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SCHOOL OF PHYSICS AND ASTRONOMY

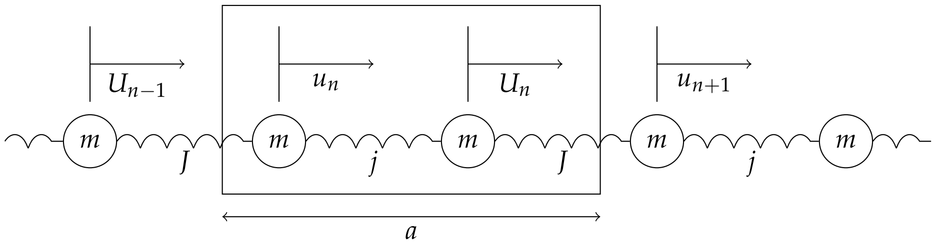
Structure and Properties of Functional Materials

Exercise Set 5

Friday, 8 February, 2013

1. *For discussion:* Why does the Einstein model fail at very low temperatures? Why does the Debye model fit low-temperature experimental data better?

2. Consider the one-dimensional diatomic chain shown below. The lattice parameter is a and the unit cell shown by a box. Every atom has the same mass m, but the bonds alternate between having spring constant J and j.



   Just as we did in class, write down the equations of motion and solve them to find ω as a function of k. Show that, just as for the case of two different masses, we have an optic and an acoustic mode. Evaluate the displacements of the two atoms at the Brillouin zone boundary $k = \pi/a$ and show that in this respect this model is different from the chain with alternating masses we discussed in class.

3. The density of allowed k values in a crystal of total volume V, in terms of k, is

$$g(k) = \frac{V}{2\pi^2}k^2.$$

   (a) Consider only acoustic phonons of low frequency, so that the speed of sound $c = \omega/k$ can be considered constant. Show that the density of phonon states in terms of ω is

$$g(\omega) = \frac{3V\omega^2}{2\pi^2 c^3}.$$

   (b) Integrate this expression to show that the total number of phonon states up to a cutoff frequency ω_{max} is $V\omega_{\text{max}}^3/2\pi^2c^3$. **Aaaaargh – another typo. Missing power of 3 in handout!!**

   (c) Explain why there are three times as many phonon modes as atoms in a material.

   (d) Hence show that the Debye frequency – the maximum occupied frequency in the Debye model – is given by

$$\omega_{\text{D}}^3 = 6\pi^2c^3n$$

   where n is the number density of atoms in the material. **Aaaaargh – same typo. Missing power of 3 in handout!!**

   (e) Why might we want to determine ω_{D} by fitting to experiment, rather than from the calculation above?