

# Eðlisfræði þéttfnis I

## Dæmablað 2

Skilafrestur 8. September 2015 kl. 15:00

### 1. Bravais lattices (10)

In each of the following cases indicate whether the structure is a Bravais lattice. If it is, give three primitive vectors; if it is not, describe it as a Bravais lattice with as small as possible a basis:

(a) Base-centered cubic: simple cubic with additional lattice points at the center of the horizontal faces of the cubic cell.

(b) Side centered cubic: simple cubic with additional lattice points at the center of the vertical faces of the cubic cell.

(c) Edge-centered cubic: simple cubic with additional lattice points at the midpoint of the lines joining the nearest neighbors of the cubic cell, i.e. at the midpoint of the edges of the cubic cell.

### 2. Linear ionic crystal (15)

Consider a line of  $2N$  ions of alternating charge  $\pm q$  with a repulsive potential energy  $A/R^n$  between nearest neighbors.

(a) Show that at the equilibrium separation

$$U(R_0) = \frac{2Nq^2 \ln 2}{4\pi\epsilon_0 R_0} \left(1 - \frac{1}{n}\right)$$

(b) Let the crystal be compressed so that  $R_0 \rightarrow R_0(1 - \delta)$ . Show that the work done in compressing a unit length of the crystal has the leading term  $\frac{1}{2}C\delta^2$ , where

$$C = \frac{(n-1)q^2 \ln 2}{4\pi\epsilon_0 R_0}$$

Note that we would not expect to obtain this result from the expression for  $U(R_0)$ , but we must use the complete expression for  $U(R)$ .

### 3. Ionic crystals (15)

We can use the form

$$u(r) = \frac{\alpha e^2}{r} + \frac{C}{r^m}$$

of the cohesive energy per ion pair to investigate the stability of the possible crystal structure an ionic crystal may assume. Assuming that the coupling constant  $C$  characterizing the contribution of the short-range repulsion is proportional to the coordination number  $Z$ , show that the equilibrium cohesive energy for different lattice types varies as  $(\alpha^m/Z)^{1/(m-1)}$ , and use the values of the Madelung constant  $\alpha$  in the table below to construct a table of relative stability according to the value of  $m$ . (Hint: First examine the case of large or small  $m$ .)

Crystal structure	Madelung constant, $\alpha$
Cesium chloride	1.7627
Sodium chloride	1.7476
Zinchblende	1.6381