PROBLEM SET 4 Due Thursday February 14

Physics 140A– WINTER 2013

[1.] In class last week we discussed getting a roughly correct value the speed of sound (300 m/s) from the expression for the phonon frequency $\omega(q) = \sqrt{2k/M}\,(\,1 - \cos qa\,)$. Notice that I have inserted a factor of the lattice constant a into this expression. This is needed for q to have the correct units (inverse length) for a wave number. Put another way, the positions of the atoms, which we labeled as integers n in class, were really na, so that our expressions e^{iqn} should really have been e^{iqna} leading us to replace q by qa.

To proceed, we need to get some estimate for the "spring constant" k. To do this, consider the following crude picture: two atoms with net charge of order the charge on an electron $e = 1.6\,\mathrm{x}\,10^{-19}$ Coulomb are located at $x = 0$ and $x = 2a$ with $a = 2\,\mathrm{x}\,10^{-10}\,m$ being a typical atomic separation in a crystal. They are pinned in position (not allowed to move). The potential $V(x)$ for an atom, also of charge e, located somewhere between them, $0 < x < 2a$, is

$$V(x) = \frac{1}{4\pi\epsilon_0}\left(\frac{e^2}{x} + \frac{e^2}{2a - x}\right)$$

with $1/4\pi\epsilon_0 = 9\,\mathrm{x}\,10^9$ in the MKS units we are using.

a. What is the equilibrium position x_0 of the in-between atom?

b. Write the Taylor expansion for $V(x)$ about $x = x_0$. What should we identify as the spring constant k in this expansion? What is its numerical value?

c. The phonon frequency $\omega(q) = \sqrt{2k/M}\,(\,1 - \cos qa\,)$ rises from $\omega = 0$ at $q = 0$ to $\omega = \sqrt{4k/M}$ at $q_{\max}a = \pi$. Approximate this as a linear rise, so that $\omega = v_s q$ (linear phonon dispersion relation) all the way from $\omega = 0$ to $\omega = v_s q_{\max}$. What do you get for the speed of sound v_s if you use an atomic mass $M = 50\,M_{\mathrm{proton}}$?

[2.] Consider a triatomic molecule with masses m at the two ends and $M \neq m$ in between. What are the normal mode frequencies if the masses are connected by springs of spring constant k? What are the normal mode eigenvectors? Explain which of these normal mode eigenvectors and eigenfrequencies are 'obvious'.