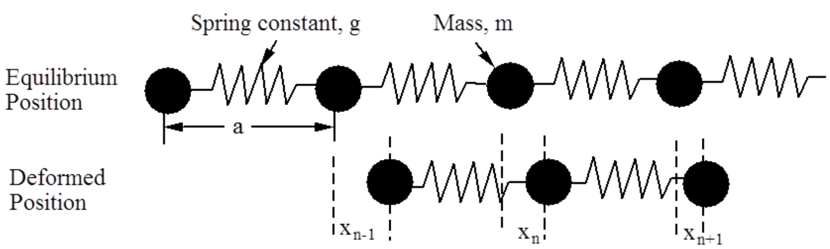
FYS3410 Spring 2018

Module II

Practical assignments:

1. Consider vibrations in an infinite 1D-lattice having one atom in the basis as shown in Fig.1 below



(a) Derive the dispersion relation for a wave propagating in this crystal;
(b) Make a graph and explain why it is sufficient knowing the dispersion relation within the 1st Brillouin zone (BZ) only;
(c) Analyze the group velocity, specifically at the center and at the edges of the 1st BZ;
(d) Assume the schematics in Fig.1 to model a longitudinal wave propagating in [100] direction in Na crystal, estimate the maximum amplitude of the vibrations.

2. Derive/analyze the phonon density of states (DOS) in 1D containing N atoms; e.g. use the following scenario:
   (a) Introduce periodic boundary conditions, derive DOS in the k-space, and plot DOS(k);
   (b) Use the 1-D dispersion relation as obtained solving problem 1, i.e. $\omega=\omega_0\sin(ka/2)$, find DOS as a function of ω, and plot DOS(ω).
   (c) Pay attention to a relative “simplicity” of DOS(k) and significantly bigger “complexity” of DOS(ω), providing an argument for calculating DOS in k-space.

3. Evaluate progress/limitations of Dulong-Petit, Einstein, and Debye models for explaining temperature dependence of the lattice heat capacity - $C_v(T)$. (Suggestion: instead of deriving formalisms in full, consider making a qualitative comparison of “oscillator models” assumed to be responsible for the corresponding $C_v(T)$ dependences.

4. A two-dimentional finite hexagonal lattice has a spacing of a = 3 Å. Assuming the sound velocity in this material to be $c = 10^3$ m·s^{-1}, what is the Debye frequency ω_D?

5. Provide a qualitative explanation of the T^3 -Debye law comparing the fraction of phonon modes occupied at a given temperature *T* versus all modes within the Debye cut-off wavevector K_D. Estimate K_D and θ_D for Na crystal.

6. The thermal conductivity coefficient κ is given by $\kappa = \frac{1}{3} C_V \Lambda$, where C_V is the heat capacity and Λ is the phonon mean free path. Consider temperature dependences for C_V (account for the 3D lattice related heat capacitance only), Λ, and κ at low/high temperature limits and fill Table I. Make a plot illustrating temperature dependence of κ and elaborate on "normal" versus "umklapp" processes.

Table I

	C_V	Λ	κ
low T			
high T			

7. Thermal properties in 1D.
   (a) Derive the formula for the low temperature heat capacity of a single 1D phonon mode in the Debye approximation;
   (b) Explain (qualitatively) the temperature behaviour of the lattice heat conductivity in nanowires