Empty lattice approximates for 100, simple cubic

\[ E(k^2, G^2) = \frac{1}{2m} \left( k^2 + G^2 \right)^2 \]

where \( k^2 \) is in \( \mathbb{R}^3 \) \( \mathbb{R}^2 \),
and \( G \) = reciprocal lattice vector.

1. \( \mathbf{k} = \mathbf{0} \) in \( \mathbf{F} \|
\] direction for this case,
\[ \mathbf{k} = (k,0,0) \]

2. simple cubic lattice.

\[ G = h \mathbf{a}^1 + k \mathbf{a}^2 + l \mathbf{a}^3 \]

where \((h,k,l)\) = integers \( (\text{this } k \text{ is not the vector!}) \)

\[ \mathbf{a}^1 = 2\pi/a \ (1,0,0) \]
\[ \mathbf{a}^2 = 2\pi/a \ (0,1,0) \]
\[ \mathbf{a}^3 = 2\pi/a \ (0,0,1) \]

\[ G^2 = \frac{4\pi^2}{a^2} (h,k,l) \]

\[ (kG)^2 = \left( k_x G_x + k_y G_y + k_z G_z \right)^2 \]
\[ = \left( k_x + G_x \right)^2 + \left( k_y + G_y \right)^2 + \left( k_z + G_z \right)^2 \]
\[ = \left( k + \frac{2\pi b}{a} \right)^2 + \left( 0 + \frac{2\pi b}{a} \right)^2 + \left( 0 + \frac{2\pi b}{a} \right)^2 \]

Define \( \mathbf{x} \) from \( \mathbf{O} \) to \( \mathbf{l} \) in the [100] direction.

\[ x = \frac{\mathbf{k}}{\mathbf{a}} = \frac{k}{2\pi} \Rightarrow k = \frac{\mathbf{a}}{x} \]

\[ E = \frac{b^2}{2m} \left( \frac{2\pi}{a} x + \frac{2\pi}{a} y \right)^2 \]
\[ = \frac{b^2}{2m} \frac{2\pi}{a^2} \left( x^2 + y^2 \right) \]

\[ E_{\text{free}} = \text{energy when } x = 1 \text{ and } (h,k,l) = 0 \]
\[ = \frac{b^2}{2m} \frac{2\pi}{a^2} \]

\[ \text{Tops.} \]
Empty lattice for 100 s.c., cont.

\[
\frac{E}{E_{\text{ref}}} = (x + 2k)^2 + y^2 + 4x^2
\]

Plots for various combinations of \( h, k, l \)

\[\uparrow \downarrow \rightarrow \frac{E}{E_{\text{ref}}} = 7\]

(Picking the best numbers can be challenging. I did it with trial and error, and by thinking about the equation.

For example, the plots with (011), (011), (011), and (011) will all be the same.)
\[ e[x_\_ , h_\_ , k_\_ , l_\_] = (x + 2h)^2 + 4k^2 + 4l^2 \]

\[ Out[1]= 4k^2 + 4l^2 + (2h + x)^2 \]

\[ In[2]= \text{Plot}\left[\{e[x, 0, 0], e[x, 1, 0, 0], e[x, -1, 0, 0], e[x, 0, 1, 0], e[x, 1, 1, 0], e[x, -1, 1, 0], e[x, 0, 1, 1]\}, \{x, -1, 1\}, \text{PlotRange} \to \{0, 9\}\right] \]

\[ Out[2]= \]