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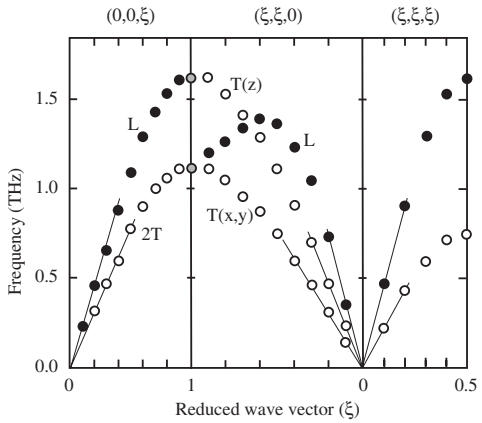
SCHOOL OF PHYSICS AND ASTRONOMY

Structure and Properties of Functional Materials

Exercise Set 4

Friday, 1 February, 2013

1. *For discussion:* Consider the dispersion curves for neon:



   (a) Why are there only two branches in the $(0,0,\xi)$ and (ξ,ξ,ξ) directions, but three in the $(\xi,\xi,0)$?

   (b) Why are the curves identical at the points $(0,0,1)$ and $(1,1,0)$? Sketch the displacements of atoms for a vibration at one of these $\mathbf{k}$ values to help your explanation.

2. Consider a hypothetical crystal structure where the motif is a molecule containing three atoms in the shape of an equilateral triangle. Sketch the Patterson map we would calculate from this crystal.

3. Prove the result claimed in class that, if we write an interatomic vector as $\mathbf{r} = (x, y, z)$ and have an interatomic potential ϕ,

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{x^2}{r^2} \frac{\partial^2 \phi}{\partial r^2}.$$

4. Consider the dispersion curves for potassium, which has a body-centred cubic structure, just as we did for neon. Show that along the $(1,0,0)$ direction all three force constants between nearest-neighbour planes are equal:

$$J_x = J_y = J_z = \tfrac{4}{3}K$$

   Note misprint in the question sheet handed out in class (which had $2K$ here) and also in Martin's book (p. 187)!

5. Consider our general expression for phonon dispersion in a 1D monoatomic chain:

$$\omega_k = \sqrt{\frac{4J}{m}} \left| \sin \frac{ka}{2} \right|$$

   Show that this gives the correct results in the limiting cases we discussed (*i.e.*, as $k \to 0$ and for $k = \pi/a$). **Note another misprint – this one really my fault – sorry! The distributed version of this sheet had $k = \pi/2$ here.**