Assignment 5

$1D$ and $2D$ Lattice Structures, Dispersion Relations
Please no AI-generated solutions. Would be your loss!

Question 1

A triangular $2D$ lattice is shown in Fig. 2. The distance between two neighbouring atoms is a.

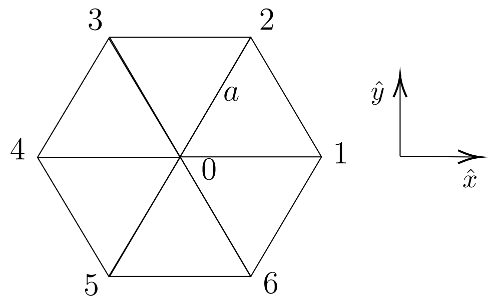

Figure 1

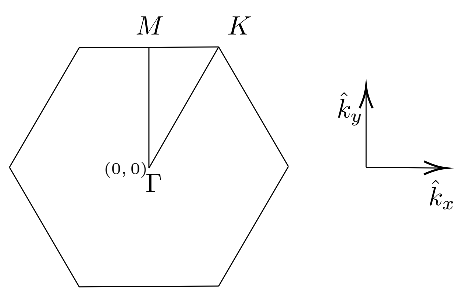

Figure 2

(a) Find the primitive lattice vectors $\vec{a}$ and $\vec{b}$.

(b) Find the lattice vectors $\vec{a}^*$ and $\vec{b}^*$ for the reciprocal lattice, which are given by:

$$\vec{a}^* = \frac{2\pi}{a}\frac{\vec{b}\times\hat{z}}{\vec{a}\cdot(\vec{b}\times\hat{z})}, \qquad \vec{b}^* = \frac{2\pi}{a}\frac{\hat{z}\times\vec{a}}{\vec{a}\cdot(\vec{b}\times\hat{z})}.$$

Show that the Wigner-Seitz cell (i.e. the first Brillouin zone) is hexagonal-shaped. What are the (k_x, k_y) coordinates for the points M and K? See Fig. 2.

(c) Given that the pairwise interaction between two atoms $\vec{w}$ apart is:

$$\Phi_{(n,i)}^{(m,j)} = -\alpha(\hat{w} \cdot \hat{x})(\hat{w} \cdot \hat{y}),$$

where α is the force constant, find all the pairwise interactions Φ, refer to the labels in Fig. 1. For example, we need $\Phi_{(0,x)}^{(0,x)}$, $\Phi_{(0,x)}^{(1,x)}$, $\Phi_{(0,x)}^{(0,y)}, \cdots$ etc.

(d) Construct the dynamical matrix elements and write a general form for the dispersion relation $\omega(k)$.

(e) Determine $\omega(k)$ along the special lines $\Gamma - M$, $M - K$, and $K - \Gamma$. Plot your results and show that the dispersion neatly stitch together at the special points Γ, M and K.

Question 2

Consider a $1D$ lattice with atoms spaced a apart. Each atom has mass M.
Suppose that the oscillations set up $s_n = u_n e^{i(kx-\omega t)}$ are damped, meaning that $k = \kappa + i\eta$, a complex wavenumber, where $\kappa, \eta \ll 1$ and $\eta \ll \kappa$. Here η and κ are real numbers.

(a) From the dynamical matrix element, find the dispersion relation and compare with the undamped case:

$$\omega^2 = \frac{2\alpha}{M} \sin^2\left(\frac{ka}{2}\right).$$

(b) Find the real and imaginary parts of ω.