Project List

1. Compute the phonon dispersion curves for a real material (solid Argon) including deformation gradient effects. Argon can be described by a Lenoard-Jones potential (see Dobbs and Jones *Reports on Progress in Physics*, **20**, 516-564, (1957) and Dobbs, Figgins, and Jones *Il Nuovo Cimento*, **9** Supplement, 32-35, 1958. Your program should allow you to compute dispersion curves for standard directions in wavevector space, select the number of neighbors to include, select the deformation gradient.

2. Find the phonon density of states function via brute force computation for an ideal 2D lattice with and without basis atoms. This is a classic technique that involves binning the possible values and computing the distribution functions. The density of states functions are used in many solid-state physics computations; see for example the discussion in Ashcroft and Mermin regarding heat capacity measurements.

3. Reproduce the computations in Chopra and Zettl *Solid State Communications* **105** 297-300 (1998).

4. Report on the glassy state model of C. Monthus an J.-P. Bouchaud *Journal of Physics. A, Mathematical and General*, **29**, 3847-3869, 1996.

5. Report on the computation of heat capacity in crystals using phonon frequencies and the Debye and Einstein approximations to the density of states.

6. Presentation and discussion of the paper of Flory, Hoeve, and Ciferri, J.Poly.Sci, Vol 34, 337-347, 1959 with special attention given to a discussion of internal energy contributions with data analysis from this and other papers. See e.g. Shen and Blatz, J.Appl.Phys v39 4937-4943 (1968).

7. Report on the effects of nearest neighbor interactions for dihedral bond potentials in linear polymers. See Chapter 5 of P.J. Flory *Statistical Mechanics of Chain Molecules* with particular emphasis on reproducing the results found in §5.4.

8. Report on the Worm-Like Chain (WLC) model. Here a polymer chain is treated like flexible continuous rod. Instead of $\boldsymbol{R} = \sum_i \boldsymbol{a}_i$, one now has an expression like $\boldsymbol{R} = \int_0^L \boldsymbol{t}(s)ds$, where $\boldsymbol{t}(s) = d\boldsymbol{r}(s)/ds$ is the tangent vector to the rod with $\boldsymbol{r}(s)$ being the position vector to a point along the rod. Such a model is popular for stiff polymers and is well-known in the DNA modeling literature. Possible potential energies can come from bending (bond angle like effects) and torsion (dihedral like effects). Some

articles to get you started: *J. Chem. Phys*, **58**, 1564-1568, 1973. *Macromolecules*, **15**, 537-541, 1982. *Biophysical Journal*, **76**, 409-413, 1999. *J Chem. Phys.*, **80**, 930-935, 1984. [N.B. Notation varies from paper to paper so you have to read carefully.]

9. Report on the thermomechanical behavior of Bose-Einstein condensates. A BE condensate is special low temperature state of a system of boson (quantum particles that whose state occupation numbers can be of any value – as opposed to, say, fermions where occupation numbers are restricted to 0 or 1). Phonons and photons are two examples of bosons. (The most common example of fermion is the electron.) See Section 4.4 of F. Schwabl *Statistical Mechanics* and Chapter 9 in F. Reif *Fundamentals of Statistical and Thermal Physics*.

10. Report on the Pruning and Enrichment Rosenbluth and Rosenbluth method of statistical importance sampling for the monte carlo simulation of polymer chains; see Grassberger *Physcial Review E*, **56**, 3682-3963, 2002.

11. Report on classical methods for computing thermal expansion in statistical mechanics and their comparison to DFT techniques.

12. Report on the statistical mechanics model for muscle behavior as presented in T.L. Hill *Progress in Biophysics and Molecular Biology*, **28**, 267-340, 1974.

13. Report on the Rouse model for dilute polymeric solutions and/or the Zimm model. References: Chapter 4 in Doi and Edwards *The Theory of Polymer Dynamics*; Chapter 4 Öttinger *Stochastic Processes in Polymeric Fluids*.

14. Report on diffusion rates in solids. Chapter 7 Weiner *Statistical Mechanics of Elasticity*.

15. Report on phonon-phonon interactions (anharmonic effects). (Could be hard). Chapter III Ziman *Electrons and Phonons*. Chapter 25 Ashcroft and Mermin *Solid State Physics*.

16. Report on non-ideal gas laws including the van der Walls gas; see Section 10.3 Reif *Fundamentals of Statistical and Thermal Physics*.

17. None of the above (but I do have to agree to it).