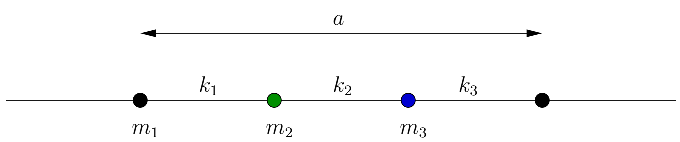
Condensed Matter Physics

Assignment II

Due: October 31, 2019

1. **Phonons in a Triatomic Chain**

   Consider a mass-and-spring model with three different masses and three different springs per unit cell as shown in this diagram.

   Assume that the masses move only in one dimension.

   (a) At $k = 0$ how many optical modes are there? Calculate the energies of these modes.

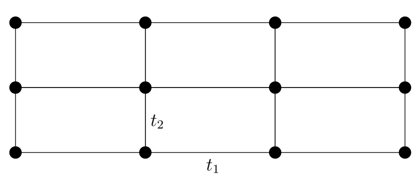
   (b) If all the masses are the same and $k_1 = k_2$, determine the frequencies of all three modes at the zone boundary $k = \pi/a$ (you should be able to guess one root of the resulting cubic equation).

   (c) Similarly, if all three spring constants are the same, and $m_1 = m_2$, determine the frequencies of all three modes at the zone boundary $k = \pi/a$.

   (25 Marks)

2. **Tight Binding Model in 2d**

   Consider an $L \times L$ rectangular lattice in two dimensions as shown in the figure.

   Now imagine a tight binding model where there is one orbital at each lattice site, and where the hopping matrix element is $\langle n|H|m\rangle = t_1$ if sites n and m are neighbors in the horizontal direction and is $= t_2$ if n and m are neighbors in the vertical direction. Consider periodic boundary conditions in both directions.

   (a) Calculate the dispersion relation for this tight binding model.

   (b) What does the dispersion relation look like near the bottom of the band?

   (25 Marks)

3. **Bloch's Theorem in 3d**

Consider a monatomic crystal arranged in an $L \times L \times L$ simple cubic lattice, with lattice constant a. Consider periodic boundary conditions in all three directions.

(a) Write the forms of the discrete translation operators $\mathbb{T}_x$, $\mathbb{T}_y$, $\mathbb{T}_z$, which perform a shift by a single lattice spacing in the x, y, z directions respectively. Show that these are mutually commuting matrices.

(b) Consider a scalar field $\phi(i, j, k, t)$ on every lattice site $\vec{r} \equiv (x, y, z) = (ai, aj, ak)$ coupled through a Hamiltonian

$$\mathcal{H} = \frac{\mathcal{K}}{2} \sum_{i,j,k} \sum_{\Delta_x=\pm 1} \sum_{\Delta_y=\pm 1} \sum_{\Delta_z=\pm 1} \left(\phi(i, j, k, t) - \phi(i + \Delta_x, j + \Delta_y, k + \Delta_z, t)\right)^2 . \tag{1}$$

Show that the equations of motion

$$\ddot{\phi}(\vec{r}, t) = -\frac{\partial \mathcal{H}}{\partial \phi(\vec{r}, t)}, \tag{2}$$

commute with the operators $\mathbb{T}_x$, $\mathbb{T}_y$, $\mathbb{T}_z$.

(c) Determine the eigenmodes of this system.

(d) Use these solutions to determine the dispersion relation.

(30 Marks)

4. **van Hove Singularities**

(a) In a linear harmonic chain with only nearest-neighbor interactions. The normal-mode dispersion relation has the form $\omega(k) = \omega_0 |\sin(ka/2)|$, where the constant ω_0 is the maximum frequency (assumed when k is on the Brillouin zone boundary). Show that the density of normal modes in this case is given by

$$g(\omega) = \frac{2}{\pi a \sqrt{\omega_0^2 - \omega^2}}. \tag{3}$$

The singularity at $\omega = \omega_0$ is a van Hove singularity.

(b) In three dimensions the van Hove singularities are infinities not in the normal mode density itself: but in its derivative. Show that the normal modes in the neighborhood of a maximum of $\omega(\mathbf{k})$ for example, lead to a term in the normal-mode density that varies as $(\omega_0 - \omega)^{1/2}$.

(20 Marks)