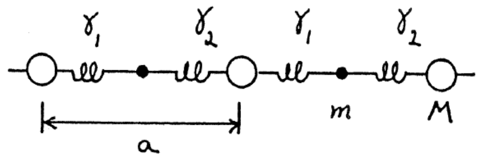
Physics 601 **Homework Set 5** **Fall, 2007**

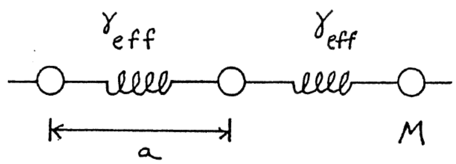
Due date: Monday Nov. 12.

Reading: Kaxiras Ch. 6

1) (25 points)
Consider the longitudinal oscillations of a linear chain consisting of alternate masses M and m, and alternate spring constants γ_1 and γ_2, as shown.

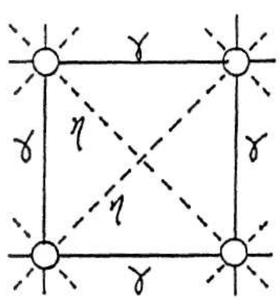


Set up the force-constant matrix $\widetilde{\Phi}(k)$. Now let the lighter mass m vanish (adiabatic approximation), and solve the resulting secular equation for the normal mode frequencies. Show that the results are identical to those of the system



with $\gamma_{\text{eff}} = \gamma_1\gamma_2/(\gamma_1+\gamma_2)$. Can you explain why, physically?

2) (40 points)
Consider a 2D square lattice with atom vibrations in the $x-y$ plane only, connected by nearest-neighbor springs of force constant γ, and next-neighbor springs of force constant η.



a) Show that

$$\widetilde{\Phi}_{\mathbf{k}} = \begin{pmatrix} 2\gamma(1-\cos k_x a) + 2\eta(1-\cos k_x a \cos k_y a) & 2\eta \sin k_x a \sin k_y a \\ 2\eta \sin k_x a \sin k_y a & 2\gamma(1-\cos k_y a) + 2\eta(1-\cos k_x a \cos k_y a) \end{pmatrix}$$

b) Find $\widetilde{\Phi}(\mathbf{k})$ at $\mathbf{k} = (\frac{\pi}{a}, 0)$ and find the frequencies at this k-point. Sketch the pattern of displacements associated with each mode, and if a mode frequency should happen to be independent of γ or η, see if you can explain why with reference to your sketch.

c) Repeat part (b) for the point $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$.

d) Expand $\widetilde{\Phi}_{\mathbf{k}}$ as a Taylor series in powers of k, keeping only terms up to quadratic order in k ("acoustic limit").

e) Using (d), solve for $\omega(\mathbf{k})$ for the special case $\eta = 0$. Find the (vector) group velocity $\mathbf{v}_g = \nabla_{\mathbf{k}}\omega$. How does the direction of energy propagation $\hat{v}_g$ vary with $\hat{k}$? Comment on the pathologies of the $\eta = 0$ case.

f) Using (d), solve for $\omega(\mathbf{k})$ for the case $\gamma = 2\eta$, find $\mathbf{v}_g$, and discuss the dependence of $\hat{v}_g$ on $\hat{k}$. *Hint: if you have done this right, the algebra should simplify strongly!* [Note that real crystals fall somewhere between the extremes of (e) and (f).]

3) (10 points)
Determine an expression for the linear momentum of a simple cubic crystal containing a single phonon of wavevector $\mathbf{k} \neq \mathbf{0}$, and show that the momentum carried is *not* $\hbar\mathbf{k}$, but zero!

4) (25 points)
Do Kaxiras problem 6.5 (fill in steps in derivation of Debye-Waller formula).