PHYSICS 555 FALL 2003

problem set 3

due Wednesday Oct. 15

1. **Localized impurity state for phonons.** Suppose you have a 1-d chain of atoms, spacing a, mass M, with nearest neighbor springs K. At the origin $\ell = 0$ is an impurity atom. The mass is $M - \Delta M$. The spring constants are unchanged.

   a. Write Newton's equation of motion for atoms ℓ = 2, -1, 0, 1, 2.

   b. Try whether a solution exists where every atom oscillates at some unknown frequency ω and the amplitudes of displacement are A for atom 0, and decaying with alternating signs in both directions (positive and negative) away from atom 0. In other words, $u_\ell = (-1)^{|\ell|}\alpha^{|\ell|}$ where α is an unknown number less than 1. If such a localized solution exists, find the values of A, α, and ω.

2. **Green's function method.** For the same problem, the Green's function method (presented in class and in Ziman's book, p. 71ff.) can be used. The equation for the frequency ω of oscillation is

$$\frac{1}{N}\sum_Q \frac{\omega^2}{\omega^2 - \omega_Q^2} = \frac{M}{\Delta M}$$

   where ω_Q is the eigenfrequency for a perfect chain with one atom per cell. With only nearest neighbor springs, ω_Q^2 is $\omega_{\max}^2 \sin^2(Qa/2)$. Ziman's book has a negative sign on the right – that is because the impurity mass was defined there as $M + \Delta M$ so ΔM has the opposite sign. Show that this gives a solution with the same frequency as in the first problem.

note: These results were derived in class by a series of elementary tricks starting from a rigorous but graphical solution of the surface state on the diatomic chain with a light mass termination.