

## Finding the $k$ -grid points inside the reciprocal cell

Let  $L_K$  be the  $k$ -grid lattice. Let  $\mathbb{K}$  be a matrix where the columns are the vectors of the generating grid. The matrix  $\mathbb{S}$  that transforms the  $k$ -grid vectors into the reciprocal vectors must have all integer elements. Its determinant is equal to the number of reducible  $k$ -points. Then, the reciprocal lattice,  $L_R$ , is given by  $\mathbb{R} = \mathbb{K}\mathbb{S}$  (where the columns of  $\mathbb{R}$  are the reciprocal lattice vectors). With no loss of generality, we may choose  $\mathbb{S}$  as Hermite Normal Form matrix.

We want to know which points of  $L_K$  are within the first unit cell of  $L_R$ . Let a point within the cell be denoted  $\vec{x}$ . The (lattice) components of  $\vec{x}$  must be  $0 \leq x_i < 1$ . Since we are interested in points in the cell that are also points of  $L_K$ , we have  $\mathbb{R}\vec{x} = \mathbb{K}\vec{z}$  where the components of  $z$  are integers. (If so, then  $\vec{x}$  is obviously a lattice point of the  $k$ -grid [that is,  $\vec{x} \in L_k$ ].)

But since  $\mathbb{R} = \mathbb{K}\mathbb{S}$ ,

$$\begin{aligned} \mathbb{R}\vec{x} &= \mathbb{K}\vec{z} \\ \mathbb{K}\mathbb{S}\vec{x} &= \mathbb{K}\vec{z} \\ \mathbb{K}^{-1}\mathbb{K}\mathbb{S}\vec{x} &= \mathbb{K}^{-1}\mathbb{K}\vec{z} \\ \mathbb{S}\vec{x} &= \vec{z} \end{aligned} \Rightarrow \begin{pmatrix} a & 0 & 0 \\ b & c & 0 \\ d & e & f \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}$$

So,

$$\begin{aligned} ax_1 &= z_1 \\ bx_1 + cx_2 &= z_2 \\ dx_1 + ex_2 + fx_3 &= z_3 \end{aligned}$$

Since the components of  $\vec{x}$  must be  $[0, 1)$ ,

$$\begin{aligned} 0 \leq x_1 = z_1/a < 1 &\rightarrow \boxed{0 \leq z_1 < a} \\ 0 \leq x_2 = \frac{z_2}{c} - \frac{b}{ca}z_1 < 1 &\rightarrow \frac{b}{ca}z_1 \leq \frac{z_2}{c} < 1 + \frac{b}{ca}z_1 \\ &\rightarrow \boxed{\frac{b}{a}z_1 \leq z_2 < c + \frac{b}{a}z_1} \\ 0 \leq x_3 = \frac{z_3}{f} - \frac{d}{f} \frac{z_1}{a} - e \left[ \frac{z_2}{c} - \frac{b}{ca}z_1 \right] < 1 \\ \frac{d}{f} \frac{z_1}{a} + \frac{e}{f} \left[ \frac{z_2}{c} - \frac{b}{ca}z_1 \right] \leq \frac{z_3}{f} < 1 + \frac{d}{f} \frac{z_1}{a} + \frac{e}{f} \left[ \frac{z_2}{c} - \frac{b}{ca}z_1 \right] \\ d \frac{z_1}{a} + \frac{e}{c} \left[ z_2 - \frac{b}{a}z_1 \right] \leq z_3 < f + z_1 \frac{d}{a} + \frac{e}{c} \left[ z_2 - \frac{b}{a}z_1 \right] \\ \boxed{z_1 \left[ \frac{d}{a} - \frac{eb}{ca} \right] + \frac{e}{c} z_2 \leq z_3 < f + z_1 \left[ \frac{d}{a} - \frac{eb}{ca} \right] + \frac{e}{c} z_2} \end{aligned}$$