MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics Department

8.231, Physics of Solids I

Due in Ses #19

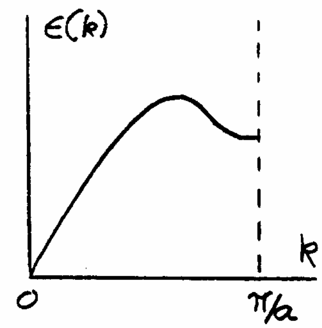
Problem Set #4

Problem 1: Density of States in One Dimension

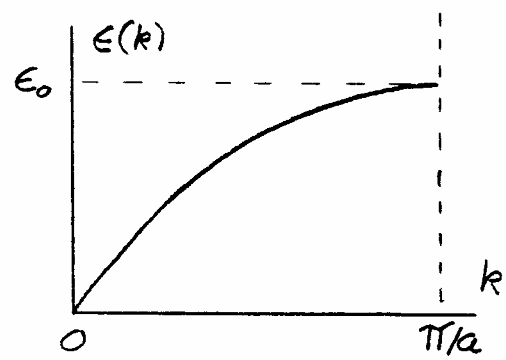
Sketch and carefully label (but do not compute analytically) the density of states as a function of energy in the following one-dimensional models:

a) The diatomic linear lattice shown in Figure 7 of Chapter 4.

b) A monatomic chain with the dispersion curve shown here.



Problem 2: Density of States in Three Dimensions



One particular acoustic phonon branch of the dispersion curve of a three dimensional solid is shown above. Near the zone edge it can be approximated by the expression

$$\varepsilon = \varepsilon_0 - A\left(k - \frac{\pi}{a}\right)^2$$

a) Calculate the contribution to the density of states from the phonons on this branch near the zone edge. Assume that this branch is isotropic in space and that the Brillouin zone boundary can be replaced by a sphere of radius π/a.

b) How many states on this branch have energies between $\varepsilon_0 - \Delta$ and ε_0, where $\Delta \ll \varepsilon_0$?

Problem 3: Two-Dimensional Debye Model

Consider a two-dimensional solid with one atom per primitive unit cell. Use a Debye model to find an approximation to the lattice heat capacity.

a) Derive expressions for the Debye wavevector k_D and the Debye temperature Θ in terms of the number of atoms per unit area N/A, the sound velocity, and Boltzmann's constant k_B.

b) Find the density of states as a function of energy for this model. Draw a carefully labeled picture of this density of states.

c) Set up, but do not evaluate, an expression for the lattice contribution to the energy of the solid.

d) Find an expression for the heat capacity. Leave your answer in terms of a dimensionless (but temperature-dependent) integral. What is the temperature dependence of the heat capacity in the low temperature limit?

e) Without doing any calculations, explain what one should expect for the temperature dependence of the heat capacity of a one-dimensional lattice in the low temperature limit.

Problem 4: Three-Phonon Interactions

Consider a crystal for which $\omega_L = v_L K$ and $\omega_T = v_T K$, where v_L and v_T are independent of K. The subscripts L and T denote longitudinal and transverse. If $v_L > v_T$, show that the normal three-phonon process T+L $\rightarrow$ T cannot satisfy conservation of energy and wavevector.

Problem 5: Decay of Elementary Excitations

A three-dimensional system has elementary excitations which at low temperature consist of a single branch with the isotropic dispersion relation

$$\varepsilon(p) = c\,p\,(1 - \gamma p^2)$$

where p is the momentum of the excitation $|\hbar \vec{k}|$, c is a velocity, and the temperature is low enough that the thermal average of $|\gamma p^2|$ is much less than 1. Show by simple conservation arguments that the sign of γ determines whether one of the excitations is able to decay into a pair of excitations, each having a lower energy. Which choice of sign leaves the excitations stable with respect to this mechanism?

Problem 6: Thermal Expansion Done Right

The thermal expansion of a crystal lattice can be understood on the basis of the assumption (verified experimentally) that the phonon frequencies increase if the lattice spacing decreases. The simplest calculation assumes that all phonon frequencies behave in a similar way under compression of the lattice:

$$\frac{d\omega(k)}{\omega(k)} = -\gamma \frac{dV}{V.}$$

The positive parameter γ (which has no relation to the γ in the previous problem) is known as Gruneisen's constant.

For a crystal in a vacuum at thermal equilibrium the pressure is zero (the crystal maintains its own shape in the absence of external influence). Thermodynamics tells us that $P = -\frac{\partial F}{\partial V}|_T$ where F is the total free energy of the solid. As far as we are concerned, F can be written as a sum of two terms: $F = \phi(V) + F_p(V,T)$. $\phi(V)$ is a structural energy associated with the geometric lattice of interacting atoms. If the atoms were stationary at their lattice sites (no degrees of freedom to be excited thermally), the volume V of the crystal would be that for which $\phi(V)$ has a minimum.

$F_p(V,T)$ is the phonon contribution to the free energy and is a sum over the free energies of each individual phonon mode, $F_p(V,T) = \sum_k F_k$.

a) The link between thermodynamics and statistical mechanics is given by the relationship $F_k = -k_B T \ln Z_k(V,T)$, where Z_k is the partition function of the individual mode. Show that at equilibrium one must have the condition

$$\frac{\partial \phi}{\partial V} = k_B T \sum_k \frac{1}{Z_k} \frac{\partial Z_k}{\partial V}.$$

b) In the canonical ensemble of statistical mechanics $Z = \sum_n e^{-E_n/k_B T}$, where the sum extends over all possible states of the subsystem being considered, in this case one phonon mode. Show that the equilibrium condition becomes

$$\frac{\partial \phi}{\partial V} = \gamma U_p/V$$

where U_p/V is the total thermal energy per unit volume in the phonon modes. This result gives the following qualitative picture of thermal expansion: as T increases, the phonon energy increases, and the equilibrium point on $\phi(V)$ shifts to larger V.

c) The linear expansion coefficient α is defined as $\alpha \equiv \frac{1}{3}\frac{1}{V}\frac{\partial V}{\partial T}\,|_P$. If $\phi(V)$ is modeled by the leading terms in a Taylor series expansion about the minimum

$$\phi(V) = -\phi_o + \frac{1}{2}K(V - V_o)^2,$$

find an expression for α. What is the temperature dependence of α at low temperatures?

Problem 7: Zero Point Energy

The lattice spacing of Li^6 is larger than that of Li^7 at absolute zero. Explain this qualitatively using the fact that the low frequency sound speed in a material is proportional to $\rho^{-1/2}$, where ρ is the mass density. The lattice spacing difference is about 0.07%. Account for this order of magnitude using a Debye model. Assume that only about 10^{-2} of the T=0 lattice constant is due to the phonons.