L \rightarrow$ length of crystal

$c_s \rightarrow$ speed of sound

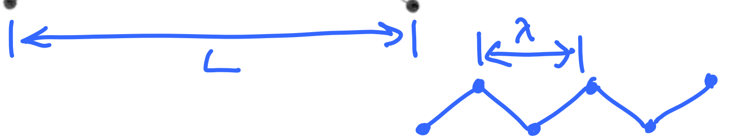
Modelling Mechanical Oscillations

- Differences between photon and phonon model
  - Can have longitudinal modes as well as transverse modes
  - Minimum wavelength for oscillation is two times the atomic spacing

$\lambda = \frac{2}{3}L$

$\lambda = L$

$\lambda = 2L$



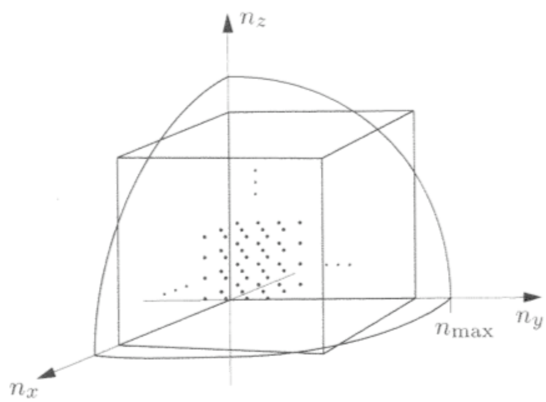
Crystal Oscillation Modes

n has a limit because of space between atoms

- Wavelength cannot be smaller than atomic spacing
- Total number of modes cannot exceed number of atoms, N
  - In 1D, $n_{max} = N$
  - In 3D, $n_{x(\max)} = \sqrt[3]{N}$

$$n_{\max} = \left(\frac{6N}{\pi}\right)^{1/3}$$

$$N = \frac{1}{8}\left(\frac{4}{3}\pi n_{max}^3\right)$$



n_{max} = radius of sphere

Total Energy for Debye Solid

- Starting from $U = 3\sum_{n_x}\sum_{n_y}\sum_{n_z} \varepsilon \bar{n}_{Pl}(\varepsilon)$

$$U = 3\iiint \frac{hc_s n}{2L} \cdot \frac{1}{e^{hc_s n/2kTL} - 1}\, dn_x\, dn_y\, dn_z$$

$$= 3\underbrace{\int_0^{\pi/2} d\phi \int_0^{\pi/2} \sin\theta\, d\theta}_{\pi/2} \int_0^{n_{max}} \frac{n^2 hc_s n\, dn}{2L} \cdot \frac{1}{e^{hc_s n/2kTL} - 1}$$

$$\Rightarrow \quad x = \frac{hc_s n}{2LkT}$$

$$U = \frac{3\pi}{2}\int_0^{x_{max}} \frac{x^3}{e^x - 1}\, dx \left(\frac{hc_s}{2L}\right)\left(\frac{2LkT}{hc_s}\right)^4$$

$$x_{max} = \frac{hc_s n_{max}}{2LkT} = \frac{hc_s}{2LkT}\left(\frac{6N}{\pi}\right)^{1/3}$$

$$= \frac{hc_s}{2k}\left(\frac{6N}{\pi V}\right)^{1/3}\frac{1}{T}$$

$$= \frac{\Theta_D}{T} = \frac{T_D}{T}$$

Θ_D Debye temperature (text uses T_D)

$$U = \frac{3\pi}{2}\,\frac{8L^3k^3}{h^3c_s^3\,6N}\,6NkT^4\int_0^{\Theta_D/T} \frac{x^3}{e^x - 1}\, dx$$

$$= \frac{9NkT^4}{\Theta_D^3}\int_0^{\Theta_D/T} \frac{x^3}{e^x - 1}\, dx$$

Total Energy

$$U = \frac{9NkT^4}{\Theta_D^3} \int_0^{\Theta_D/T} \frac{x^3}{e^x - 1}$$

high T $\rightarrow \Theta_D \ll T$

$e^x \approx 1 + x$

integral

$\hookrightarrow \int_0^{\Theta_D/T} x^2 dx = \frac{1}{3} x^3 \Big|_0^{\Theta_D/T}$

$= \frac{1}{3}\left(\frac{\Theta_D}{T}\right)^3$

$U = 9NkT^4 \frac{1}{3T^3} = 3NkT$

$\hookrightarrow C_V = 3Nk \qquad T \gg \Theta_D$

$\hookrightarrow$ equipartition theorem

low T $\quad \Theta_D \gg T$

$\frac{\Theta_D}{T} \rightarrow \infty$

$\int_0^{\infty} \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}$

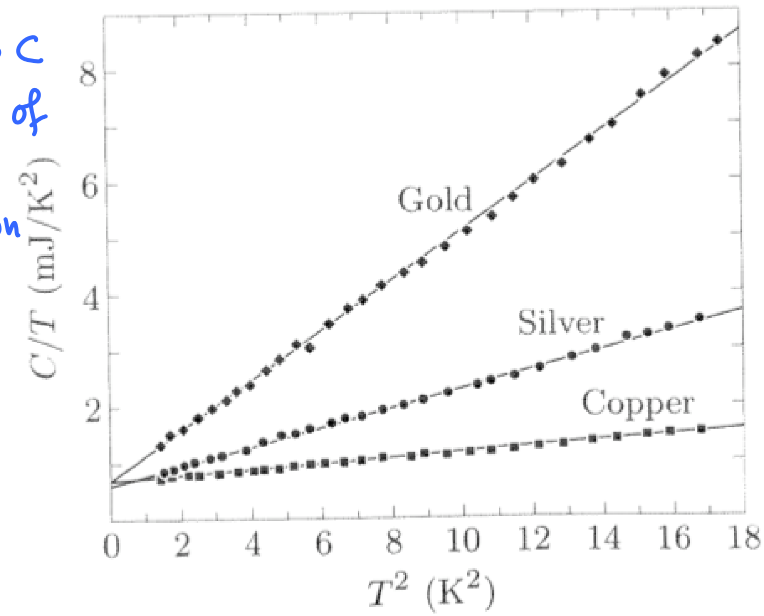
$U = \frac{3\pi^4}{5} \frac{NkT^4}{\Theta_D^3}$

$\hookrightarrow C_V = \frac{12\pi^4}{5}\left(\frac{T}{\Theta_D}\right)^3 Nk \qquad T \ll \Theta_D$

$C_V \propto T^3$

Experimental Results

in metals:
2 contrib. to C
→ vibrations of lattice
+ conduction electrons



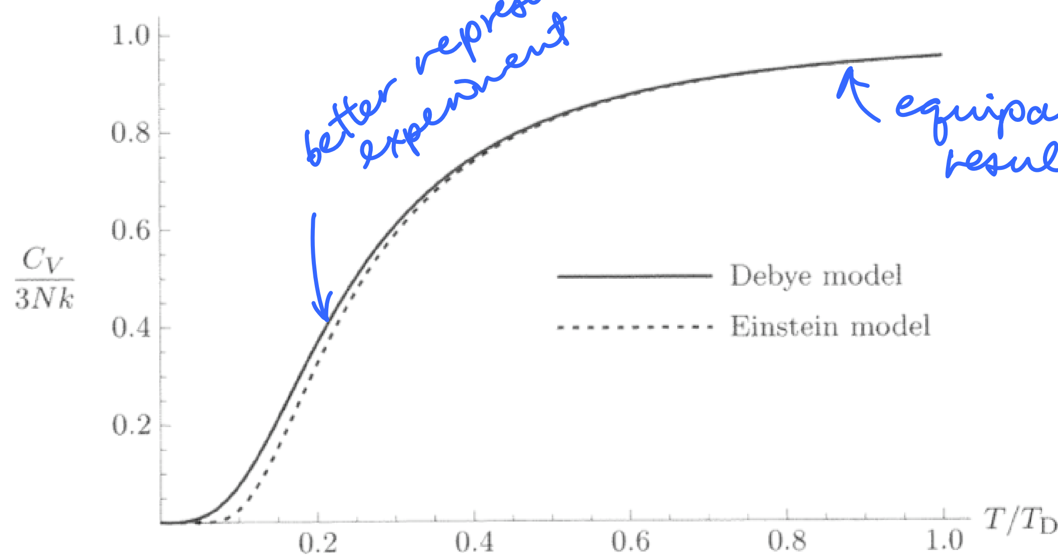
$\frac{C}{T}$ vs T^2

$$C = \gamma T + \frac{12\pi^4 N k}{5\Theta_D^3} T^3$$

Comparing Model Results

better represents experiment

equipartition result



Θ_D gives estimate of C_V over full range of T for non-metallic crystal