

Condensed Matter Computer Project

Deadline: 10:00 a.m., April 29, 2013.

You must write a user-friendly program that allows the user to plot the following:

- (a) Dispersion relations for single atom- and two atom- type one dimensional chains.
- (b) Lattice vibrations similar to what can be observed in the following links
<http://www.chembio.uoguelph.ca/educmat/chm729/Phonons/movies.htm> or
<http://en.wikipedia.org/wiki/Phonon>

Each item described above is independent of each other, that is, you will not need to allow the plotting of dispersion relation and lattice vibrations in a single graph. When plotting (a) the user should be able to plot the single atom, the double atom or both types of dispersion relations. Lattice vibrations for both transverse and longitudinal waves should be shown on the same screen. At least 12 atoms should be observable.

Assume default values as needed. Allow the user to rescale. In case (a) the user should be allowed to input or select masses, atomic spacing, and spring constants. Be sure to indicate to the user the units in which you want the required data. Your program should be as foolproof as possible.

Grading:

60 pts	program works: it plots all graphs required without crashing, should have default values, variables used should not be identical to those used by peers, in case that two programs are nearly identical you will lose 50 pts.
+15 pts	program allows for user input but does not accept unrealistic values such as negative masses, has tooltips for data input.
+15 pts	program is user friendly, allows for graph rescaling, colors are used in graphs, descriptions of program sections available in pull down or popup menus
+10	be creative and impress reviewer (i.e. me!!) in a unique way (i.e., don't look at the work of your peers)

You will need to e-mail me your executable program by the deadline indicated above.