PROBLEM SHEET 3

Introduction to Condensed Matter Theory

(To be submitted on Monday, 01.06.2015 directly to the tutor in the class)

1. **Lennard-Jones potential** The interaction between two (neutral) noble gas atoms i and j is well described by the so-called *Lennard-Jones potential* which has the general form

$$V_{ij}(r_{ij}) = V(r) = A\left(\frac{\sigma}{r}\right)^{12} - B\left(\frac{\sigma}{r}\right)^{6} \quad (1)$$

where A, B and σ are the characteristic atomic parameter.

(a) Plot V(r) and find the equilibrium distance r_0 and the binding energy of this configuration with respect to the above parameters. [2]

(b) Now take the case of $A = B$ and investigate the stability for small aggregate of atoms (N = 2,3). Now take r_0 as the minimum interatomic distance and determine in each case the minimum potential energy for different geometric configurations. [1]

For sufficiently low temperature and under atmospheric pressure, the noble gases Ne, Ar, Kr, Xe crystallizes into a face-centered cubic lattice. The binding energy per particle (energy required to remove the individual particles from the lattice) u is dependent on the distance r of the atoms and is given for a particle by the sum of the potentials of the neighbors (as in problem (3) of problem sheet 2). u is then described by a Lennard-Jones potential as:

$$u = 2\varepsilon\left[A_{12}\left(\frac{\sigma}{r}\right)^{12} - A_6\left(\frac{\sigma}{r}\right)^{6}\right] \quad (2)$$

where the coefficients $A_{12} = 12.13$ and $A_6 = 14.45$ as the lattice sum (similiar to the Madelung constant in Problem sheet 2). In the following we also assume that the values for the paramters ε and σ as known (N. Bernardes, Physical Review 112, 1534(1958)):

	Ne	Ar	Kr	Xe
ε (meV)	3.1	10.4	14	20
σ (nm)	0.274	0.340	0.365	0.398

(c) Determine also here the equilibrium distance r_0 of the atoms in the lattice as a function of σ and the equilibrium potential as a function of ε and determine the values for the various elements. [2]

2. **Lattice dynamics of monoatomic linear chain:** In the lecture, we introduced phonons in general. Here we will consider the lattice vibrations of a concrete example.

Consider a linear chain of N atoms of mass m, separated by an equlibrium distance a from one another and subject to periodic boundary conditions. As is known from the lecture, the potential around the equilibrium state can be developed for small displacements u_i in the so-called harmonic approximation described by the second order term of the series. Suppose further that interactions between next neighbouring atoms dominate and is the same for all atoms. So the effective potential describes the chain of atoms, which are linked via spring with spring constant K with their neighbours.

(a) Write the effective potential and determine the equation of motion for a particle at lattice point n. [2]

(b) With the solution for the equation of motion

$$u_n = Ae^{-i\omega t}e^{ikna} \tag{3}$$

there is a relation between frequency ω and wave number k, known as the *dispersion relation*. Obtain this. [2]

(c) What possible values follow for k from the periodic boundary conditions? Why is it possible to limit the view of the lattice vibrations in the Brillouin zone $(-\frac{\pi}{a} < k < \frac{\pi}{a})$? [1]

(d) Show that the equation of motion in (a) for large wavelength $(ka << 1)$,i.e. in the continuum can transform into a continous wave equation. Compare the propogation velocity of such waves with the speed of sound in the lattice defined as $v_g = \frac{\partial \omega}{\partial k}$. [2]

3.**Lattice dynamics of diatomic linear chain** Let's take a linear chain of atoms with alternating masses m_1 and m_2. The distance between the identical atoms is a and the effective potential is described by a system of harmonic oscillators with spring constant K.

(a) Write again the equation of motion in the system. [1]

(b) Then use the following ansatz

$$u_{2n+1} = Ae^{-i\omega t}e^{ik(2n+1)\frac{a}{2}} \tag{4}$$

$$u_{2n} = Be^{-i\omega t}e^{ik2n\frac{a}{2}} \tag{5}$$

with $n \in \mathbb{Z}$ and deduce the eigen value problem. [2]

(c) Solve the eigen value problem and obtain the dispersion relation. How many eigen modes does the linear chain have (for a fixed wave number)? What periodicity does the linear chain have? [3]

(d) What happens to the two dispersion curves in the points $k = 0$ and $k = \frac{\pi}{a}$. How does the neighbouring ions oscillate with respect to each other? [2]