Technische Universität Berlin
Institut für Theoretische Physik
Lecture Course: Prof. Dr. Matthias Scheffler, Dr. Christian Carbogno
Exercises: Dr. Christian Carbogno, Henrik Kowalski et al.

June 13,2017

http://www.itp.tu-berlin.de/menue/lehre/lv/ss_2017/pflichtveranstaltungen_masterstudium/theoretische_physik_vi_vertiefung_theoretische_festkoerperphysik_i_ii/

Theoretical Material Science: Exercise Sheet 8

Please hand in solutions by: Tuesday, June 20, start of the exercise class

Exercise 19 (4 points): *Phonon dispersion relation for the diatomic chain*
Consider a one-dimensional chain with 2 alternating types atoms of masses M_A and M_B. Let the potential between any two neighbouring atoms be the same as that caused by a classical elastic spring with spring constant C. For simplicity, the atoms are assumed to move only in one dimension along the chain and interactions past the nearest neighbors shall be ignored.

a) Derive the classical equation of motion for the problem.

b) Use an appropriate ansatz to solve the equation derived in part a.
Sketch the results, how do the nuclei move at the Γ-point ($q = 0$)?

Exercise 20 (4 points): *Phonon density of states*
Calculating Brillouin zone integrals of a given property $\Pi_s(\omega(\mathbf{q}))$ can be a exhausting task. For this purpose the phonon density of states $g(\omega)$ can be introduced to reduce the computational effort.

a) Show that using the phonon density of states $g(\omega) = \sum_s \int_{\mathrm{BZ}} \frac{1}{(2\pi)^3}\delta(\omega - \omega_s(\mathbf{q}))d\mathbf{q}$ any integral $\Pi = \sum_s \int_{\mathrm{BZ}} \frac{1}{(2\pi)^3}\Pi_s(\omega(\mathbf{q}))d\mathbf{q}$ can be written as $\Pi = \int g(\omega)\Pi(\omega)d\omega$.

b) In the one dimensional case the phonon density of states can be written as
$g(\omega) = \sum_s \int \frac{1}{2\pi}\delta(\omega - \omega_s(q))dq$. Calculate the phonon density of states under the assumption of the dispersion curve for a linear chain $\omega_s(q) = \omega_0|\sin(\frac{qa}{2})|$.

Exercise 21 (4 points): *Vibrational properties of real materials*
In the lecture and the last two exercises you got acquainted with the phonon dispersion relation and the phonon density of state. However in modern theoretical material science one most often faces problems that can not be treated analytically anymore. In this task you will see how to practically assess vibrational properties of crystals in the harmonic approximation in a way that is widely used in modern theoretical material science.

a) Calculate the phonon band structure of diamond silicon along the path
$\Gamma \to X \to W \to K \to \Gamma \to L$ in the first cubic supercell.
What happens to the acoustic modes at the Γ-point and why?
Redo the calculation for the primitive unitcell and compare and plot the results for the primitive, the first cubic, the second cubic supercell, and the fourth cubic supercell. Do we reach convergence (the *ab-initio* results for the second and fourth cubic supercell will be given)?

b) Calculate the phonon density of states for all four supercell sizes. Compare and plot the results. Does it converge faster or slower than the band structure? Can you give an explanation?
Also take a closer look at the density of states where do the peaks occure?