P3.1 Typical compressibilities and frequencies The interatomic potential in a noble gas like argon is well represented by the Lennard-Jones form of Eq. 20.2. A crystal of argon has a close-packed FCC structure, and most of the interaction occurs between each atom and its twelve nearest neighbors. Thus the cohesive energy per atom is about 6ϵ.

a) If external pressure is applied to an argon crystal, the separation between all the atoms decreases by the same amount. Roughly how many Joules of energy are required to compress a cubic centimeter of argon by one percent? Use Eq. 20.2 and the table at the bottom of page 398. You need only consider nearest-neighbor interaction.

b) Compare the energy in a) to that for i) iron and ii) liquid water, using table values for their bulk moduli.

c) Find the vibrational frequency ω of small oscillations for a single argon atom displaced from equilibrium, supposing that all the other atoms are fixed. This is a typical vibrational frequency of the real crystal. What electromagnetic wavelength corresponds to this frequency? How large is $\hbar\omega$ compared to k_BT at room temperature? How large is $\hbar\omega$ compared the energy to flip an electron spin in a one-Tesla magnetic field?

The interaction potential between carbon atoms in diamond has a much different origin than that between argon atoms. Nevertheless, the Lennard-Jones form is an adequate qualitative represention for the interaction. For diamond, the minimum energy ϵ is 3 eV and the separation $2^{1/6}\sigma$ is .15 nanometer.

d) Using this representation of the potential, roughly how many Joules of energy are required to compress a cubic centimeter of diamond by one percent? Compare with a) and b) above. Again, consider only interactions between neighboring carbon atoms.

e) Estimate the vibration frequency of one carbon atom if all the others are held fixed. For this estimate you can assume that a small displacement costs the same energy for all the nearest neighbors. Compare with c) above.

P3.2 Lennard-Jones chain A line of N atoms interacts by the Lennard-Jones potential of Eq. 20.2. Interactions beyond nearest neighbors can be neglected. Its equilibrium length is evidently $2^{1/6}N\sigma$. This line of atoms is pulled at its ends, so that the separation is increased to $(1+\gamma)2^{1/6}\sigma$.

a) Find the tension force F needed to give this increase in length, for $\gamma \ll 1$.

b) Find the change in the speed of long-wavelength compressional waves for $\gamma \ll 1$. Does the speed increase or decrease as γ increases?

c) Find the speed of *transverse* waves relative to that of longitudinal waves of the same wavelength.

P3.3 Two-dimensional specific heat A certain two-dimensional simple-square lattice of lattice constant a has the dispersion relation $(\omega_L(k))^2 = c_L^2k^2$, for longitudinal vibrations and $(\omega_L(k))^2 = c_T^2k^2$ for transverse vibrations for $ka \ll 1$.

a) What is the density of vibrational frequencies $g(\omega)$ for an $N-$atom crystal at frequencies ω described by the dispersion relation above? That is, what is the number of modes between ω and $\omega + d\omega$?

Suppose that for some wave-vector $\vec{k}_0$, the $\omega_L(k)$ has an absolute maximum. Near this maximum $\omega_L(k) = \omega_0 - A(\vec{k} - \vec{k}_0)^2$. You can assume $\omega_T(k)$ always lies below ω_0.

b) Find the form of $g(\omega)$ when $\omega \lesssim \omega_0$, and when $\omega \gtrsim \omega_0$.

P3.4 Phonon numbers in a mode A vibrational normal mode of frequency ω has allowed energies $(n+\frac{1}{2})\hbar\omega$, for some integer n, as noted in Chapter 23. When such a mode is in equilibrium with a reservoir at temperature $T = 1/\beta$ the average of n, denoted $\langle n\rangle$, is given by $\langle n\rangle = (e^{\beta\hbar\omega} - 1)^{-1}$.

a) For a given $\langle n\rangle$ what is the *most probable* value of n?

b) For a given $\langle n\rangle$ what is the variance of n, *i.e.,* $\big\langle (n - \langle n\rangle)^2\big\rangle$.