PH207 - Solid State Physics

Problem set N. 4

Handed out 16/03 – Due in 23/03

Consider a linear (i.e. 1-dimensional) array of neutral atoms. Model the electronic charge density and the nuclear charge density as pointlike charges of value $-q$ and q respectively and assume that their interaction is described by an harmonic oscillator potential:

$$V_a(r) = \frac{1}{2}kr^2 \tag{1}$$

where k is given.

1. Consider two such atoms at distance $R \gg r_1, r_2$, where r_1 and r_2 are the distances of the positive and negative charges in each of the two atoms. Write the exact expression of the electromagnetic interaction potential in terms of R, r_1 and r_2 and approximate it at the second order in the Taylor expansion, not considering the interaction (1). [*5 marks*]

2. Reintroduce the interaction (1). Show that the effect of the interaction computed in the previous point is to couple the two oscillators and compute the normal modes. [*5 marks*]

3. Write down also the kinetic term of the energy. By taking the difference between the zero point energy of two uncoupled oscillators and the zero point energy of the two coupled oscillators, show that the interaction goes like $-1/R^6$, i.e. the interaction is of the Van der Vaals type (you need to expand a square root to second order in $1/R^3$). [*5 marks*]

4. A crystal of those atoms will be interacting according to the Lennard-Jones potential

$$V_{LJ} = 2\epsilon N \left(-A_6 \left(\frac{\sigma}{R} \right)^6 + B_{12} \left(\frac{\sigma}{R} \right)^{12} \right) \tag{2}$$

   Taking the elastic constant from the above expression, write down the dispersion relation for the corresponding one-dimensional phonon as a function of ϵ and σ. [*5 marks*]