

Solid state physics (winter term 2015/2016)

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Exercise sheet 6

1. Einstein Model

Einstein model of lattice heat capacity assumes that all lattice vibration modes are at the same frequency.

- a) Assuming Einstein approximation, how many phonon modes (Density of States) exist for a crystal of N unit cells each containing 2 atoms.
- b) Write down the total energy in the phonon representation.
- c) Calculate the specific heat of phonons for this model and describe the low and high temperature behaviours.
- d) Is Delong-Petit law fulfilled at high temperatures?

2. Thermal Expansion

a) Show that the temperature dependence of thermal expansion coefficient α can be predicted using the inter-atomic potential as in:

$$U(x) = cx^2 - gx^3 - fx^4$$

b) Calculate the average displacement $\langle x \rangle$ according to their thermodynamically probability using $\beta = \frac{1}{k_B T}$ and expand the exponentials by approximated functions as given in lecture.



3. Density of States in a Simple Cubic lattice

A simple cubic lattice is defined with a period "L" along all three cubic axis, "N" atoms within the volume L^3 and having "a" as lattice constant.

a) Write down the periodic conditions for k_x , k_y , k_z and calculate the density of states D(w) per unit frequency in a volume $V = L^3$

b) In Debye approximation, also known as long-wavelength or continuum approximation, the dispersion relation is reduced to a simple isotropic linear relation w = v.k because the wavelength is much longer than the lattice constant ($\lambda \gg$ a). Reduce accordingly the density of state found in part (3.a)

c) Write down the Debye density of states found in part (3.b) as the sum of that of all three polarizations and plot it against "*w*".

Please return on 26/11/2015