Homework - 3

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Question 1

The following are the point group operations which leaves the cluster unchanged:
Identity (E) : $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, Inverse (I) : $\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$, Mirror-x ($\mathrm{M_x}$) : $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$, Mirror-y ($\mathrm{M_y}$) : $\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$.

The force constant matrix can be expressed as a sum over tensor basis:

$$\begin{bmatrix} \phi_{\mathrm{xx}} & \phi_{\mathrm{xy}} \\ \phi_{\mathrm{yx}} & \phi_{\mathrm{yy}} \end{bmatrix} = \phi_{\mathrm{xx}} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \phi_{\mathrm{xy}} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \phi_{\mathrm{yx}} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} + \phi_{\mathrm{yy}} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \tag{1}$$

To find the symmetry invariant basis, apply Reynold's operator :

$$\tilde{\Lambda}_i = \frac{1}{|\mathrm{S}|} \sum_{\mathrm{S}} \mathrm{S}^{\mathrm{T}} \Lambda_i \mathrm{S} \tag{2}$$

where S can be any of the symmetry operator which leaves the cluster unchanged $(\mathrm{E}, \mathrm{I}, \mathrm{M_x}, \mathrm{M_y})$.

Applying Reynold's operator on $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ gives:

$$\tfrac{1}{4}\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

$$= \tfrac{1}{4} \begin{bmatrix} 4 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

Applying Reynold's operator on $\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ gives:

$$\tfrac{1}{4}\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

$$= \tfrac{1}{4} \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

Applying Reynold's operator on $\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$ gives:

$$\tfrac{1}{4}\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

$$= \tfrac{1}{4} \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

Applying Reynold's operator on $\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ gives:

$$\tfrac{1}{4}\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

$$= \tfrac{1}{4} \begin{bmatrix} 0 & 0 \\ 0 & 4 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

The force constant matrix (Φ) expressed in the symmetry invariant tensor basis is,

$$\Phi = \alpha_1 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \alpha_2 \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \boxed{\begin{bmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{bmatrix}} \tag{3}$$

Question 2

Dynamical matrix (D) is given by,

$$\boxed{\mathrm{D} = \frac{1}{\mathrm{m}}\sum_{\vec{\mathrm{r}}_l} \Phi(0, \vec{\mathrm{r}}_l) \mathrm{e}^{-\mathrm{i}\vec{\mathrm{k}}.\vec{\mathrm{r}}_l}} \tag{4}$$

where $\vec{\mathrm{r}}_l$ is position vector of the neighboring atoms, $\vec{\mathrm{k}}$ is the crystal momentum and Φ is the force constant matrix. To obtain D, we need Φ of all the nearest neighbors. It can be obtained using the relation: $\Phi(0, \vec{\mathrm{r}}_l) = \mathrm{S}^{\mathrm{T}}\Phi(0, \vec{\mathrm{r}}_1)\mathrm{S}$, where S is the symmetry operation which transforms the cluster $(0, \vec{\mathrm{r}}_1)$ to $(0, \vec{\mathrm{r}}_l)$. The following are the force constant matrices for all the 6 pair clusters.

$$\Phi(0, \mathrm{r}_1) = \begin{bmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{bmatrix}$$

$$\Phi(0, \mathrm{r}_2) = \begin{bmatrix} \frac{1}{4}\alpha_1 + \frac{3}{4}\alpha_2 & \frac{\sqrt{3}}{4}(\alpha_1 - \alpha_2) \\ \frac{\sqrt{3}}{4}(\alpha_1 - \alpha_2) & \frac{3}{4}\alpha_1 + \frac{1}{4}\alpha_2 \end{bmatrix}$$

$$\Phi(0, \mathrm{r}_3) = \begin{bmatrix} \frac{1}{4}\alpha_1 + \frac{3}{4}\alpha_2 & \frac{\sqrt{3}}{4}(\alpha_2 - \alpha_1) \\ \frac{\sqrt{3}}{4}(\alpha_2 - \alpha_1) & \frac{3}{4}\alpha_1 + \frac{1}{4}\alpha_2 \end{bmatrix}$$

$$\Phi(0, \mathrm{r}_4) = \begin{bmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{bmatrix}$$

$$\Phi(0, \mathrm{r}_5) = \begin{bmatrix} \frac{1}{4}\alpha_1 + \frac{3}{4}\alpha_2 & \frac{\sqrt{3}}{4}(\alpha_1 - \alpha_2) \\ \frac{\sqrt{3}}{4}(\alpha_1 - \alpha_2) & \frac{3}{4}\alpha_1 + \frac{1}{4}\alpha_2 \end{bmatrix}$$

$$\Phi(0, \mathrm{r}_6) = \begin{bmatrix} \frac{1}{4}\alpha_1 + \frac{3}{4}\alpha_2 & \frac{\sqrt{3}}{4}(\alpha_2 - \alpha_1) \\ \frac{\sqrt{3}}{4}(\alpha_2 - \alpha_1) & \frac{3}{4}\alpha_1 + \frac{1}{4}\alpha_2 \end{bmatrix}$$

Plugging in the force constant matrices in Equation. 4, gives:

$$\mathrm{D} = \frac{1}{\mathrm{m}} \begin{bmatrix} 2\alpha_1 \cos(\mathrm{ak_x}) + (\alpha_1 + 3\alpha_2)\cos(\frac{\mathrm{a}}{2}\mathrm{k_x})\cos(\frac{\mathrm{a}\sqrt{3}}{2}\mathrm{k_y}) & -\sqrt{3}(\alpha_1 - \alpha_2)\sin(\frac{\mathrm{a}}{2}\mathrm{k_x})\sin(\frac{\mathrm{a}\sqrt{3}}{2}\mathrm{k_y}) \\ -\sqrt{3}(\alpha_1 - \alpha_2)\sin(\frac{\mathrm{a}}{2}\mathrm{k_x})\sin(\frac{\mathrm{a}\sqrt{3}}{2}\mathrm{k_y}) & 2\alpha_2 \cos(\mathrm{ak_x}) + (3\alpha_1 + \alpha_2)\cos(\frac{\mathrm{a}}{2}\mathrm{k_x})\cos(\frac{a\sqrt{3}}{2}\mathrm{k_y}) \end{bmatrix} \tag{5}$$

Question 3

Considering $(\mathrm{a}, 0)$, $(\frac{a}{2}, \frac{a\sqrt{3}}{2})$ to be the real space lattice vectors of the triangular lattice, the reciprocal lattice vectors are given by: $\frac{2\pi}{a}(0, \frac{2}{\sqrt{3}})$ and $\frac{2\pi}{a}(1, \frac{-1}{\sqrt{3}})$.

Figure.1 shows the first Brillouin zone (shaded portion) and some of the high symmetry points (black dots) of the triangular lattice.

Question 4

The analytical expression for the eigen values of the Dynamical matrix obtained in Question 2 is given by,

$$\begin{aligned} e = \frac{1}{\mathrm{m}}\Bigg(& (\alpha_1 + \alpha_2)\Big(\cos(\mathrm{ak_x}) + 2\cos(\frac{\mathrm{a}}{2}\mathrm{k_x})\cos(\frac{\mathrm{a}\sqrt{3}}{2}\mathrm{k_y})\Big) \\ & \pm (\alpha_1 - \alpha_2)\sqrt{\Big(\cos(\mathrm{ak_x}) - \cos(\frac{a}{2}\mathrm{k_x})\cos(\frac{a\sqrt{3}}{2}\mathrm{k_y})\Big)^2 + 3\sin^2(\frac{a}{2}\mathrm{k_x})\sin^2(\frac{a\sqrt{3}}{2}\mathrm{k_y})}\Bigg) \end{aligned} \tag{6}$$

Figure.2 shows the dispersion curves along some high symmetry directions $(\Gamma, \mathrm{K}, \mathrm{M})$ for $\mathrm{m} = 1$, $\alpha_1 = 0.1$, and $\alpha_2 = 0.2$.

Question 5

The displacement field corresponding to an eigen vector (e_α) at a k point $(\vec{\mathrm{k}})$ is given by:

$$\vec{\mathrm{u}}(\vec{\mathrm{k}}) = \mathrm{c}\vec{e}_\alpha(\vec{\mathrm{k}}) \tag{7}$$

Figure. 3 shows the displacement field corresponding to the two eigen vectors at M point. The black and blue arrows represent displacement fields corresponding to 2 different eigen vectors.

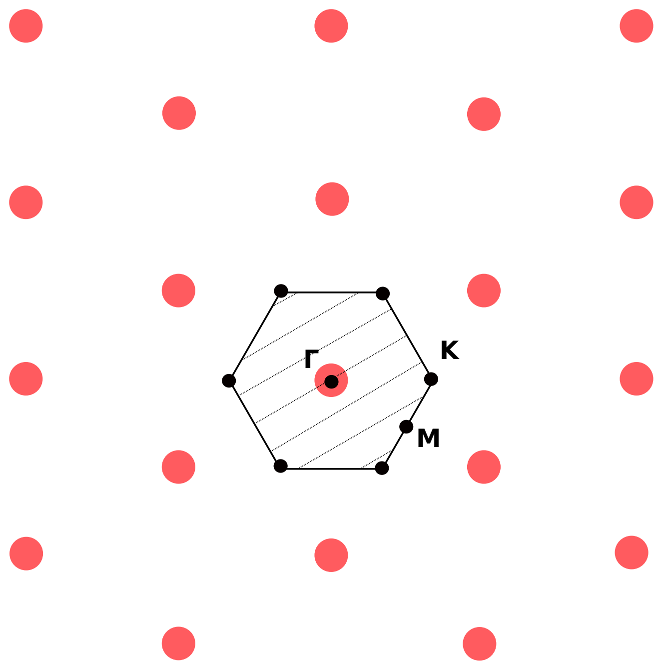

Figure 1: Reciprocal lattice

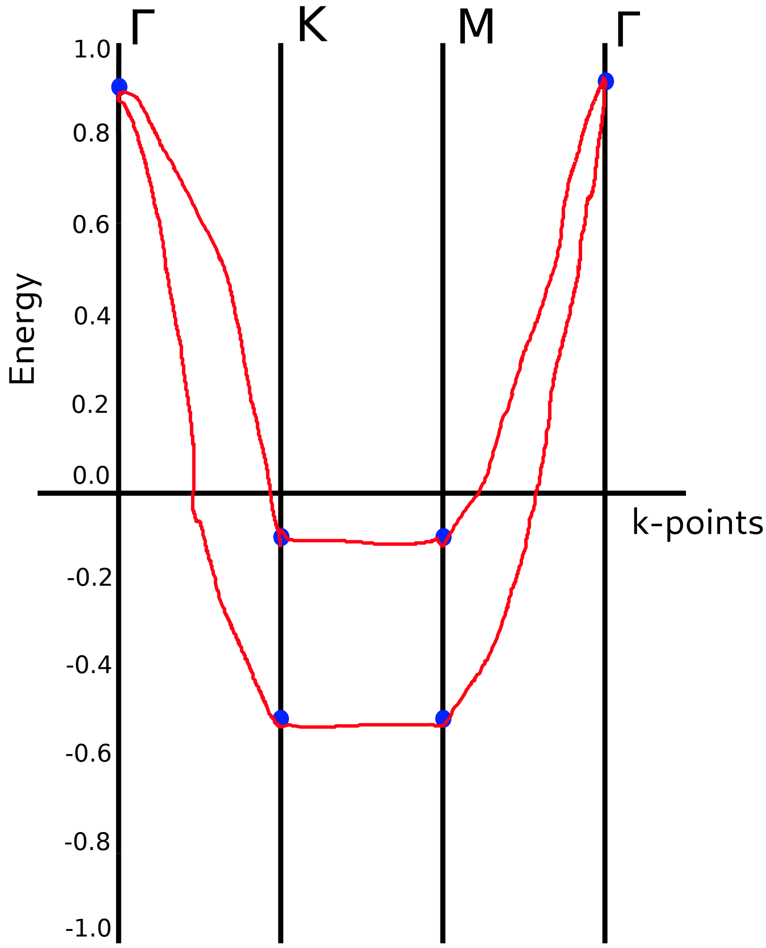

Figure 2: Dispersion curves

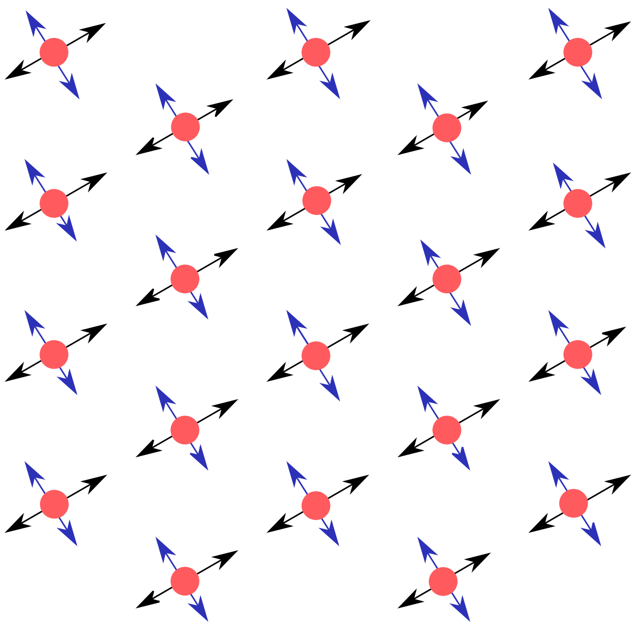

Figure 3: Displacement field