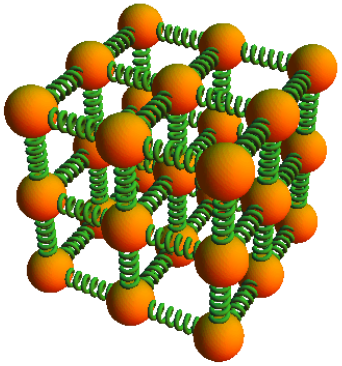
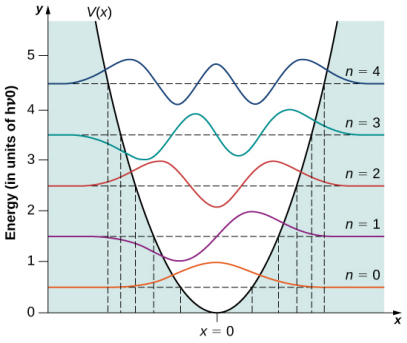
Phonon gas and Debye crystal model

Lecture 20, Fys2160

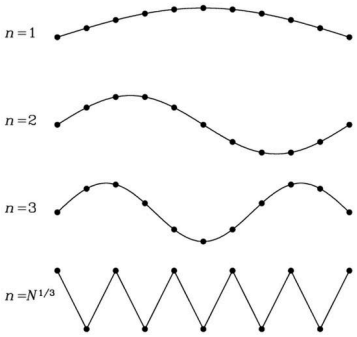
Thermal vibrations in solids:





Einstein crystal model:

- Each atom in 3D has 3 one-dimensional quantum harmonic oscillators
- The harmonic oscillators are independent



Debye crystal model

- Thermal vibrations are coupled

Einstein crystal model

1 quantum harmonic oscillator

Hamiltonian $\widehat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}\kappa\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$

Quantized energy levels $E = \left(n + \frac{1}{2}\right)\hbar\omega = \left(n + \frac{1}{2}\right)\varepsilon$

Relative to ground state $\Delta E = E - \frac{1}{2}\varepsilon = n\varepsilon$

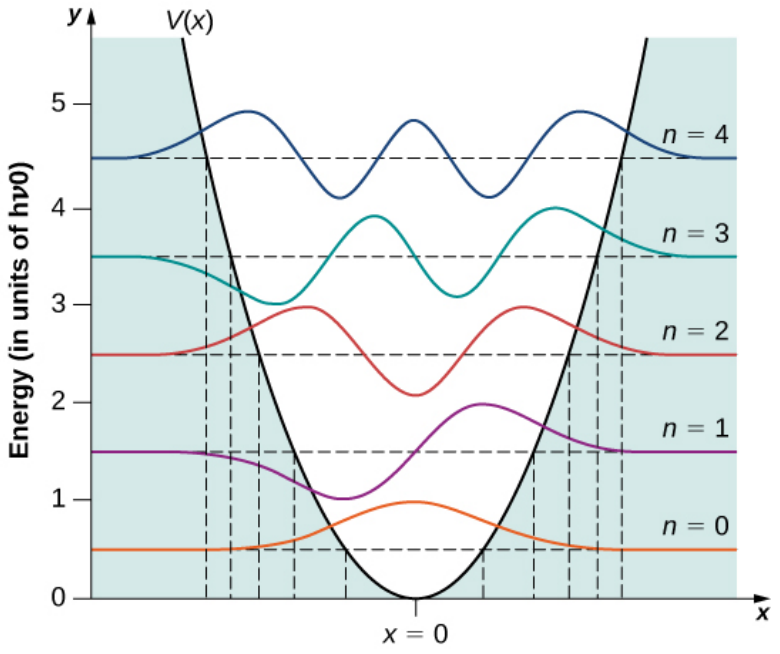
N quantum harmonic oscillators

Total energy $U_N = \sum_{i=1}^{N} E_i = \sum_{i=1}^{N} n_i\,\varepsilon \left(+\frac{N}{2}\varepsilon\right)$

$= q\varepsilon \left(+\frac{N}{2}\varepsilon\right)$

Energy units $\mathrm{q} = \frac{U_N}{\varepsilon}\left(-\frac{N}{2}\right)$

Multiplicity $\Omega(q, N) = \frac{(N-1+q)!}{q!(N-1)!}$



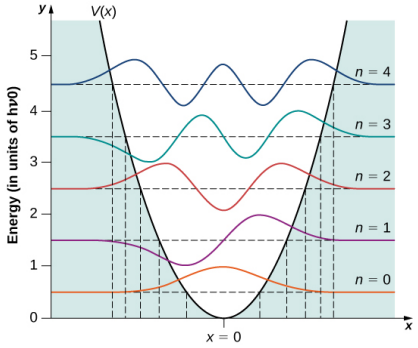
Einstein crystal model

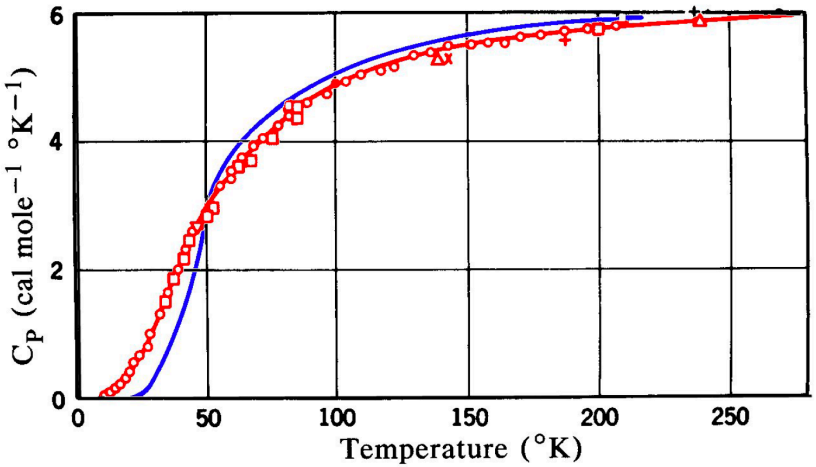
Total energy $U_N = q\varepsilon$

Energy units $\mathrm{q} = \frac{U_N}{\varepsilon}$

Multiplicity $\Omega(q,N) = \frac{(N-1+q)!}{q!(N-1)!}$

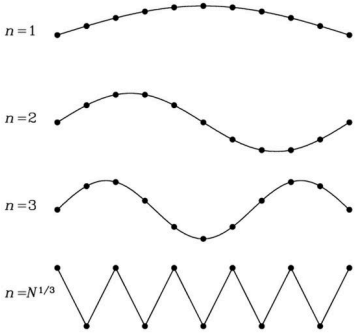
Heat capacity $C_V = 3Nk\frac{\left(\frac{\varepsilon}{kT}\right)^2 e^{\varepsilon/kT}}{\left(e^{\varepsilon/kT}-1\right)^2}$



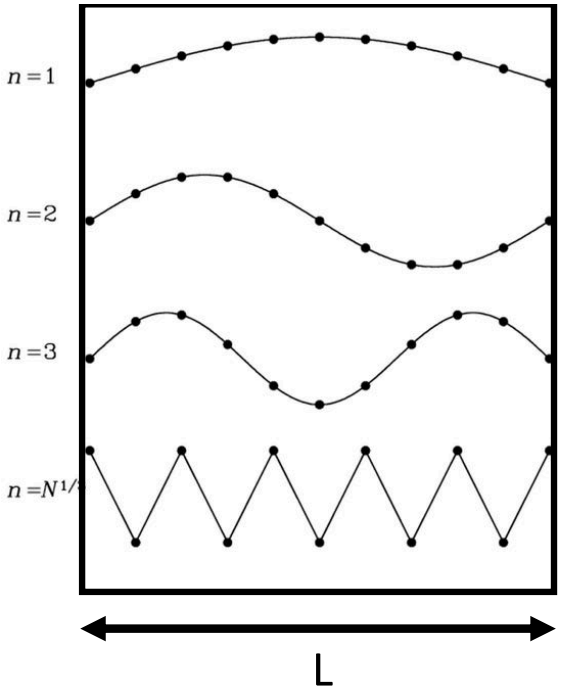


Einstein model C_V is too small at low T

Lacks low frequency (long wavelength, low energy collective modes



Debye crystal model



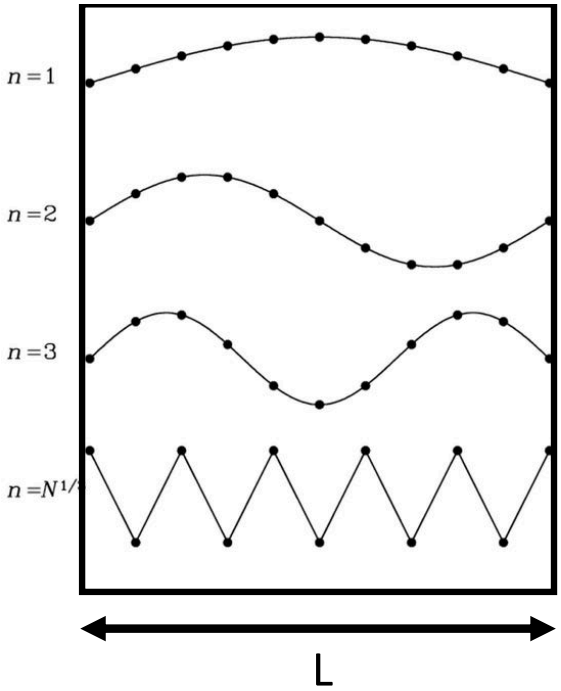
Collective modes of motion (vibration) of atoms in crystal

= Standing (sound) waves in solid of size L:

- wavelength $\lambda_n = \frac{2L}{n}$
- minimum wavelength λ_{min} = 2 * interatomic distance
- sound velocity assumed constant c_s
- energy $\varepsilon = h\nu = \frac{hc_s}{\lambda} = \frac{hc_s n}{2L}$
- waves -> phonons -> bosons with $\mu = 0$
- average number of energy units $\bar{n}_{BE}(\varepsilon, T) = \frac{1}{e^{\beta\varepsilon} - 1}$
- 3 polarizations: 1 long, 2 transv.
- total energy $U = 3 \sum_{n_x} \sum_{n_y} \sum_{n_z} \varepsilon \, \bar{n}_{BE}$
- sum in 1/8 sphere of volume N $n_{max} = \left(\frac{6N}{\pi}\right)^{1/3}$
- almost same integral as photons $U = \int_0^{n_{max}} dn \int_0^{\pi/2} d\theta \int_0^{\pi/2} d\varphi \, n^2 \sin\theta \frac{3hc_s n}{2L} \frac{1}{e^{\beta \frac{hc_s n}{2L}} - 1}$
- integrate over angles $= \frac{3\pi}{2} \int_0^{n_{max}} dn \frac{hc_s}{L} \frac{n^3}{e^{\beta \frac{hc_s n}{2L}} - 1}$

*Unlike photons

Debye crystal model



Collective modes of motion (vibration) of atoms in crystal

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- integrate over angles $U = \frac{3\pi}{2}\int_0^{n_{max}} dn \frac{hc_s}{L} \frac{n^3}{e^{\beta\frac{hc_s n}{2L}}-1}$
- $x = \frac{\varepsilon}{kT} = \frac{hc_s n}{2LkT}, \quad \frac{dx}{dn} = \frac{hc_s}{2LkT}$ $x_{max} = \frac{hc_s n_{max}}{2LkT} = \frac{hc_s}{2LkT}\left(\frac{6N}{\pi}\right)^{1/3} \equiv \frac{\boldsymbol{T_D}}{\boldsymbol{T}}$
- not analytical $U = \frac{9nkT^4}{T_D^3}\int_0^{T_D/T} \frac{x^3}{e^x-1} dx$
- Heat capacity $C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V} = 9NkT\left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^4 e^x}{(e^x-1)^2} dx$

Debye crystal model

Debye temperature $T_D = \frac{hc_s}{2Lk}\left(\frac{6N}{\pi}\right)^{1/3}$

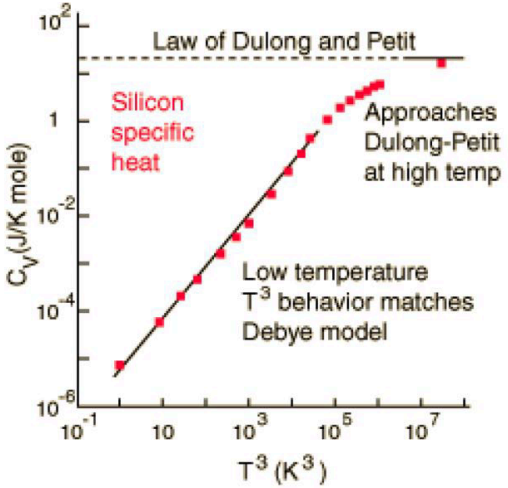
Total energy $U = \frac{9nkT^4}{T_D^3}\int_0^{T_D/T}\frac{x^3}{e^x-1}\,dx$

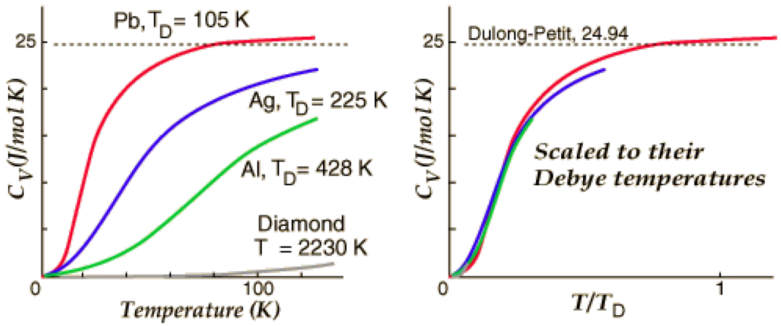
Heat capacity $C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V} = 9NkT\left(\frac{T}{T_D}\right)^3\int_0^{T_D/T}\frac{x^4e^x}{(e^x-1)^2}\,dx$

Low temperature $T \ll T_D$ $U = \frac{3\pi^4}{5}\frac{NkT^4}{T_D^3}$

$C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V} = \frac{12\pi^4}{5}\left(\frac{T}{T_D}\right)^3$

free electron model $C_V = \gamma T,\ \ \gamma = \frac{\pi^2 nk^2}{2\varepsilon_F}$

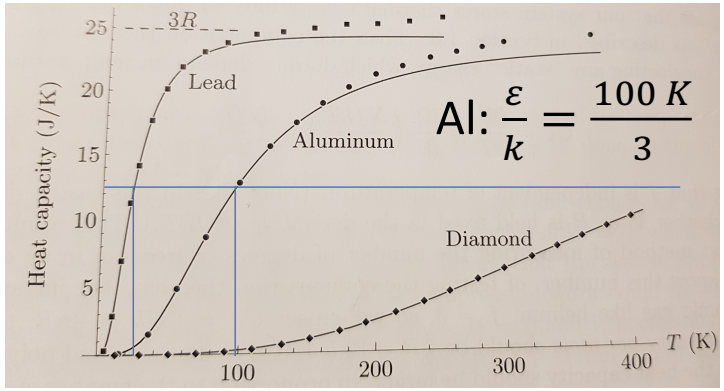




How do we relate models to materials?

Einstein model

- harmonic oscillators:
  - energy quanta, $\varepsilon = h\nu$, ε only material parameter
  - temperature scale, kT/ε
  - ex., $\frac{C_V(\frac{kT}{\varepsilon}=3)}{3Nk} = 0.4963$
- no coupling between atoms => no elasticity
- no volume, pressure...
- $U, N, T, S, C_V, \mu, \ldots$



Debye models

- elastic waves:
  - energy quanta, $\varepsilon = h\nu = \frac{hc_s n}{2L}$, c_s only material parameter
  - temperature scale, kT/ε
  - same empirical fit possible
- coupling between atoms => elasticity, $c_s = \sqrt{\frac{B}{\rho}}$, B- bulk modulus