



SUMMARY LECTURE 5

Specific Heat, Density of states.

SPECIFIC HEAT

- Def : Energy required to raise the temperature of a unit mass of a substance by one degree.
- Mathematical Formulation:

$$C_v = \left(\frac{\partial U}{\partial T} \right)_v$$

Thus the rate of change of the internal energy U with respect to the change in temperature while the Volume is held constant.

ENUMERATION OF MODES AND DENSITY OF STATES

- Why?

→ We are interested in the internal energy of the solid as to be able to establish a relationship with its specific heat.

→ To get the energy (*for the Debye Model*) we need to know how many states are present in a given frequency range, since we treat the atoms as oscillators.

ENUMERATION OF MODES AND DENSITY OF STATES

- How?

→ Implement periodic boundary condition. (Doesn't really matter, but makes our life easier.)

→ Linear Dispersion Relation : $\omega = v_s k$

→ Mathematical formulation: (1D)

$$D(\omega) = \frac{L}{\pi} \frac{1}{\frac{d\omega}{dk}}$$

ENUMERATION OF MODES AND DENSITY OF STATES

- In 3D it looks a bit different, however the derivation is almost identical:

→Mathematical formulation:

$$D(\omega) = \frac{3V}{2\pi^2} \frac{\omega^2}{v_s^3}$$

Remarks : $V = L^3$; Notice symmetry factors in 2 and 3 dimensions!

SPECIFIC HEAT – EXPERIMENTAL OBSERVATIONS

- At high temperatures (Dulong – Petit) $\rightarrow C_v \approx 3R$
- At low temperatures $\rightarrow C_v \propto T^3$

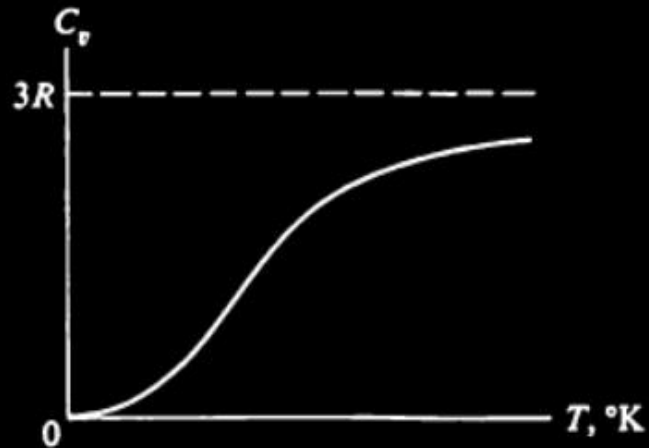


Fig. 3.7 Dependence of specific heat of solids on temperature.

WHY THE NEED FOR NEW MODELS?

- Classical physics of a harmonic force predicted a specific heat, independent of temperature, namely:

$$C_v = 3R$$

EINSTEIN'S MODEL

- Einstein liked QM better than CM.
- He also liked independent atoms.
- His equation for the energy:

$$E = 3N_A \frac{\hbar\omega_E}{e^{\hbar\omega_E/kT} - 1}$$

- His corresponding specific heat equation:

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

- Remarks : θ_E - Einstein temperature given by : $k\theta_E = \hbar\omega_E$, it is chosen to produce the best fit to the measured values over the whole temperature range, from which then ω_E is determined.

WHAT'S WRONG WITH EINSTEIN MODEL?

- Although giving a good general shape , his model fails at low temperatures. It falls off exponentially and not with the 3rd power of T as experiments show.

DEBYE'S MODEL

- Debye considered the motion of the lattice as a whole and not as a single independent atom – *collective lattice modes*.
- He used the prototype of the sound wave - linear dispersion relation.
- Debye model frequency covered a wider range of values.
- Subtle point : Ignorance of the discreteness of the lattice.

DEBYE'S MODEL (MATHS)

- Debye Model Energy:

$$E = \int \varepsilon D(\omega) d\omega$$

- Debye Model Specific Heat:

$$C_v = 9R \left(\frac{T}{\theta_D} \right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

- Remarks: $x = \frac{\hbar\omega}{kT}$, Debye temperature is determined in the same sense as Einstein's.

WHAT'S WRONG WITH DEBYE?

- It still is just an approximation since the discreteness of the lattice is ignored with the current dispersion relation.



CLOSING REMARKS