1 Triangular lattice: nearest neighbor tensor basis

The basis vectors of a triangular lattice are $\vec{a} = \hat{i} + 0\hat{j}$ and $\vec{b} = \frac{1}{2}\hat{i} + \frac{\sqrt{3}}{2}\hat{j}$. We select one of any of the nearest neighbor pairs, such as $\vec{s_0} = 0\vec{a} + 0\vec{b}$ and $\vec{s_1} = \vec{a} + 0\vec{b}$. The goal is to find a symmetrized tensor basis for the force constant matrix of this pair.

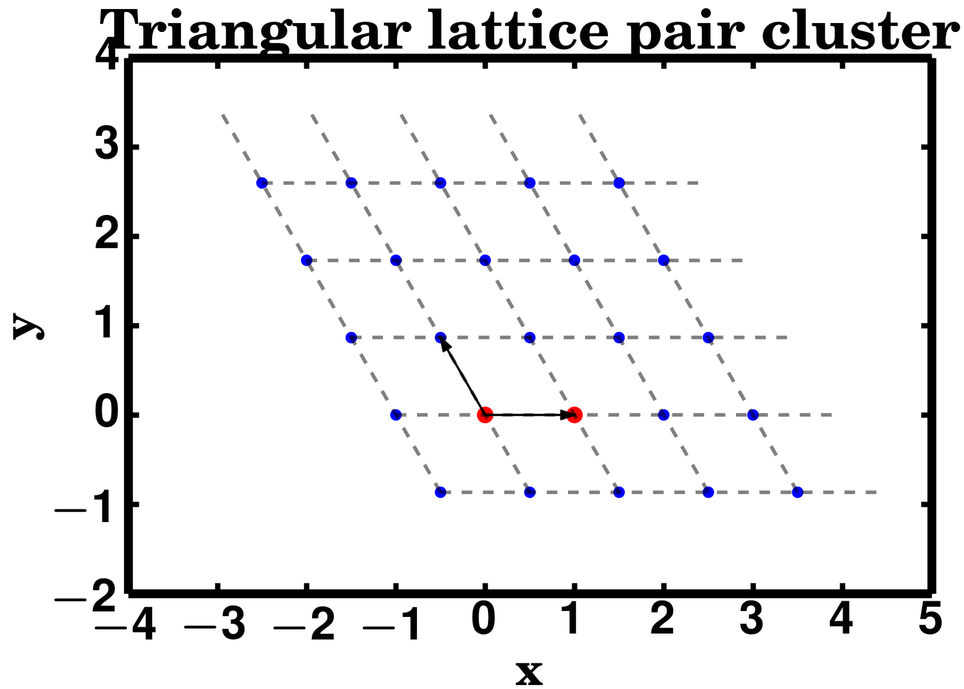

Figure 1: Selected pair cluster (red) in a triangular lattice.

$$\Phi = \Phi_{xx}\Lambda_{xx} + \Phi_{xy}\Lambda_{xy} + \Phi_{yx}\Lambda_{yx} + \Phi_{yy}\Lambda_{yy} \tag{1}$$

Where Φ is the force constant matrix for the particular pair we're looking at and Λ is the appropriate starting tensor basis that reconstruct Φ.

There is a total of 4 symmetry operations that leave the cluster invariant. Two of them map the sites back onto themselves, while the other two result in the sites exchanging places.
The following operations map the cluster sites onto themselves:

I0

$$S = \begin{pmatrix} 1.0 & 0.0 \\ 0.0 & 1.0 \end{pmatrix}, \vec{\tau} = \begin{pmatrix} 0.0 \\ 0.0 \end{pmatrix} \tag{2}$$

M0

$$S = \begin{pmatrix} 1.0 & 0.0 \\ 0.0 & -1.0 \end{pmatrix}, \vec{\tau} = \begin{pmatrix} 0.0 \\ 0.0 \end{pmatrix} \tag{3}$$

The following operations map the cluster sites onto each other:

R180

$$S = \begin{pmatrix} -1.0 & 0.0 \\ 0.0 & -1.0 \end{pmatrix}, \vec{\tau} = \begin{pmatrix} 1.0 \\ 0.0 \end{pmatrix} \tag{4}$$

M90

$$S = \begin{pmatrix} -1.0 & 0.0 \\ 0.0 & 1.0 \end{pmatrix}, \vec{\tau} = \begin{pmatrix} 1.0 \\ 0.0 \end{pmatrix} \tag{5}$$

We apply the Reynolds operator to each Λ with the first set of symmetry operations, and repeat the process on Λ^T with the second set of operations. After applying these operations and normalizing by number of operations, the tensor basis becomes:

$$\Lambda_{xx} = \begin{pmatrix} 1.0 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} \tag{6}$$

$$\Lambda_{xy} = \begin{pmatrix} 0.0 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} \tag{7}$$

$$\Lambda_{yx} = \begin{pmatrix} 0.0 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} \tag{8}$$

$$\Lambda_{yy} = \begin{pmatrix} 0.0 & 0.0 \\ 0.0 & 1.0 \end{pmatrix} \tag{9}$$

A QR decomposition (or simple observation in this case) reveals that only Λ_{xx} and Λ_{yy} are needed to form the tensor basis, since the other two values are linearly dependent.

2 Honeycomb structure: nearest neighbor tensor basis

The process can be repeated for the nearest neighbor pair in a honeycomb structure.

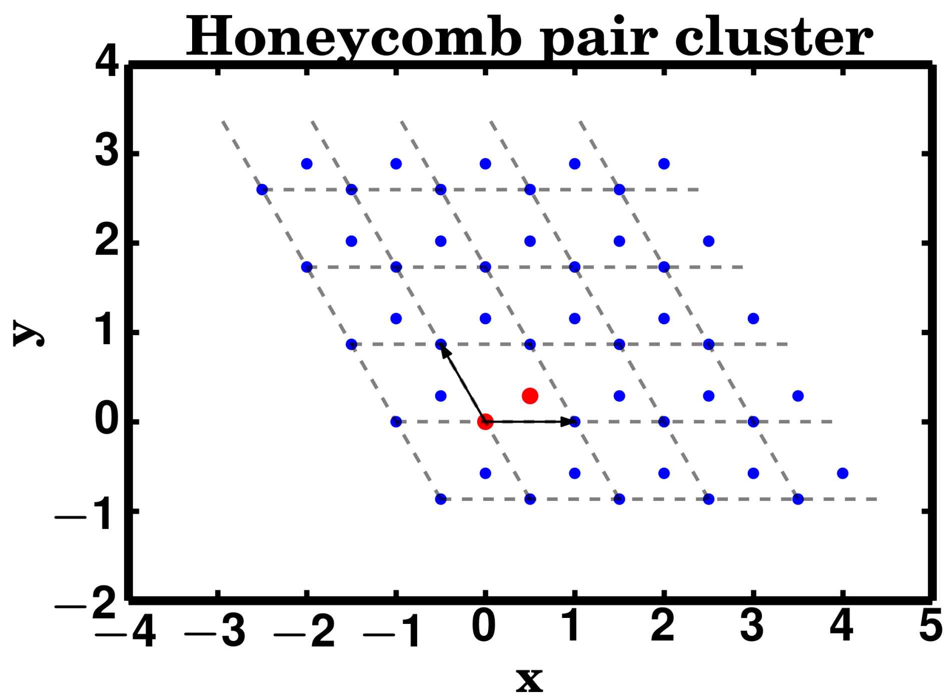

Figure 2: Selected pair cluster (red) in a triangular lattice.

There is a total of 4 symmetry operations that leave the cluster invariant. Two of them map the sites back onto themselves, while the other two result in the sites exchanging places.
The following operations map the cluster sites onto themselves:

I0

$$S = \begin{pmatrix} 1.0 & 0.0 \\ 0.0 & 1.0 \end{pmatrix}, \vec{\tau} = \begin{pmatrix} 0.0 \\ 0.0 \end{pmatrix} \tag{10}$$

M30

$$S = \begin{pmatrix} 0.5 & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -0.5 \end{pmatrix}, \vec{\tau} = \begin{pmatrix} 0.0 \\ 0.0 \end{pmatrix} \tag{11}$$

The following operations map the cluster sites onto each other:

R180

$$S = \begin{pmatrix} -1.0 & 0.0 \\ 0.0 & -1.0 \end{pmatrix}, \vec{\tau} = \begin{pmatrix} 0.5 \\ \frac{\sqrt{3}}{6} \end{pmatrix} \tag{12}$$

M120

$$S = \begin{pmatrix} -0.5 & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & 0.5 \end{pmatrix}, \vec{\tau} = \begin{pmatrix} 0.5 \\ \frac{\sqrt{3}}{6} \end{pmatrix} \tag{13}$$

We apply the Reynolds operator to each Λ with the first set of symmetry operations, and repeat the process on Λ^T with the second set of operations. After applying these operations and normalizing by number of operations, the tensor basis becomes:

$$\Lambda_{xx} = \begin{pmatrix} \frac{5}{8} & \frac{\sqrt{3}}{8} \\ \frac{\sqrt{3}}{8} & \frac{3}{8} \end{pmatrix} \tag{14}$$

$$\Lambda_{xy} = \begin{pmatrix} \frac{\sqrt{3}}{8} & \frac{3}{8} \\ \frac{3}{8} & -\frac{\sqrt{3}}{8} \end{pmatrix} \tag{15}$$

$$\Lambda_{yx} = \begin{pmatrix} \frac{\sqrt{3}}{8} & \frac{3}{8} \\ \frac{3}{8} & -\frac{\sqrt{3}}{8} \end{pmatrix} \tag{16}$$

$$\Lambda_{yy} = \begin{pmatrix} \frac{3}{8} & -\frac{\sqrt{3}}{8} \\ -\frac{\sqrt{3}}{8} & \frac{5}{8} \end{pmatrix} \tag{17}$$

A QR decomposition reveals that only Λ_{xx} and Λ_{xy} are needed to form the tensor basis, since the other two values are linearly dependent.