Empty Lattice Approximation
by Dr. Colton, Physics 581 (last updated: Fall 2020)

1) Actual Band Structures

![Energy bands of Si](image1)

*Fig. 2.10. Electronic band structure of Si calculated by the pseudopotential technique. The solid and the dotted lines represent calculations with a nonlocal and a local pseudopotential, respectively.*

![Energy bands of GaAs](image2)

*Fig. 2.14. Electronic band structure of GaAs calculated by the pseudopotential technique.*

2) Empty Lattice Approximation (also from Yu and Cardona)

![Band structure of diamond](image3)

*Fig. 2.9. Band structure of nearly free electrons for a diamond-type crystal in the reduced zone scheme. The numbers in square brackets denote corresponding reciprocal lattice vectors in the extended zone scheme in units of \((2\pi/a)\), \(a\) being the size of the unit cube.*

![Band structure of zinc-blende](image4)

*Fig. 2.8. Band structure of nearly free electrons in a zinc-blende-type crystal in the reduced zone scheme.*
3) Empty Lattice Approximation
4) Calculating the Empty Lattice Approximation – Example, Simple Cubic, [100] direction

\[ \epsilon(\vec{k}, \vec{G}) = \frac{\hbar^2}{2m} (\vec{k} + \vec{G})^2 \]

Where \( \vec{k} \) is in the first B.Z and \( \vec{G} \) is any reciprocal lattice vector.

(1) \( \vec{k} \) is in the [100] direction for this problem \( \rightarrow \vec{k} = (k,0,0) \)

(2) Simple Cubic Lattice

\[ \vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3 \quad (h,k,\ell) \in \mathbb{Z} \quad \text{(this k is not the wavevector!)} \]

and

\[ \vec{b}_1 = \frac{2\pi}{a}(1,0,0) \]
\[ \vec{b}_2 = \frac{2\pi}{a}(0,1,0) \]
\[ \vec{b}_3 = \frac{2\pi}{a}(0,0,1) \]

\[ \Rightarrow \vec{G} = \frac{2\pi}{a}(h,k,\ell) \]

\[(k + \vec{G})^2 = (k + G_x, k_y + G_y, k_z + G_z) \cdot (k_x + G_x, k_y + G_y, k_z + G_z) \]
\[= (k_x + G_x)^2 + (k_y + G_y)^2 + (k_z + G_z)^2 \]
\[= (k + 2\pi h/a)^2 + (0 + 2\pi k/a)^2 + (0 + 2\pi \ell/a)^2 \]

Define x to go from 0 to 1 first BZ in the [100] direction,

\[ x = \frac{k}{k_{max}} = \frac{k}{\pi/a} \rightarrow k = \frac{\pi}{a} x \]

\[ E = \frac{\hbar^2}{2m} \left[ \left( \frac{\pi}{a} x + \frac{2\pi}{a} h \right)^2 + \left( \frac{2\pi}{a} k \right)^2 + \left( \frac{2\pi}{a} \ell \right)^2 \right] \]
\[= \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} [(x + 2h)^2 + 4k^2 + 4\ell^2] \]

Define a reference energy, \( E_{ref} = E(x = 1, (h,k,\ell) = 0) = \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} \)

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

Plots for variations combinations of (h,k,l) up to \( \frac{E}{E_{ref}} = 7 \)

(picking the h,k,l numbers for the plots 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.)
\textbf{In[1]:= } \text{e[x_, h_, k_, l_] = (x+2 h)^2 + 4 k^2 + 4 l^2}

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

\textbf{In[2]:= } \text{Plot[} \{\text{e[x, 0, 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\}\text{]}

\textbf{Out[2]=}