Empty Lattice Approximation for S.C. in [100] direction - Dr Colton

Simple Cubic, [100] direction

$$E(\vec{k}, \vec{G}) = \frac{\hbar^2}{2m}(\vec{k} + \vec{G})^2$$ where $\vec{k}$ is in 1st B.Z. and $\vec{G}$ = any reciprocal lattice vector

(1) $\vec{k}$ is in [100] direction for this case

$$\Rightarrow \vec{k} = (k, 0, 0)$$

(2) simple cubic lattice

$$\Rightarrow \vec{G} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3}$$

with (h, k, l) = integers (this k is not the wavevector!)

and $\vec{b_1} = 2\pi/a\ (1,0,0)$

$\vec{b_2} = 2\pi/a\ (0,1,0)$

$\vec{b_3} = 2\pi/a\ (0,0,1)$

$$\Leftrightarrow \vec{G} = \frac{2\pi}{a}(h, k, l)$$

$$(\vec{k}+\vec{G})^2 = (k_x + G_x, k_y + G_y, k_z + G_z) \cdot (k_x + G_x, k_y + G_y, k_z + G_z)$$

$$= (k_x + G_x)^2 + (k_y + G_y)^2 + (k_z + G_z)^2$$

$$= \left(k + \frac{2\pi h}{a}\right)^2 + \left(0 + \frac{2\pi k}{a}\right)^2 + \left(0 + \frac{2\pi l}{a}\right)^2$$

Define x to go from 0 to 1 across the 1st BZ in the [100] direction

$$x = \frac{k}{k_{max}} = \frac{k}{\frac{\pi}{a}} \rightarrow k = \frac{\pi}{a}x$$

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

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

E_{ref} = energy when $x = 1$ and $(h, k, l) = 0$

$$= \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}$$

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Empty lattice for 100 s.c., cont.

$$\boxed{\frac{E}{E_{ref}} = (x+2h)^2 + 4k^2 + 4l^2}$$

Plotted for various combinations of h k, l

up to $\frac{E}{E_{ref}} = 7$

(Picking the hkl 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), $(0\bar{1}1)$, $(01\bar{1})$, and $(0\bar{1}\bar{1})$ will all be the same.)

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In[1]:= `e[x_, h_, k_, l_] = (x + 2 h)^2 + 4 k^2 + 4 l^2`

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

In[2]:=
```
Plot[{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}, PlotRange → {0, 9}]
```

Out[2]=