PROBLEM SHEET 2

Introduction to Condensed Matter Theory

(To be submitted on Wednesday, 13.05.2015 directly to the tutor in the class or alternately you can drop them in the insititute mail box –, KOMET 337 one day before)

1. Geometric Structure Factor: The Geometric structure factor of a crystal is defined as follows:

$$S_{\mathbf{K}} = \sum_{j=1}^{n} e^{i\mathbf{K}\cdot\mathbf{d}_j} \tag{1}$$

where $\mathbf{K}$ is the reciprocal lattice vector and $\mathbf{d}_j$ corresponds to n-atomic basis (n identical atoms at positions $\mathbf{d}_1, \mathbf{d}_2, ...\mathbf{d}_n$) of a monoatomic, hexagonal close-packed crystal as shown in figure 1. The conventional basis is given by the vector:

$$\mathbf{a}_1 = a\mathbf{e}_x, \mathbf{a}_2 = \frac{a}{2}\mathbf{e}_x + \frac{a\sqrt{3}}{2}\mathbf{e}_y, \mathbf{a}_3 = c\mathbf{e}_z \tag{2}$$

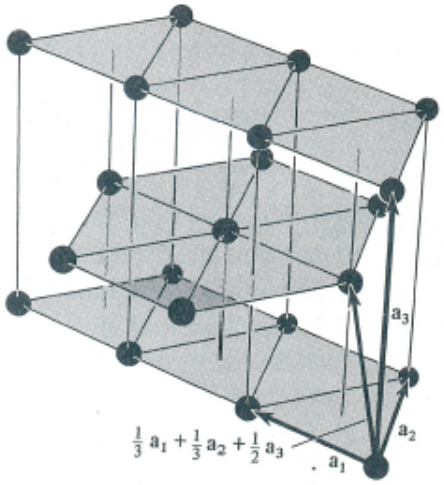

Figure 1: Hexagonal close-packed crystal

(a) Show that the geometrical structure factor for such a lattice can take exactly the values

$$S_{\mathbf{K}} = 1 + e^{im\frac{\pi}{3}}, m = 1, ..., 6 \tag{3}$$

when **K** passes through the points of the reciprocal lattice of the simple hexagonal lattice. [2]

(b) Show that you can find the points with Structure factor $S_{\mathbf{K}} = 0$ in the alternating planes of the family of lattice planes perpendicular to the z-axis. [2]

(c) Show that all the reciprocal lattice points have a non-vanishing structure factor in the plane perpendicular to the z-axis containing **K** = 0. [2]

(d) Show that in the alternating planes with zero structure factor, the point that is located on the z-axis has structure factor 0. [1]

(e) Show that the removal of all points with structure factor 0 from such a level reduces the triangular structure of the reciprocal lattice to a honeycomb structure. [2]

2.Born-Oppenheimer approximation: Consider the following Hamiltonian for the problem of two coupled oscillator

$$\hat{H} = \frac{\hat{p_1}^2}{2M} + \frac{\hat{p_2}^2}{2m} + \frac{K}{2}\hat{x_1}^2 + \frac{k}{2}(\hat{x_1} - \hat{x_2})^2, \hat{p_j} = \frac{\hbar}{i}\frac{\partial}{\partial x_j}(j = 1, 2) \tag{4}$$

(a) Determine the exact eigen values of $\hat{H}$. [4]
Note: To make it more clear, write $\frac{m}{M} = \gamma, \frac{k}{m} = \omega_2^2$ *and* $\frac{K}{m} = \omega_1^2 \Rightarrow \frac{K}{M} = \gamma\omega_1^2$, *and substitute* $\hat{\tilde{x_1}} = \sqrt{M}\hat{x_1}$, $\hat{\tilde{p}}_1 = \frac{\hat{p_1}}{\sqrt{M}}$, $\hat{\tilde{x_2}} = \sqrt{m}\hat{x_2}$, $\hat{\tilde{p}}_2 = \frac{\hat{p_2}}{\sqrt{m}}$.

(b) Now assume that the masses are very different $(m << M)$ so that the approximation can be applied. Now take $\hat{H_1} = \frac{\hat{p_1^2}}{2M}$ (negligible energy of the atoms) and solve the problem for the "electron" $\hat{H_0} = \hat{H} - \hat{H_1}$ for a fixed paramter x_1, that is, determine the eigen values $E_{n2}(x_1)$. Then find the eigen values for the " atomic" problem, that is, for $\hat{H_{BO}} = \hat{H_1} + E_{n2}(x_1)$. [3]

(c) Compare this with the exact solution. Derive the result of (a) in γ. [2]

3. Madelung constant in one dimension: Let's consider a hypothetical one dimensional crystal (infinite length) which is composed of Cl^- anions and Li^+ cations alternately. The distance between the atoms is given by $a = r^+ + r^-$ where $r^{\pm}$ is the radius of the respective ions.

(a) Show that the energy of the electrostatic interaction of the cation with its neighbours (all!) is [1]

$$U = -M\frac{e^2}{4\pi\varepsilon_0 a} \tag{5}$$

(b) The dimensionless factor M is known in crystallography as the Madelung constant (and is used in determining the electrostatic potential of a single ion in a crystal by approximating the ions by point charges). Determine M. Remember the power series of the natural logarithm. Is the lattice stable? [1]