Physics 474 Problem Set 4 Due before class, Wednesday, March 7

1) The point of this problem is to check that, for a weak periodic potential U, at a value of $\vec{k}$ where 2 degenerate energy levels occur at U=0, the corrections to the degenerate perturbation theory formula we have been using are indeed of order U^2. Let's label the two degenerate levels at U=0 by ε_1^0. Let's label the Fourier mode of U which connects them U_{12}. For simplicity, let's only consider 1 other energy level whose unperturbed energy is ε_3^0 and only consider the Fourier modes of U which connect these 3 levels. We label these Fourier modes U_{12}, U_{13} and U_{23}. Then the 3x3 matrix eigenvalue equation becomes:

$$\begin{pmatrix} \varepsilon_1^0 & U_{12} & U_{13} \\ U_{21} & \varepsilon_1^0 & U_{23} \\ U_{31} & U_{32} & \varepsilon_3^0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \varepsilon \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}.$$

Assuming that $|U_{ij}| << |\varepsilon_3^0 - \varepsilon_1^0|$, develop perturbation theory for the two nearly degenerate energy levels, which are close to ε_1^0.

a) Confirm that to first order in U_{ij} we recover the result obtained by ignoring mixing with other levels, $\varepsilon_\pm = \varepsilon_1^0 \pm |U_{12}|$.

b) Show that the next correction to these energy levels is second order in U_{ij} and find it explicitly.

HINT: Show that the eigenvalue equation can be written in the form $(\varepsilon - \varepsilon_1^0)^2 - |U_{12}|^2 + \frac{1}{\varepsilon_3^0 - \varepsilon}\left[(\varepsilon_1 - \varepsilon) f(U) + g(U)\right]$ where f(U) is quadratic in the U_{ij} and g(U) is cubic in the U_{ij}. Then give an argument why we can approximate $\frac{1}{\varepsilon_3^0 - \varepsilon}$ by $\frac{1}{\varepsilon_3^0 - \varepsilon_1^0}$ in solving for the order U^2 corrections to $\varepsilon_\pm$. Making that approximation you have a quadratic equation for ε which can be solved exactly. Taylor expand the solution in powers of U to obtain the correction to the above result which is quadratic in U.

2) Consider a 1 dimensional lattice of ions with 2 inequivalent ions at equilibrium positions na and na+d with dislpacements from eqilibrium $u_1(na)$ and $u_2(na)$ as in the Feb. 14 lecture. Assume only nearest neighbour interactions of the form considered in class:

$$U = \sum_n \left[\frac{K}{2}\left[u_1(na) - u_2(na)\right]^2 + \frac{G}{2}\left[u_2(na) - u_1\left((n+1)a\right)\right]^2 \right].$$

Now let atom 1 have mass M_1 and atom 2 have mass M_2.

a) By writing and solving the Euler-Lagrange equations, find an exact formula for the dispersion relations $\omega_{\pm}(k)$ for the two branches of plane-wave solutions, as in class.

b) Show that the acoustic branch has a frequency at small wave-vector which can be approximated: $\omega_{-} \approx v_s |k|$ and find the velocity of sound, v_s.

3) Consider a simple cubic lattice of atoms with a 1 atom basis and lattice spacing a. Keep only nearest neighbour interactions in the potential energy:

$U = \frac{1}{2} \sum_{<\vec{R},\vec{R}'>} \phi\left[\left|\vec{R} - \vec{R}' + \vec{u}(\vec{R}) - \vec{u}(\vec{R}')\right|\right]$ where only nearest neighbours are kept in the sum, with each nearest neighbour pair occurring once. Note that we are assuming that ϕ only depends on the instantaneous *distance* between the atoms, not the direction.

a) Taylor expanding to second order in $\vec{u}$, show that the potential energy can be written in the form assumed in class:

$$U = \frac{1}{2} \sum_{\vec{R},\vec{R}',\mu,\nu} u_{\mu}(\vec{R}) D_{\mu\nu}(\vec{R} - \vec{R}') u_{\nu}(\vec{R}')$$

and determine the matrix $D_{\mu\nu}(\vec{R} - \vec{R}')$ in terms of the derivatives of $\phi(r)$. You may assume that $\left.\frac{d\phi}{dr}\right|_{r=a} = 0$ since otherwise the equilibrium energy could be lowered by changing the separation of the atoms, a. Note that $D_{\mu\nu}(\vec{R} - \vec{R}')$ is only non-zero for $|\vec{R} - \vec{R}'| = a$ or 0.

b) Calculate the Fourier transform

$D_{\mu\nu}(\vec{k}) = \sum_{\vec{R}} D_{\mu\nu}(\vec{R}) e^{-i\vec{k}\cdot\vec{R}}$, where the sum is over only 7 terms.

c) Calculate the dispersion relations $\omega_i(\vec{k})$ for the 3 branches of phonons, i=1,2,3.

(Note: a somewhat unphysical result occurs because we are ignoring longer range interactions.)