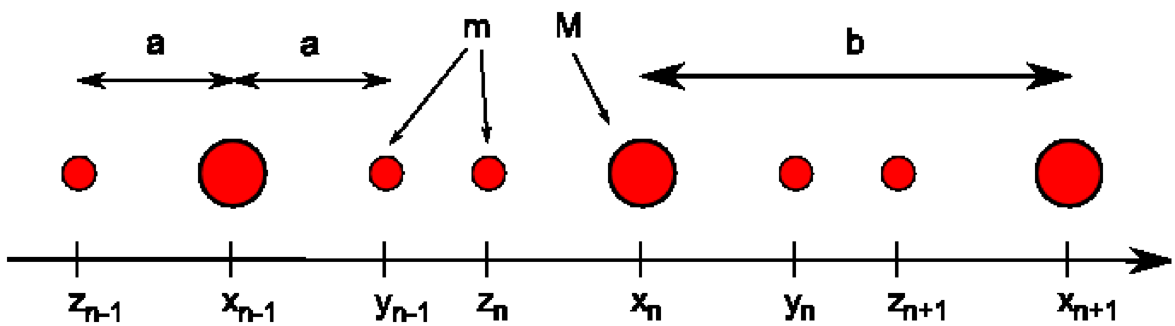
## Physics 501 Problem Set 3

Due at the end of class, Friday February $29^{th}$ (late assignments will not be accepted).

### 1. Vibrations in 1D solid.

Consider a one dimensional solid made up of two kinds of atoms the masses $M$ and $m$, as shown on the diagram. The Lagrangian for longitudinal motion of the atoms is

$$L = \sum_{i=0}^{N-1} \left( \frac{M}{2}\dot{x}_n^2 + \frac{m}{2}\dot{y}_n^2 + \frac{m}{2}\dot{z}_n^2 - \frac{\alpha}{2}(x_n - y_n + a)^2 - \frac{\alpha}{2}(x_n - z_n - a)^2 - \frac{\beta}{2}(z_{n+1} - y_n - b + 2a)^2 \right)$$




**(a)** Write down a third-degree polynomial whose roots give you the branches of $\omega(k)$.

**(b)** Compute the possible values of $\omega$ at $k = 0$ and explain/sketch the nature of normal modes of oscillation at $k = 0$ for each value of $\omega$.

**(c)** For $M = 2m$ and $\alpha = \beta$ plot (using your favourite computer tool) the dependence of $\omega$ on $k$ in all branches in the first Brillouin zone.

**2.** Consider a cubic lattice of identical atoms, with lattice spacing $a$, where the interaction is *not* limited to nearest neighbour atoms. Let the potential energy due to interaction between any two atoms separated by $\vec{r}$ be $\varphi(|\vec{r}|)$.

**(a)** Compute $D_{\mu\nu}(\bar{n})$ in terms of derivatives of $\varphi(|\vec{r}|)$: $\varphi'$ and $\varphi''$. Recall that to quadratic order, the total potential energy is

$$U = \sum_{\bar{n},\bar{n}'} \varphi(|u(\bar{n}) - u(\bar{n}') + a(\bar{n} - \bar{n}')|) \sim U_0 + \frac{1}{2} \sum_{\bar{n},\mu,\bar{n}',\nu} D_{\mu\nu}(\bar{n} - \bar{n}') u_\mu(\bar{n}) u_\nu(\bar{n}')$$

Hint: there are two cases, $\bar{n} = 0$ and $\bar{n} \neq 0$ which need to be considered separately.

**(b)** Making the continuum approximation, prove that the dynamical matrix $D_{\mu\nu}(k)$ has a form

$$D_{\mu\nu}(k) = \frac{k_\mu k_\nu}{|k|^2} G_1(|k|) + \delta_{\mu\nu} G_2(|k|)$$

where $G_1$ and $G_2$ are some functions which depend on $\varphi$. You do not need to find an explicit formula for $G_1$ and $G_2$. The continuum approximation simply means that you can replace the sum over lattice sites with an integral:

$$\sum_{\bar{n}} \longrightarrow \int d^3 n$$

You may also assume that the solid is infinite.

Note: if you can't do part (b), please go on and do (c) and (d).

**(c)** Using the dynamical matrix given in part (b), find the polarization vectors $\epsilon_\mu^{(s)}(k)$ and dispersion relations $\omega_\mu^{(s)}(k)$ in each of the three branches in terms of $G_1$ and $G_2$. Hint: the answers are different in the longitudinal and transverse cases.

**(d)** Assume that at times $t < 0$, the lattice was static (nothing was vibrating). At time $t = 0$, a single atom at $\bar{n} = 0$ is suddenly given a velocity $u_\mu(0,0,0) = v_\mu$ (lets say it was hit by a very energetic cosmic ray). Using the normal modes you have computed in part (c), compute the positions of all the atoms in the lattice for all $t > 0$. Please make sure your answer is a *real* expression. You may leave it as a sum over modes.

**3.** Consider one-phonon neutron scattering. The crystal can be assumed to have 3 different acoustic branches, with different speeds of sound depending on which branch you are in, and the on direction of $\vec{k}$: $\omega^{(s)}(\vec{k}) \sim c^{(s)}(\vec{k}/|k|)|k|$. Let $c_{min} > 0$ be the smallest of $c^{(s)}(\vec{k}/|k|)$ for all $s$ and $\vec{k}/|k|$.

**(a)** Show that if the incoming neutron's momentum is too small, it cannot excite a phonon.

**(b)** Find the minimum neutron momentum necessary to produce a phonon, in terms of $c_{min}$.

**(c)** What direction must the neutron be initially traveling in to produce a phonon when it has only this minimum momentum?