

Finding the interior points

\mathbb{A} is a matrix where the columns are the vectors of the parent lattice, L_A . \mathbb{S} is an HNF matrix. Then, the superlattice is L_b , given by $\mathbb{B} = \mathbb{A}\mathbb{S}$.

We want to know which points of L_A are within one tile of L_B . Let a point within the tile be denoted \vec{x} . The components of \vec{x} must be $0 \leq x_i < 1$. Since we are interested in points in the tile that are also points of L_A , we have $\mathbb{B}\vec{x} = \mathbb{A}\vec{z}$ where the components of z are integers.

But since $\mathbb{B} = \mathbb{A}\mathbb{S}$,

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

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 $[0, 1)$,

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