PH207 - Solid State Physics

Problem set N. 2

Handed out 06/03 – Due in 13/03

Consider a biatomic crystal in ONE dimension, with atoms of species A and B equally spaced and alternated, such that the distance between nearest-neighbour atoms is a and each atom of one species has two atoms of the other species as nearest neighbours. The interaction potential is

$$V(x) = \pm q^2 \frac{e^{-c|x|}}{|x|} \tag{1}$$

where the + sign is for atoms of the same species and - for atoms of different species.

1. Show that the interaction produced by all other atoms on a given one can be written as

   $$\tilde{V} = 2q^2 \sum_{m=1}^{\infty} (-1)^m \frac{e^{-2mac}}{2ma} \tag{2}$$

   [*3 marks*]

2. Use the identities

   $$\int_1^{+\infty} e^{-\beta r} = \frac{e^{-\beta}}{\beta} \qquad \text{and} \qquad \sum_{n=0}^{\infty} (-1)^n y^n = \frac{1}{1+y} \tag{3}$$

   to compute the sum. You need to rewrite each term in the sum as an integral and change the order of the sum and integration. Using this result, show that V can be written in the form

   $$V(a) = -\alpha \frac{q^2}{a} \tag{4}$$

   and give the expression for α (the Mandelung "constant" of our problem) in terms of a and c.
   [*7 marks*]

3. Now assume that the atoms experience also an hard core repulsion potential, such that the resulting interaction for each atom is described by

   $$V(r) = -\alpha \frac{q^2}{r} + \frac{C}{r^m} \tag{5}$$

Suppose we can determine from experiments the value of

$$B = \left.\frac{\mathrm{d}^2\mathrm{V}}{\mathrm{dr}^2}\right|_{r=a} \tag{6}$$

Describe how we can use this information and the knowledge of a to determine C and m (you just need to write down the system of equations that determines those quantities, not to solve it).
[*5 marks*]

4. Determine the coesion energy per atom (defined as the energy needed to separate the two ionic species) in terms of the parameters of the potential. Which other information would one need to determine the energy needed to separate the ionic crystal into its constituent atoms?
[*5 marks*]

Note that each question can be solved independently of the others