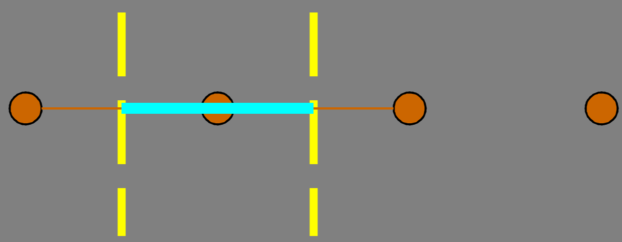
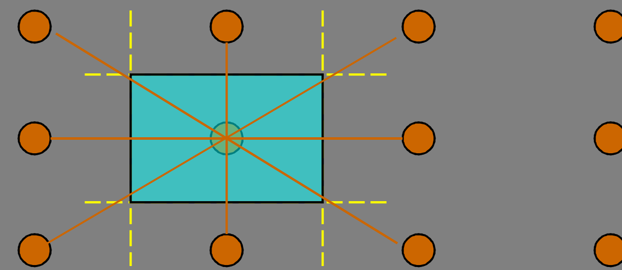
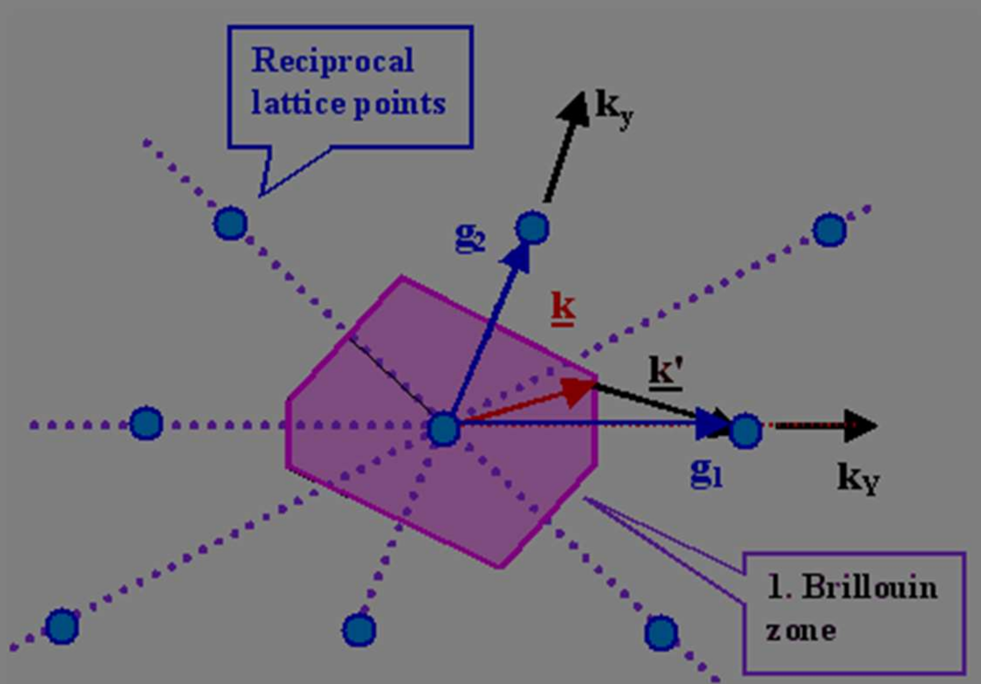
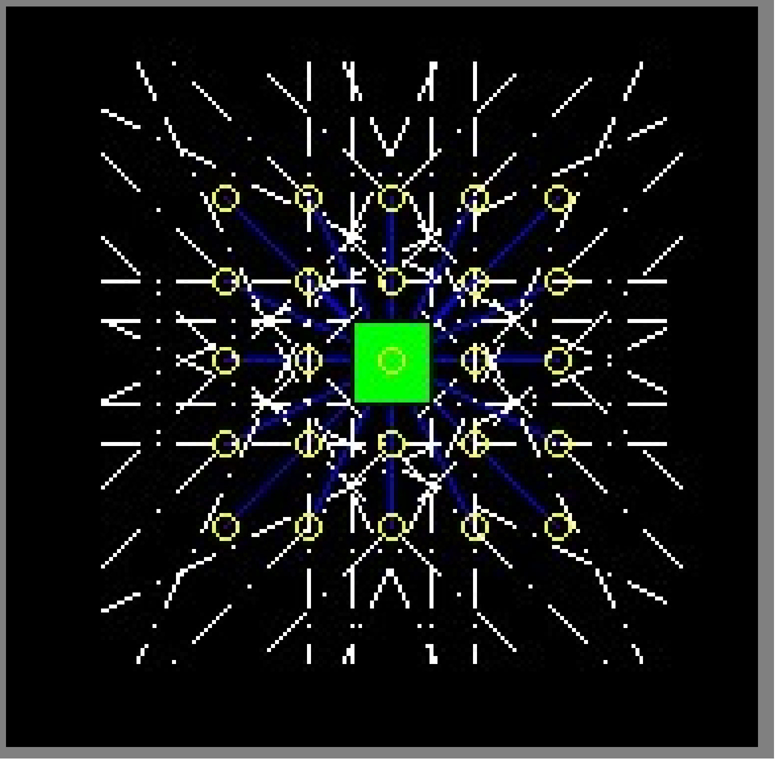
Band Structure plotting of empty 3 dimensional lattices

Before learning how to plot band structure in an empty space, it is useful to remind you that how one can draw various zones of Brillouin.



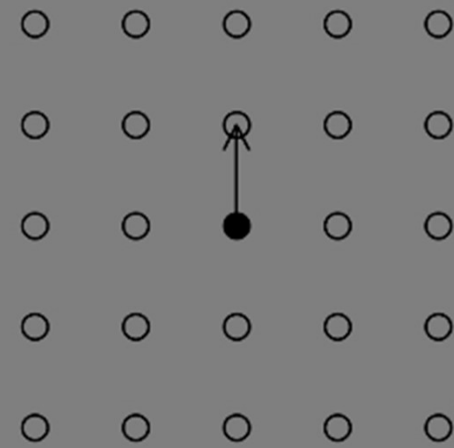


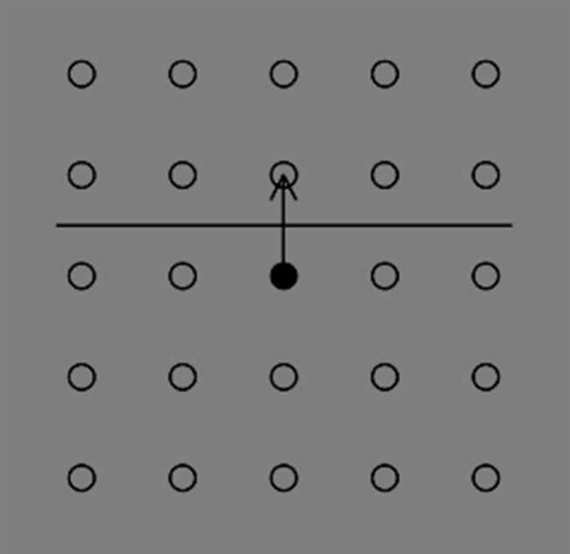




http://www.doitpoms.ac.uk/tlplib/brillouin_zones/zone_construction.php

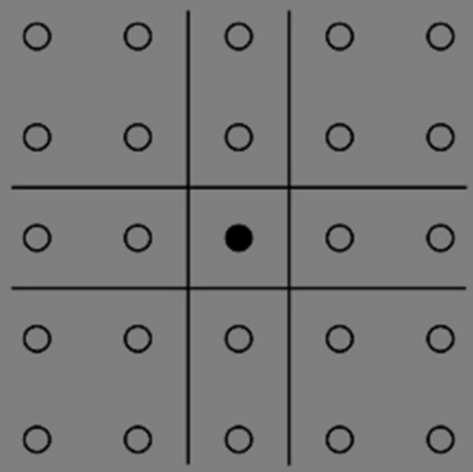
Draw a line connecting this origin point to one of its nearest neighbors. This line is a reciprocal lattice vector as it connects two points in the reciprocal lattice.



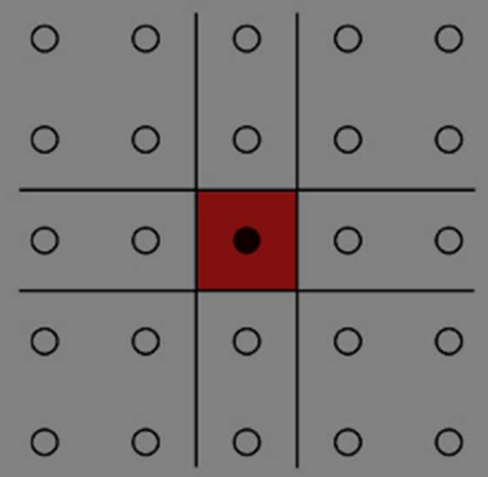


Then draw on a perpendicular bisector to the first line. This perpendicular bisector is a Bragg Plane.

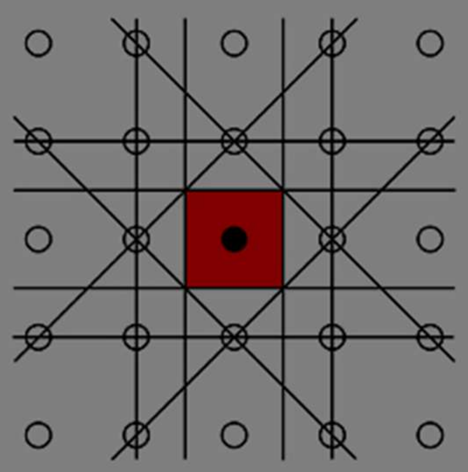
Add the Bragg Planes corresponding to the other nearest neighbours.



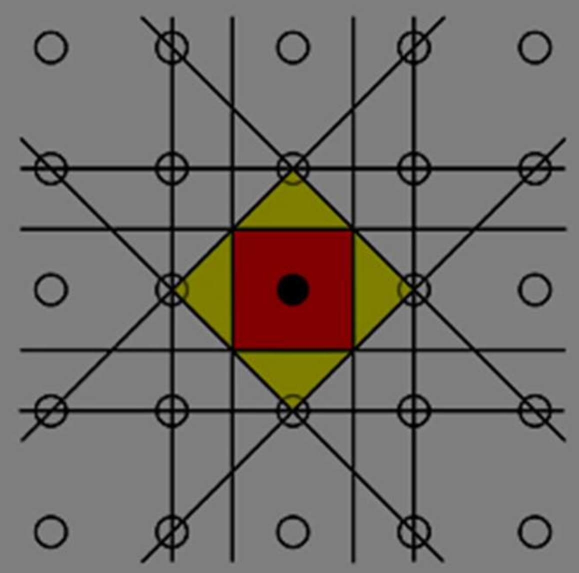
The locus of points in reciprocal space that have no Bragg Planes between them and the origin defines the first Brillouin Zone. It is equivalent to the Wigner-Seitz unit cell of the reciprocal lattice. In the picture below the first Zone is shaded red.



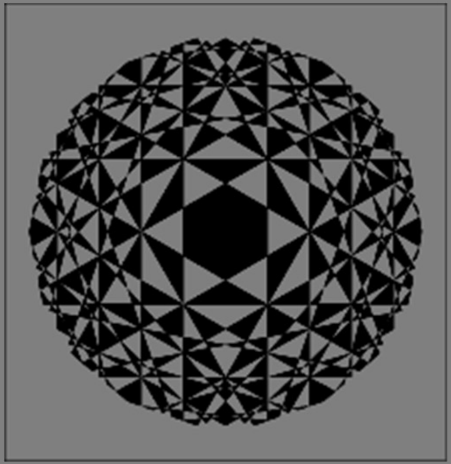
Now draw on the Bragg Planes corresponding to the next nearest neighbours.

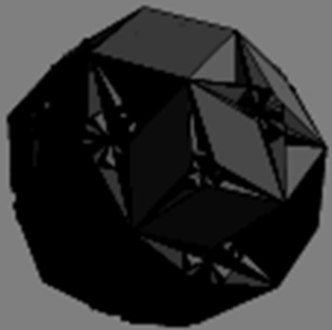


The second Brillouin Zone is the region of reciprocal space in which a point has one Bragg Plane between it and the origin. This area is shaded yellow in the picture below. Note that the areas of the first and second Brillouin Zones are the same.



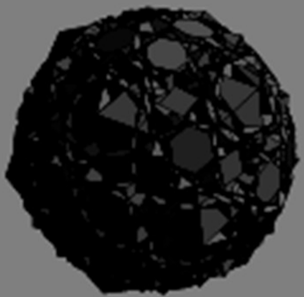
The first twenty Brillouin zones of a 2D hexagonal lattice.

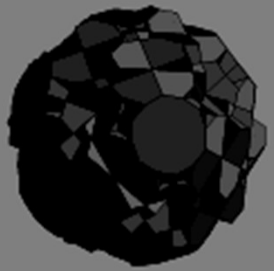




The (outside of) 15th Brillouin zone for the simple cubic.

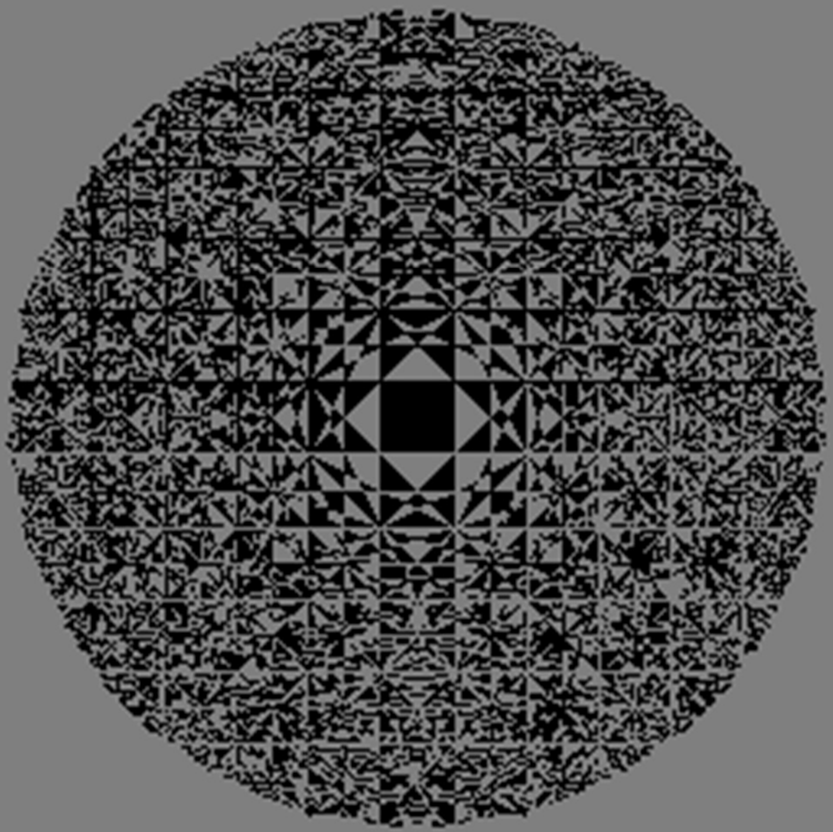
The (outside of) 18th Brillouin zone for the face-centered cubic

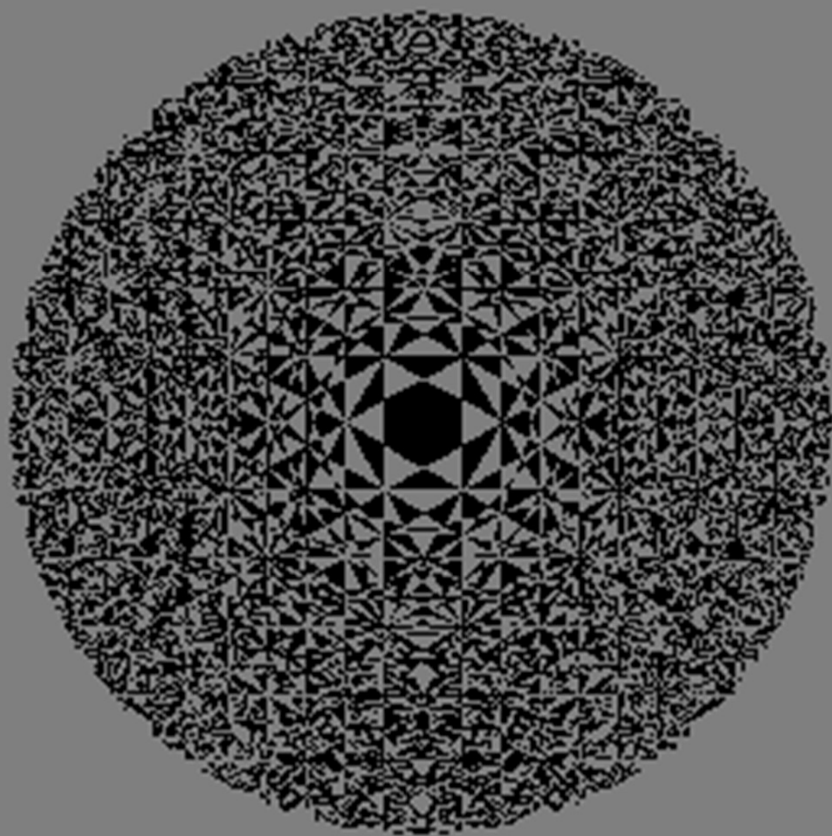




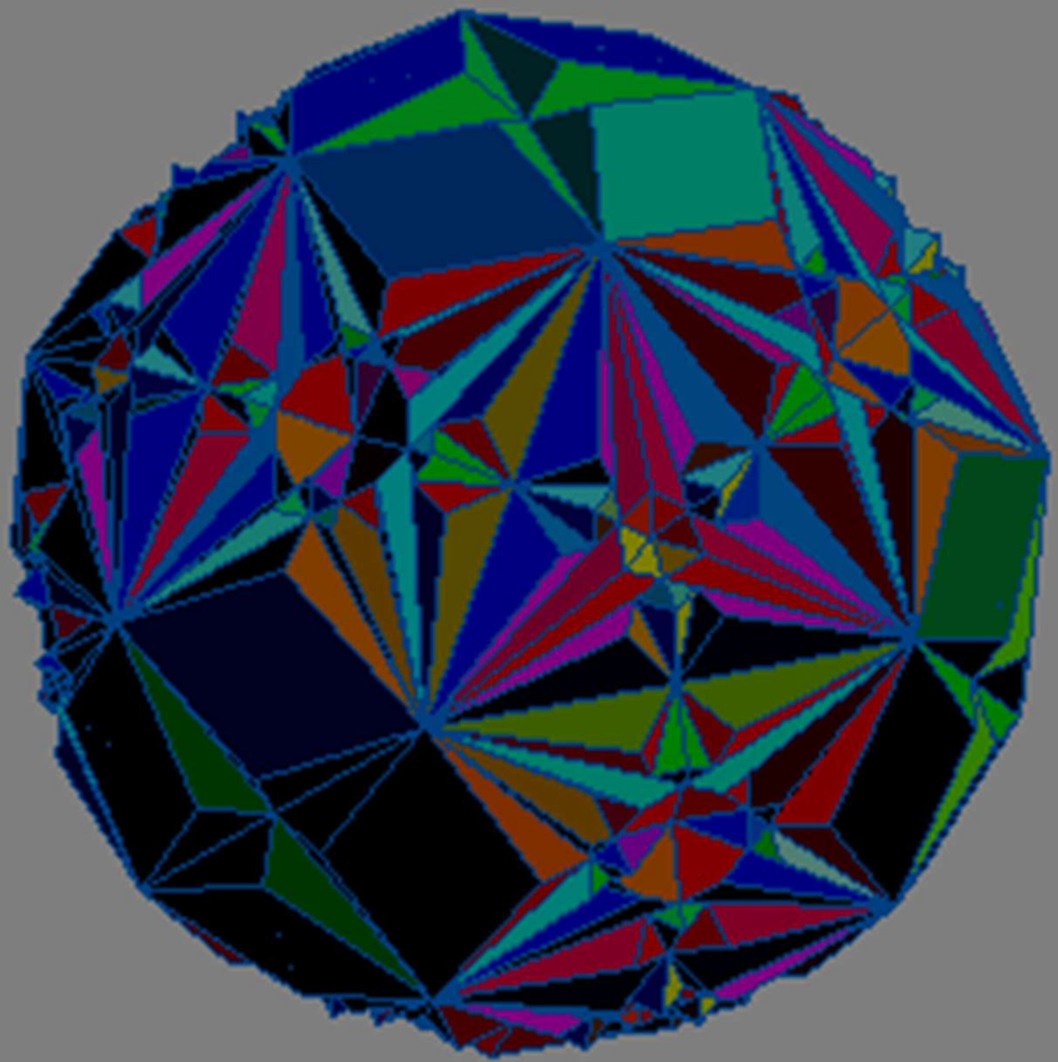
The (outside of) 10th Brillouin zone for the body-centered cubic lattice.

Two dimensional Brillouin zone

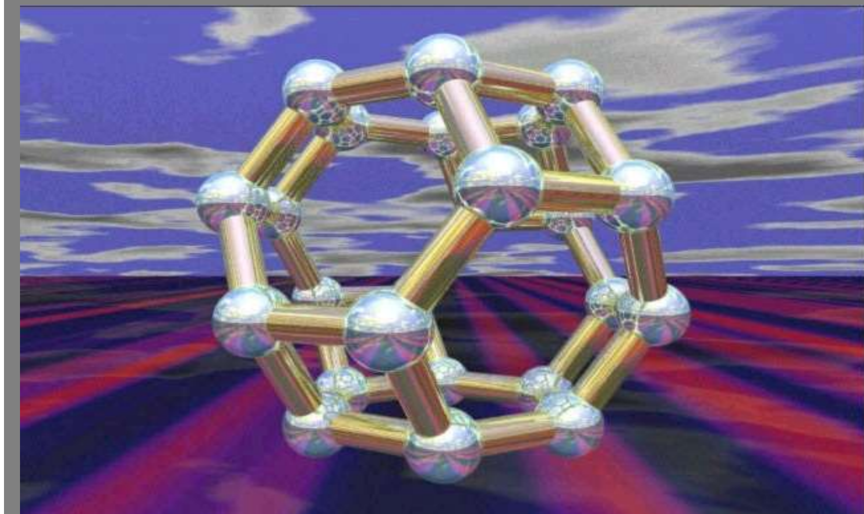


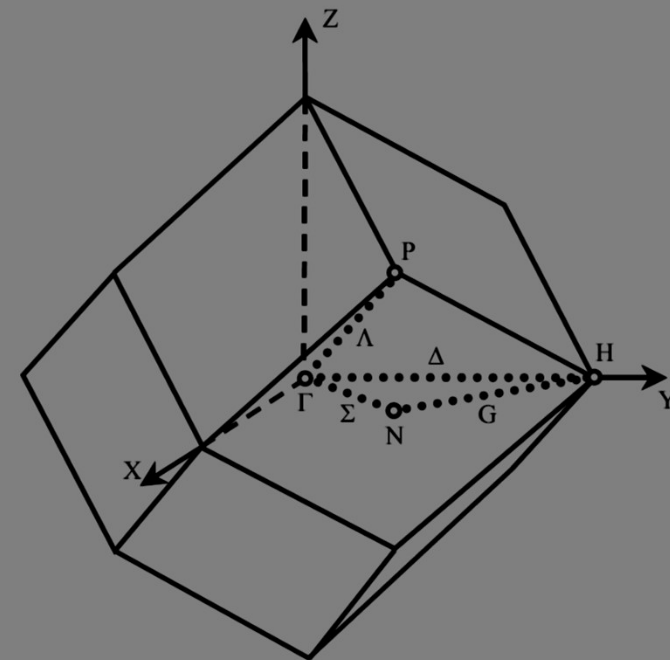


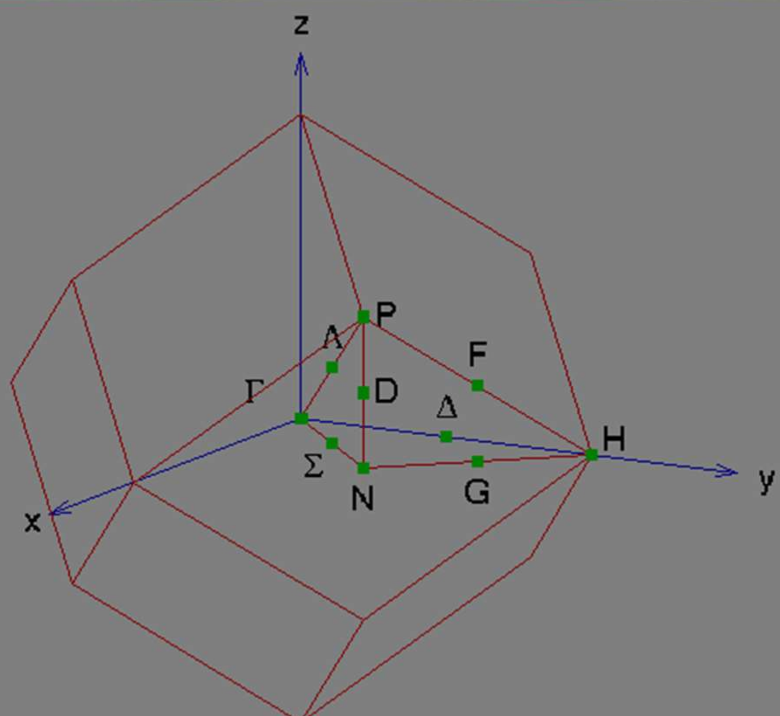
Three dimensional Brillouin zone

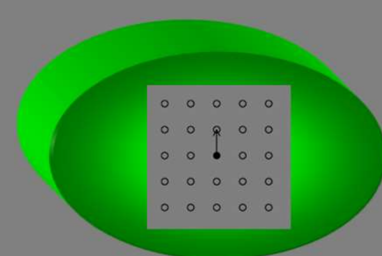


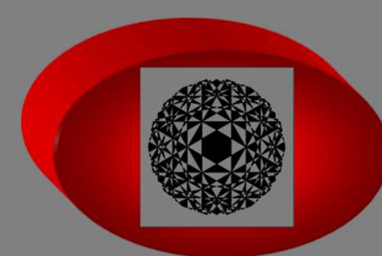
First Brillouin Zone BCC



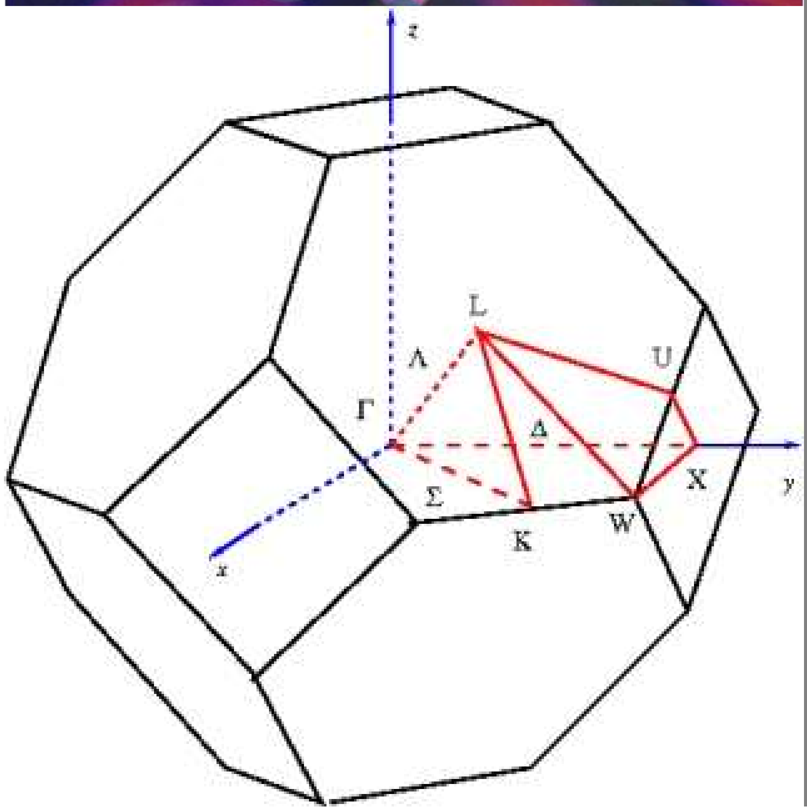


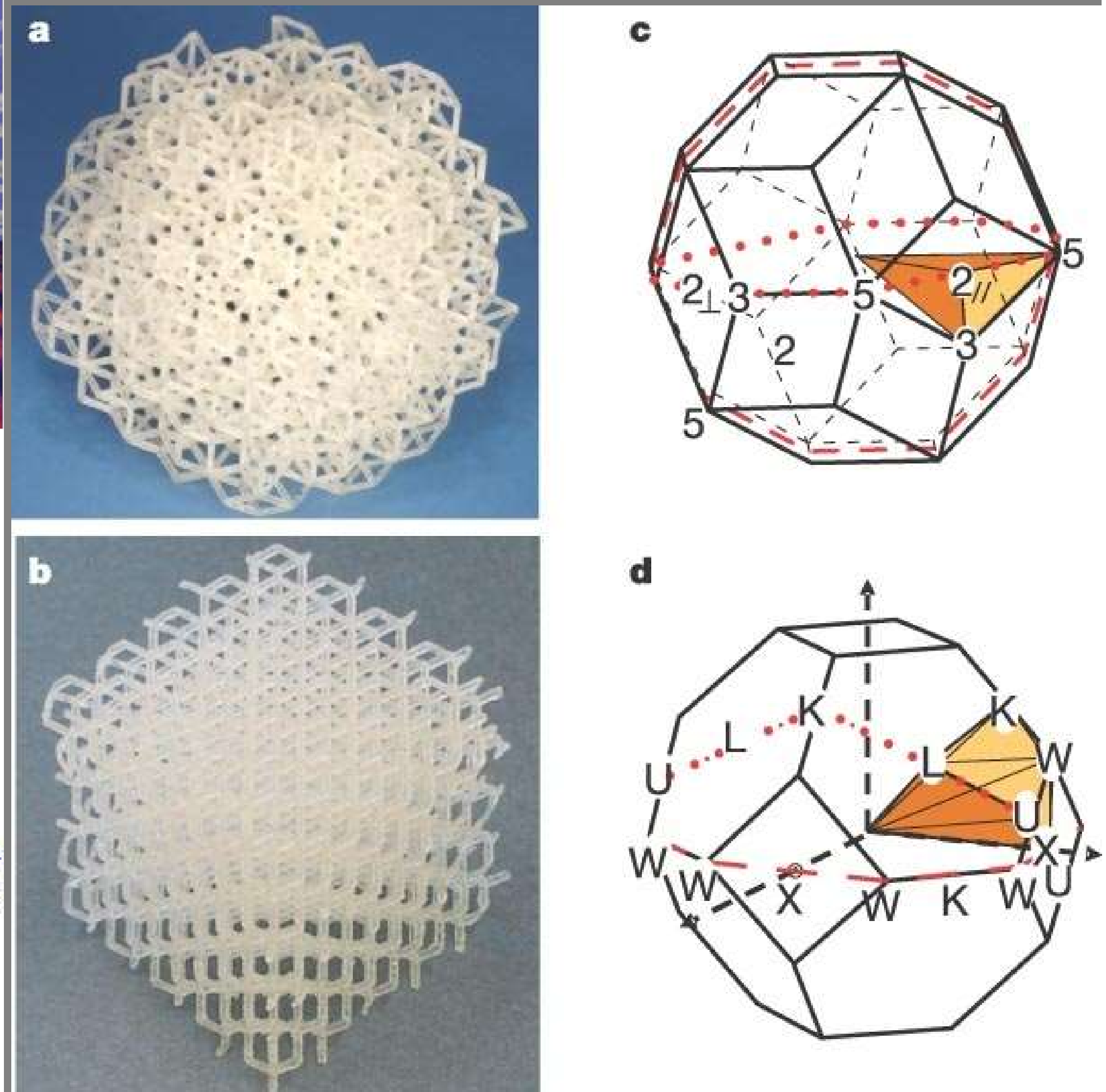


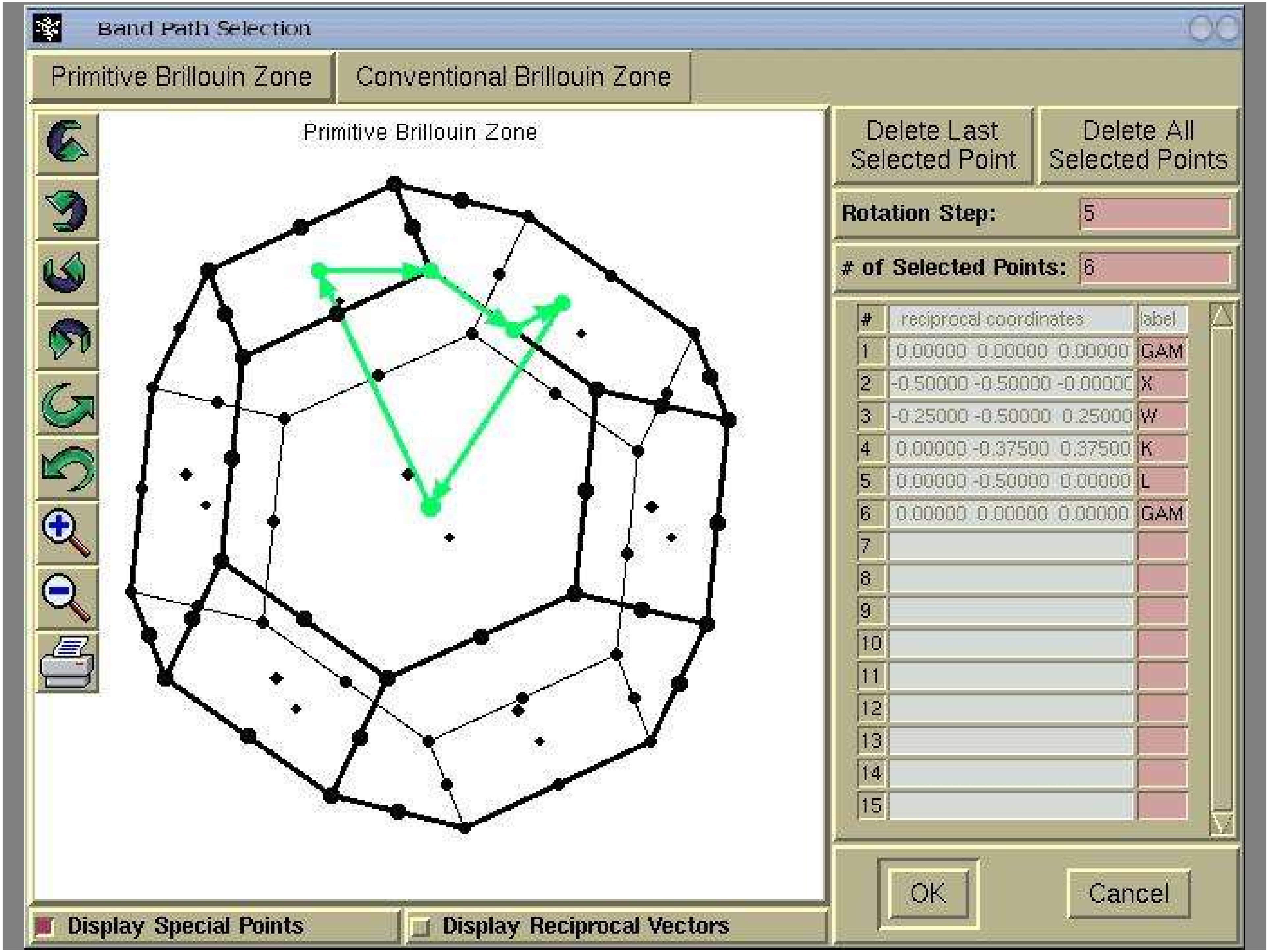




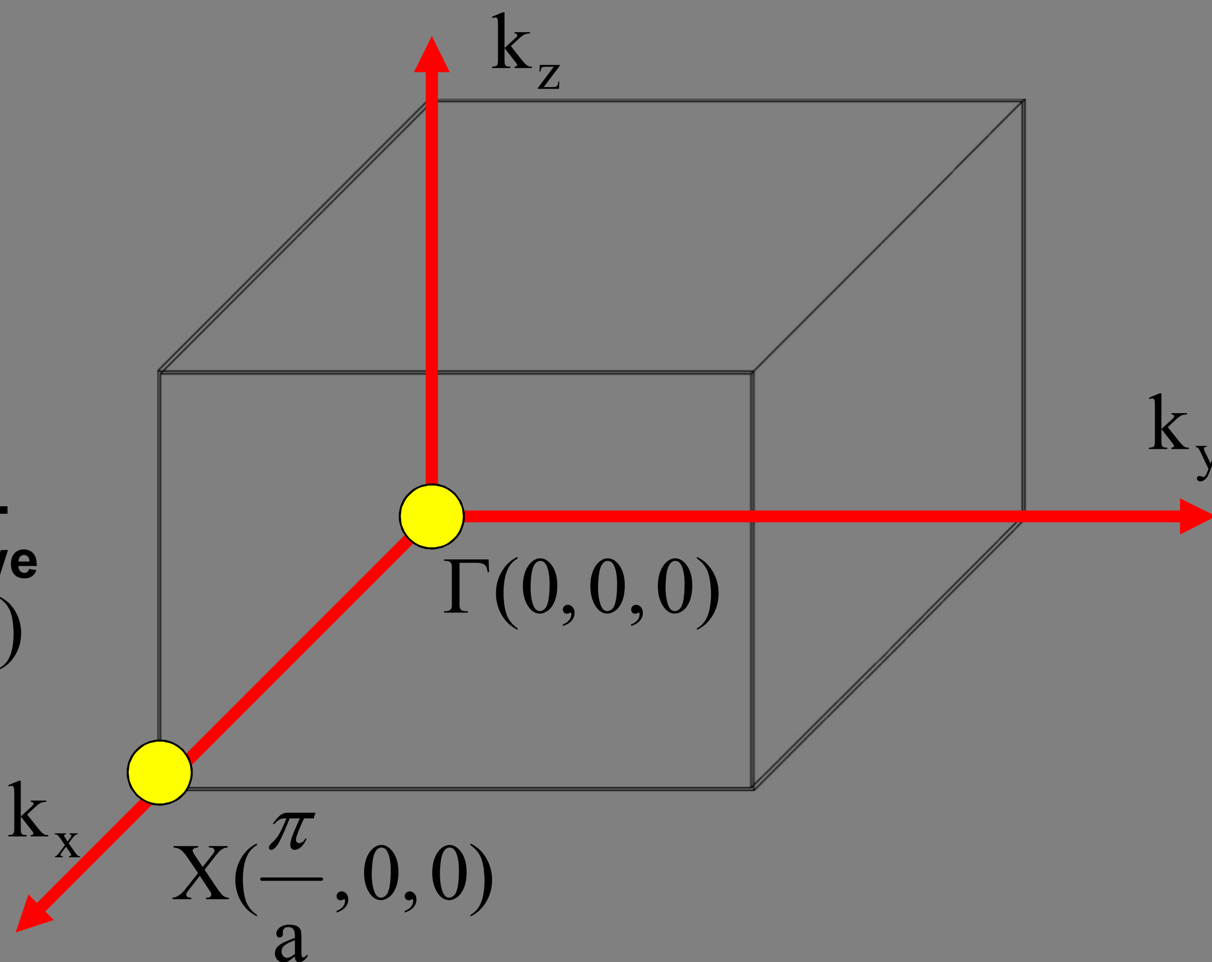
First Brillouin Zone FCC






Band Path Selection
Primitive Brillouin Zone
Conventional Brillouin Zone
Primitive Brillouin Zone
Delete Last Selected Point
Delete All Selected Points
Rotation Step:
5
# of Selected Points:
6
#
reciprocal coordinates
label
1 0.00000 0.00000 0.00000 GAM
2 -0.50000 -0.50000 -0.00000 X
3 -0.25000 -0.50000 0.25000 W
4 0.00000 -0.37500 0.37500 K
5 0.00000 -0.50000 0.00000 L
6 0.00000 0.00000 0.00000 GAM
7
8
9
10
11
12
13
14
15
OK
Cancel
Display Special Points
Display Reciprocal Vectors

Band structure of a simple cubic lattice along Γ to X direction. Along this direction we have: $\mathbf{k} = (k_x, 0, 0)$

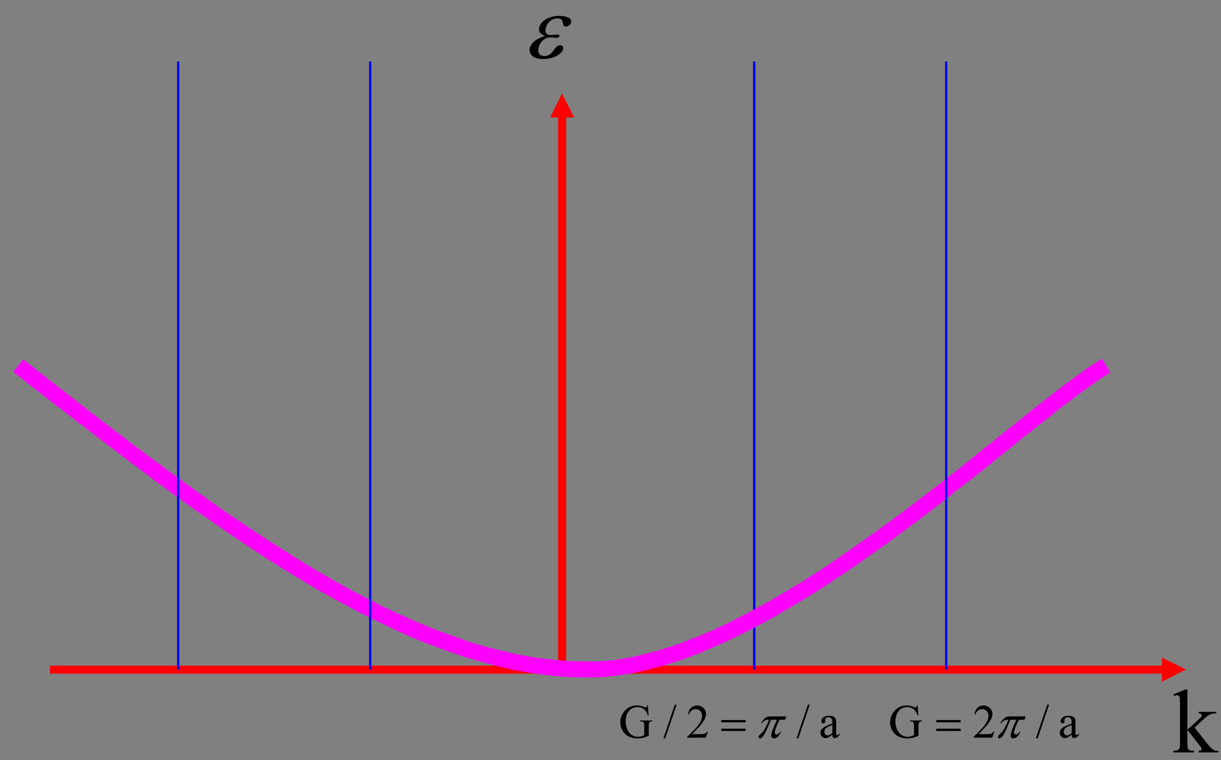


$$\Gamma(0,0,0) \Longrightarrow X(\frac{\pi}{a},0,0)$$

$$\mathbf{K} = \mathbf{k} + \mathbf{G}$$

Inside of the 1BZ

Outside of the 1BZ



$$\varepsilon = \frac{\hbar^2}{2m}(\mathbf{k}+\mathbf{G})^2 = \frac{\hbar^2}{2m}\left((k_x + G_x)^2 + (k_y + G_y)^2 + (k_z + G_z)^2\right)$$

Thus one would take some allowed shortest G vectors and try to plot their corresponded bands

Inside of the 1BZ

$$\Gamma(0,0,0) \Rightarrow X\left(\frac{\pi}{a},0,0\right)$$

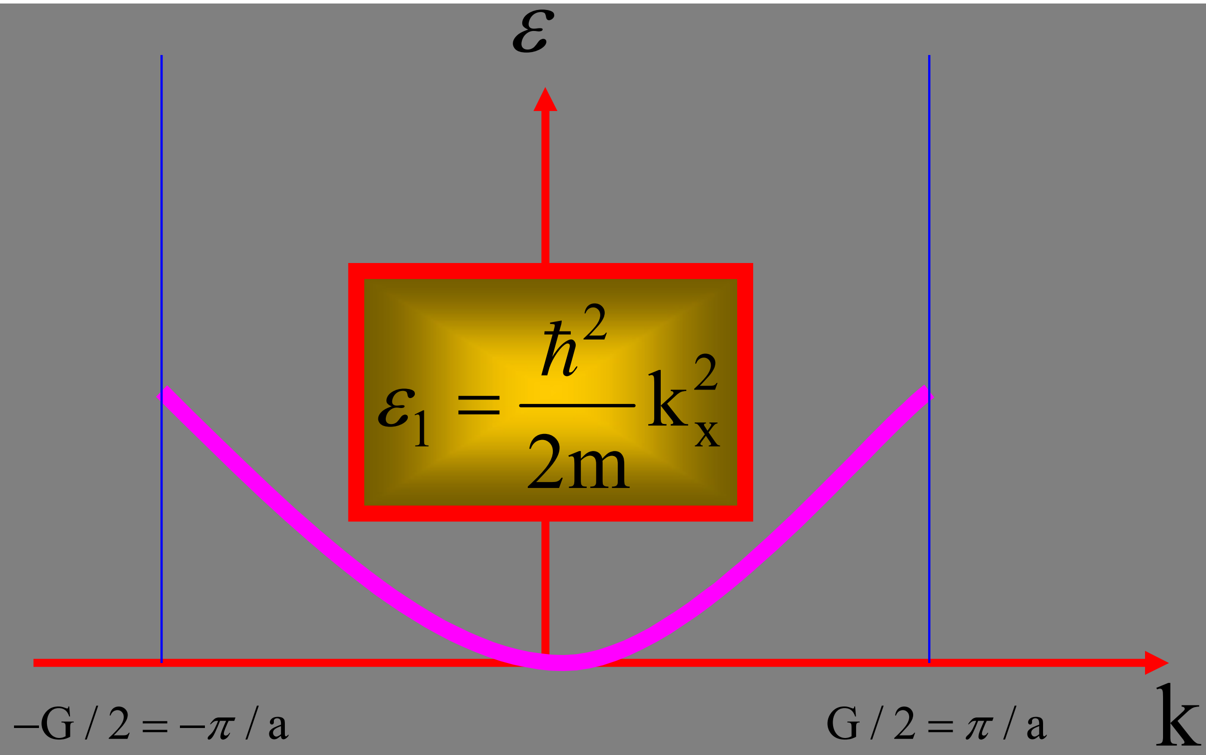
$$\mathbf{k} = (k_x, 0, 0)$$

$$k_y = k_z = 0$$

$$\varepsilon = \frac{\hbar^2}{2m}\left(\mathbf{k}+\mathbf{G}\right)^2 = \frac{\hbar^2}{2m}\left(\left(k_x + G_x\right)^2 + G_y^2 + G_z^2\right)$$

If $\mathbf{G} = 0 \Rightarrow G_x = G_y = G_z = 0 \Rightarrow$

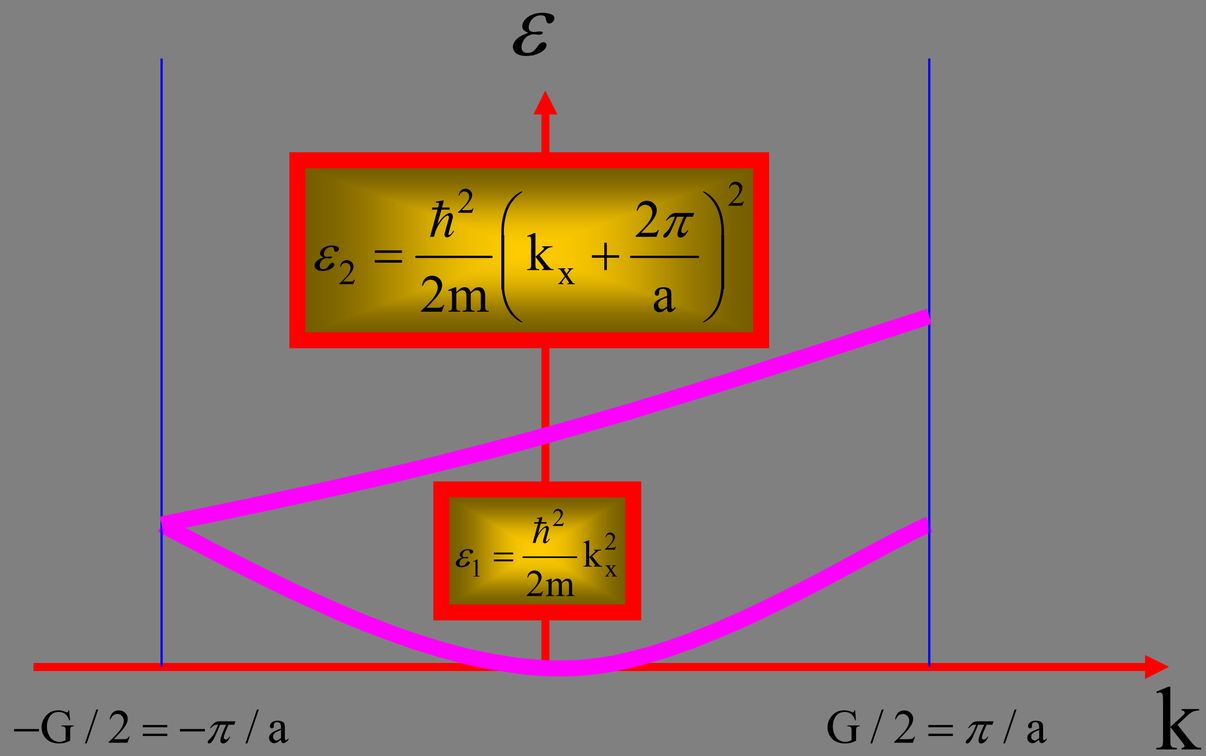
$$\varepsilon_1 = \frac{\hbar^2}{2m} k_x^2$$



$$\varepsilon_1 = \frac{\hbar^2}{2m} k_x^2$$

If $\mathbf{G} = \frac{2\pi}{a}(1,0,0)$ $\rightarrow$ $G_x = \frac{2\pi}{a}, G_y = G_z = 0$

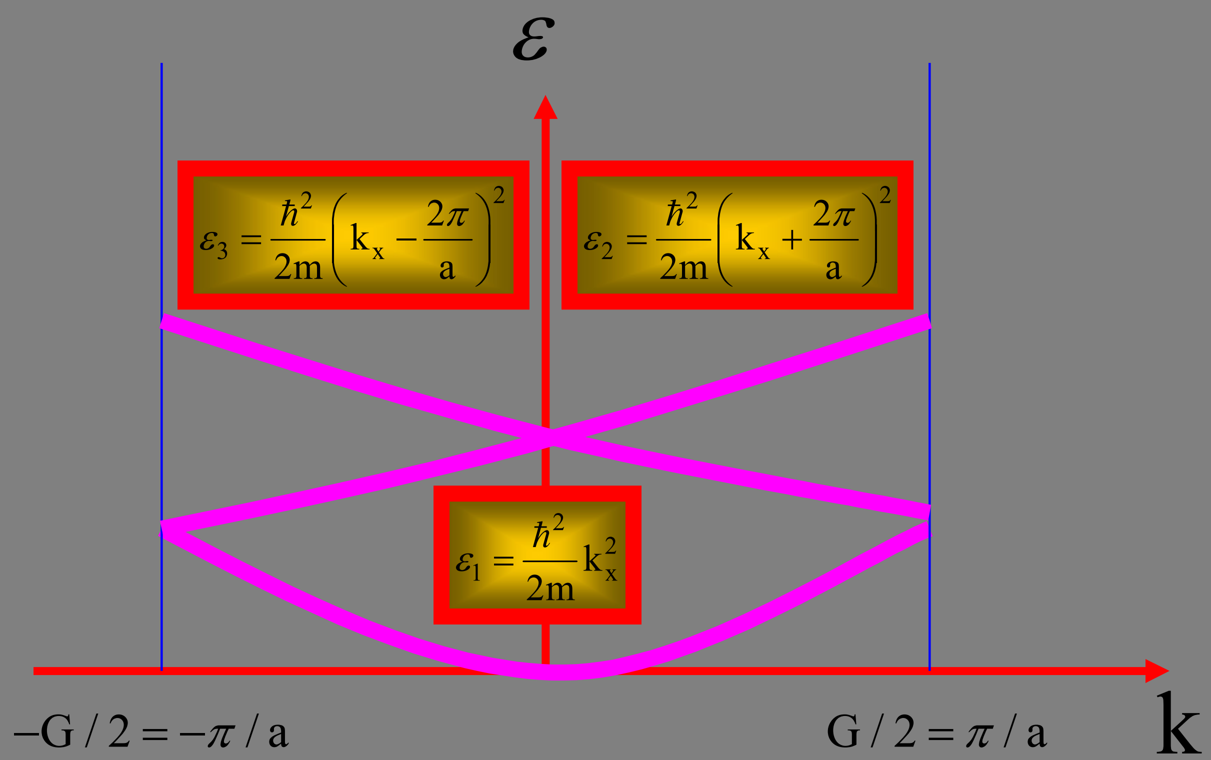
$$\varepsilon_2 = \frac{\hbar^2}{2m}\left(k_x + \frac{2\pi}{a}\right)^2$$



If $\mathbf{G} = \frac{2\pi}{a}(\bar{1},0,0)$

$$G_x = -\frac{2\pi}{a}, G_y = G_z = 0$$

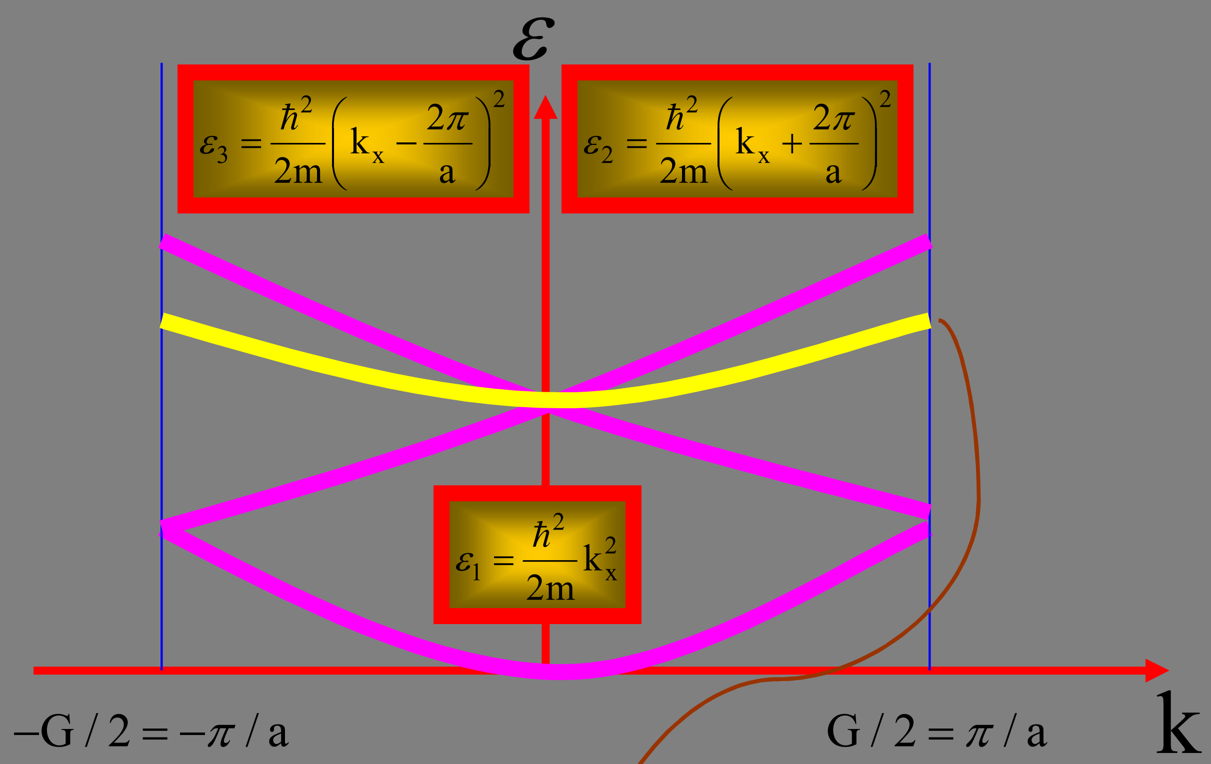
$$\varepsilon_3 = \frac{\hbar^2}{2m}\left(k_x - \frac{2\pi}{a}\right)^2$$



If

$$\mathbf{G} = \frac{2\pi}{a}(0,1,0) = \frac{2\pi}{a}(0,\bar{1},0) = \frac{2\pi}{a}(0,0,1) = \frac{2\pi}{a}(0,0,\bar{1})$$

$$\varepsilon_4 = \frac{\hbar^2}{2m}\left(k_x^2 + \left(\frac{2\pi}{a}\right)^2\right) = \varepsilon_5 = \varepsilon_6 = \varepsilon_7$$

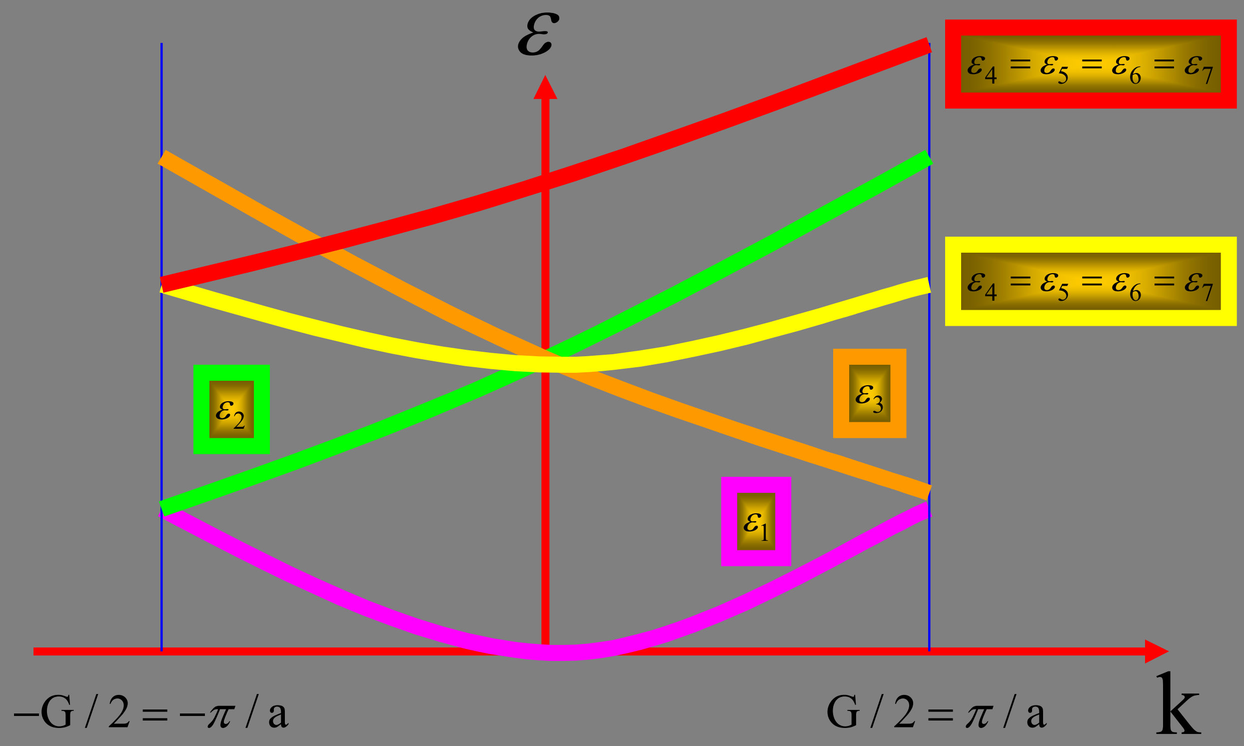


$$\boxed{\varepsilon_4 = \frac{\hbar^2}{2m}\left(k_x^2 + \left(\frac{2\pi}{a}\right)^2\right) = \varepsilon_5 = \varepsilon_6 = \varepsilon_7}$$

This band is four fold degenerated

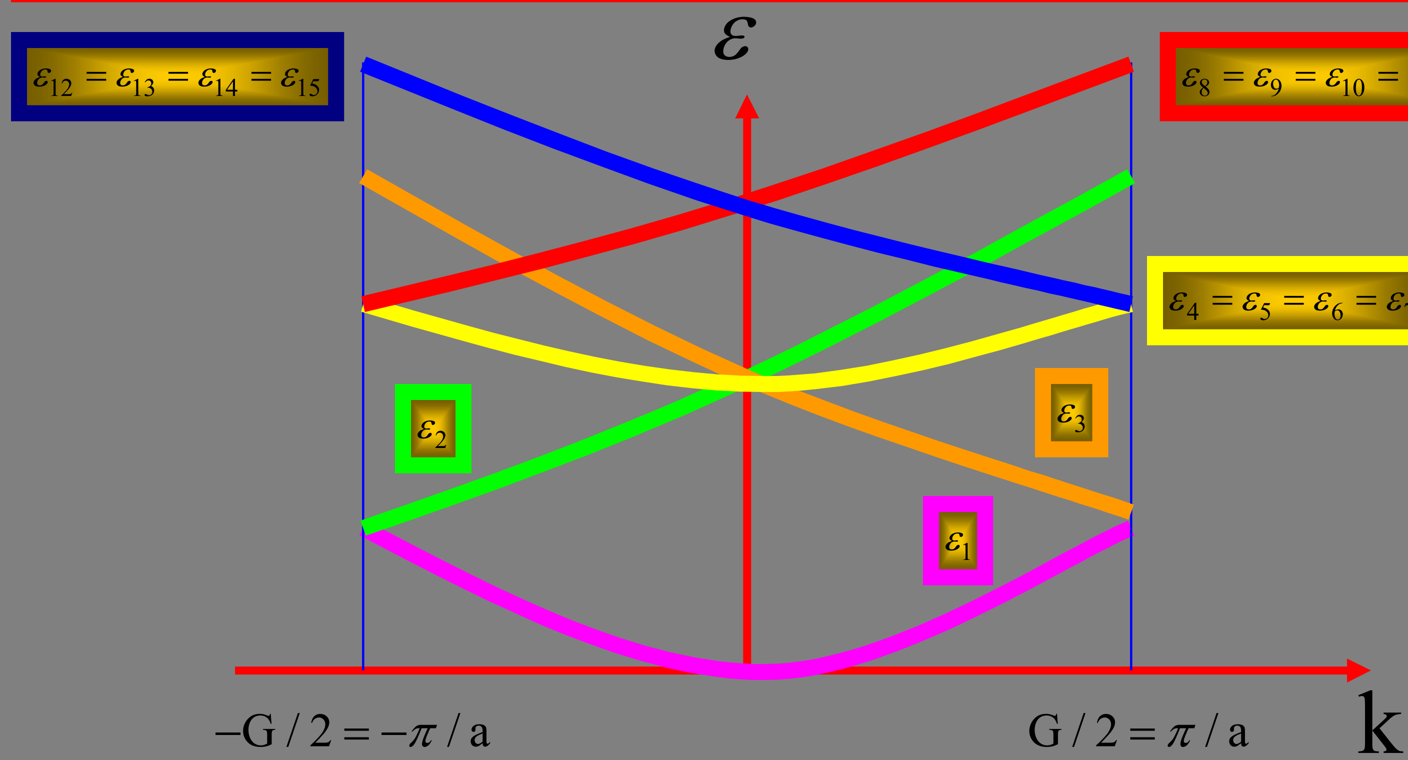
If $\mathbf{G} = \dfrac{2\pi}{a}(110;101;1\bar{1}0;10\bar{1})$

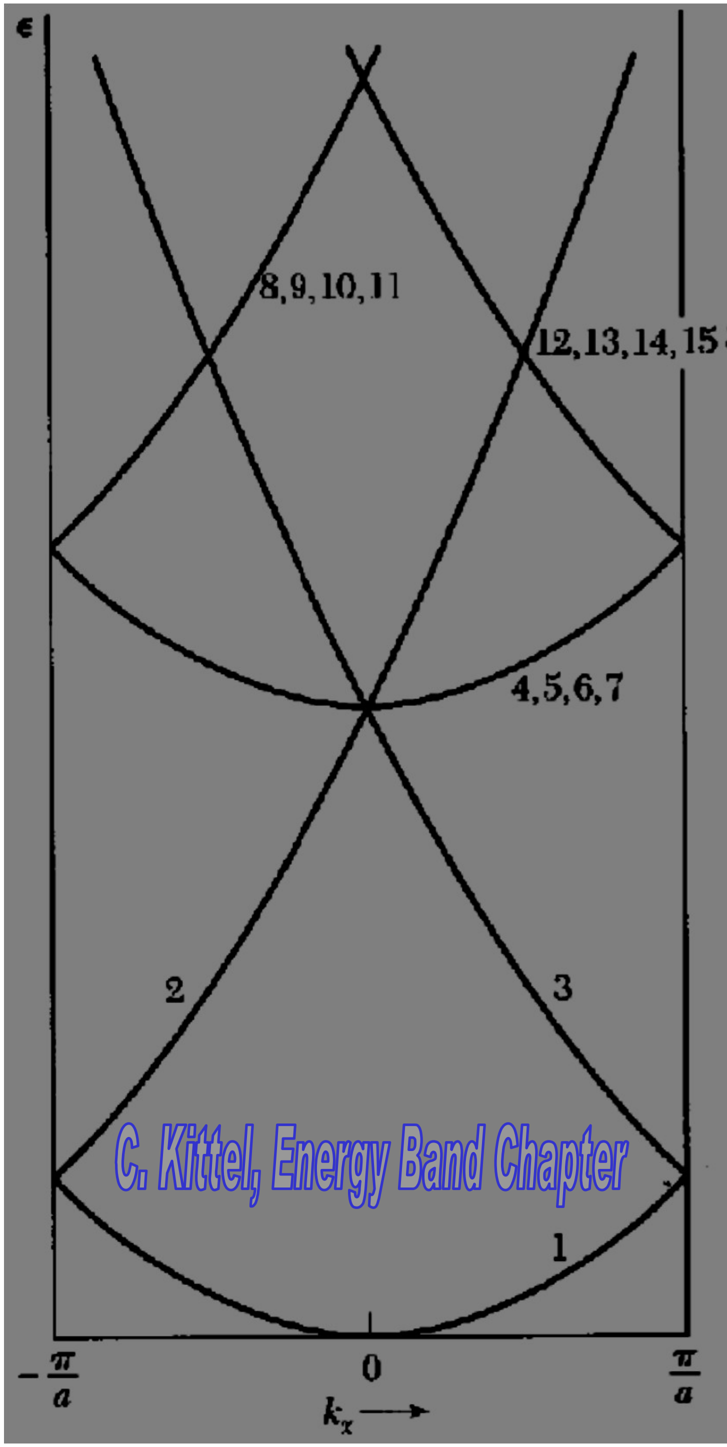
$$\varepsilon_8 = \frac{\hbar^2}{2m}\left(\left(k_x + \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2\right) = \varepsilon_9 = \varepsilon_{10} = \varepsilon_{11}$$



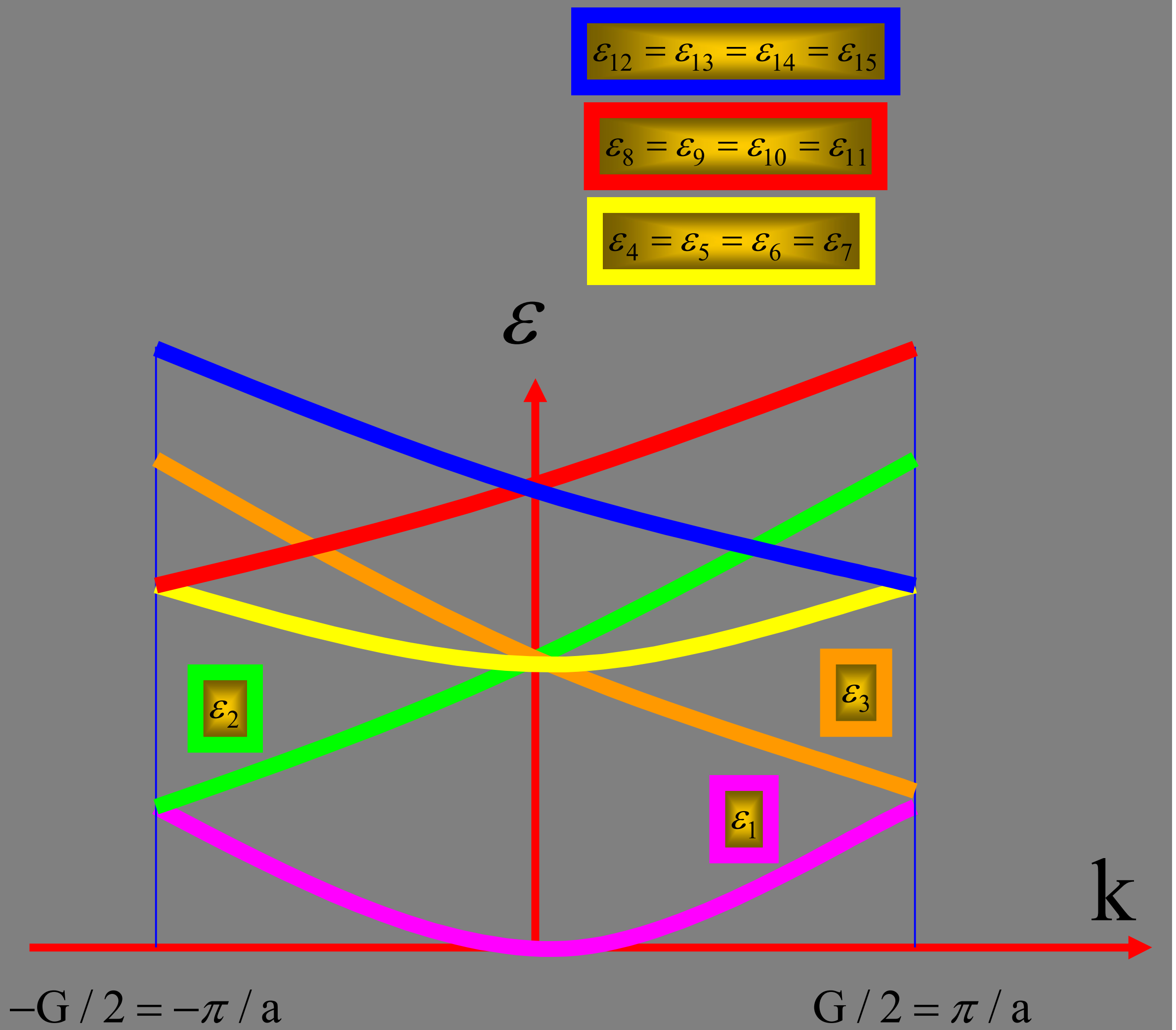
If $\mathbf{G} = \frac{2\pi}{a}(\bar{1}10; \bar{1}01; \bar{1}\bar{1}0; \bar{1}0\bar{1})$

$$\varepsilon_{12} = \frac{\hbar^2}{2m}\left(\left(k_x - \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2\right) = \varepsilon_{13} = \varepsilon_{14} = \varepsilon_{15}$$





ϵ
8, 9, 10, 11
12, 13, 14, 15
4, 5, 6, 7
2
3
1
C. Kittel, Energy Band Chapter
$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
k_x



$\varepsilon_{12} = \varepsilon_{13} = \varepsilon_{14} = \varepsilon_{15}$
$\varepsilon_{8} = \varepsilon_{9} = \varepsilon_{10} = \varepsilon_{11}$
$\varepsilon_{4} = \varepsilon_{5} = \varepsilon_{6} = \varepsilon_{7}$
ε
ε_2
ε_3
ε_1
k
$-G/2 = -\pi/a$
$G/2 = \pi/a$

PRACTICE

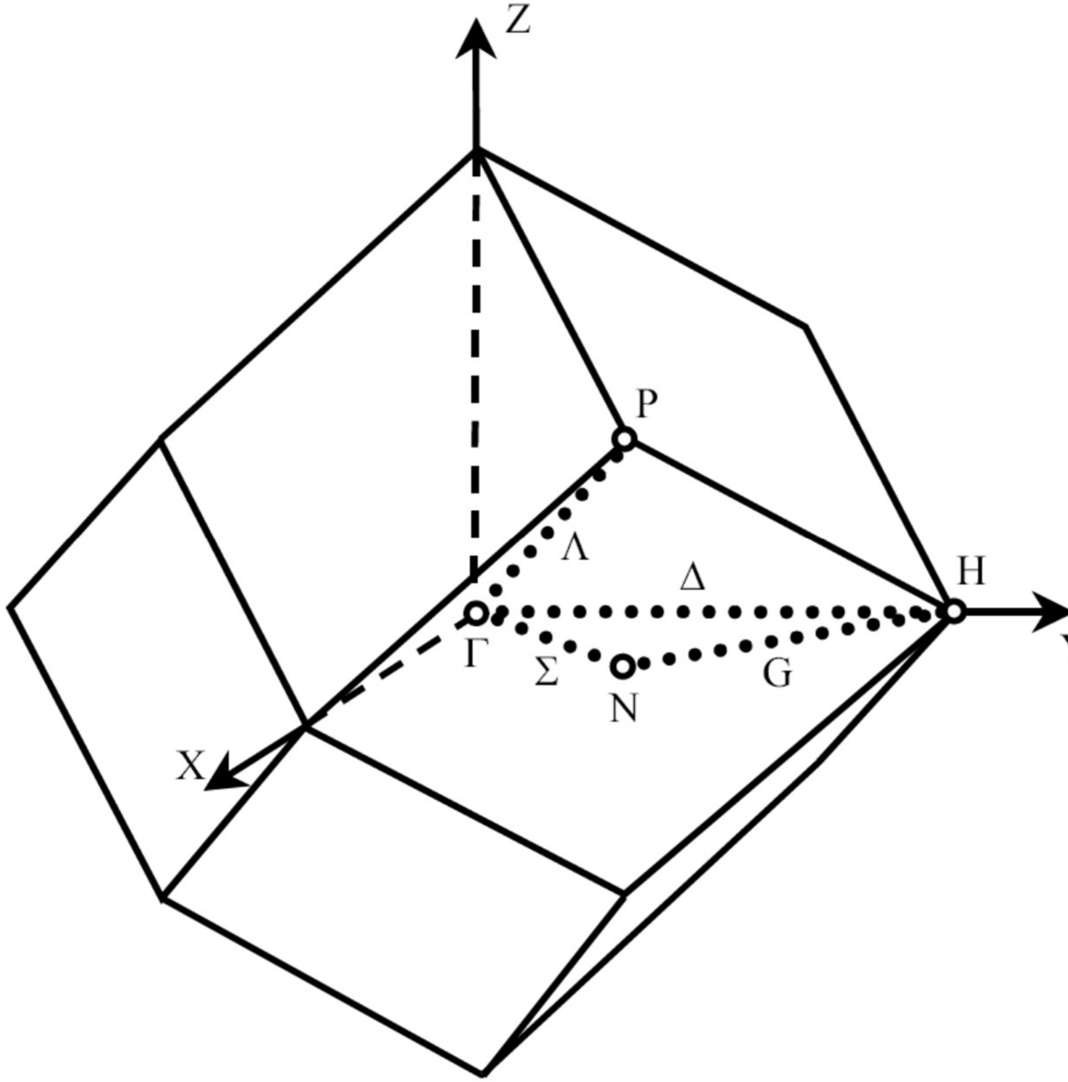
Find the band structure of an empty simple cubic (SC) along (111) direction

Find the band structure of an empty body centered cubic (bcc) along Γ(000) to H(010) for the first four allowed G vectors taking bcc structure factor into account

$$S_{\mathbf{K}} = 1 + e^{i\pi(n_1+n_2+n_3)} = 1 + (-1)^{n_1+n_2+n_3}$$
$$= \begin{cases} 2, & n_1 + n_2 + n_3 \quad \text{even,} \\ 0, & n_1 + n_2 + n_3 \quad \text{odd.} \end{cases}$$

$$\mathbf{G} = \frac{2\pi}{a}\left(n_1\hat{k}_x + n_2\hat{k}_y + n_3\hat{k}_z\right)$$

Miller indexes h, k, l

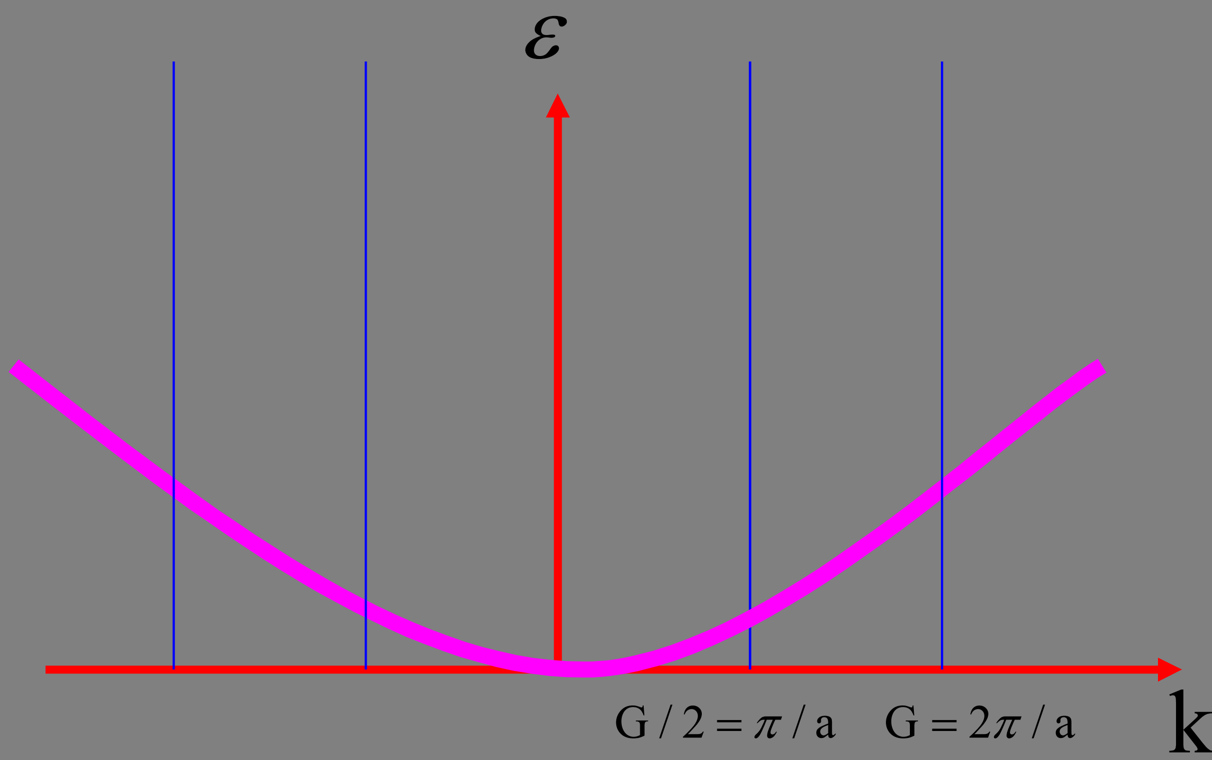


$$\Gamma(0,0,0) \Rightarrow \Delta\left(\frac{\pi}{a}(010)\right) \Rightarrow H\left(\frac{2\pi}{a}(010)\right)$$

$$\boxed{\mathbf{K}} = \boxed{\mathbf{k}} + \mathbf{G}$$

Inside of the 1BZ

Outside of the 1BZ



$$\varepsilon = \frac{\hbar^2}{2m}(\mathbf{k}+\mathbf{G})^2 = \frac{\hbar^2}{2m}\left(\left(\boxed{k_x}+G_x\right)^2+\left(\boxed{k_y}+G_y\right)^2+\left(\boxed{k_z}+G_z\right)^2\right)$$

Thus one would take some allowed shortest G vectors and try to plot their corresponded bands

Inside of the 1BZ

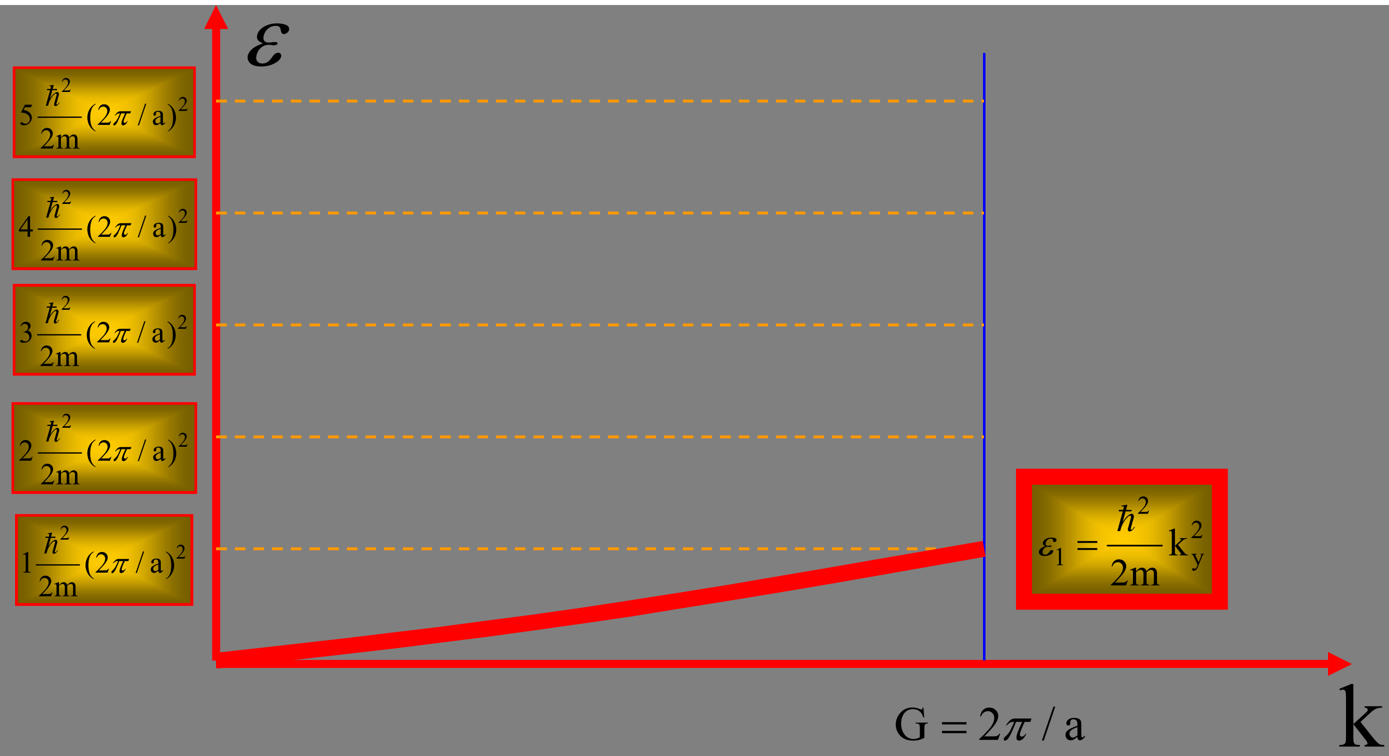
$$\Gamma(0,0,0) \Rightarrow H\left(0, 2\frac{\pi}{a}, 0\right)$$

$$\mathbf{k} = (0, k_y, 0)$$

$$k_x = k_z = 0$$

$$\boxed{\varepsilon = \frac{\hbar^2}{2m}\left(\mathbf{k}+\mathbf{G}\right)^2 = \frac{\hbar^2}{2m}\left(G_x^2 + \left(k_y + G_y\right)^2 + G_z^2\right)}$$

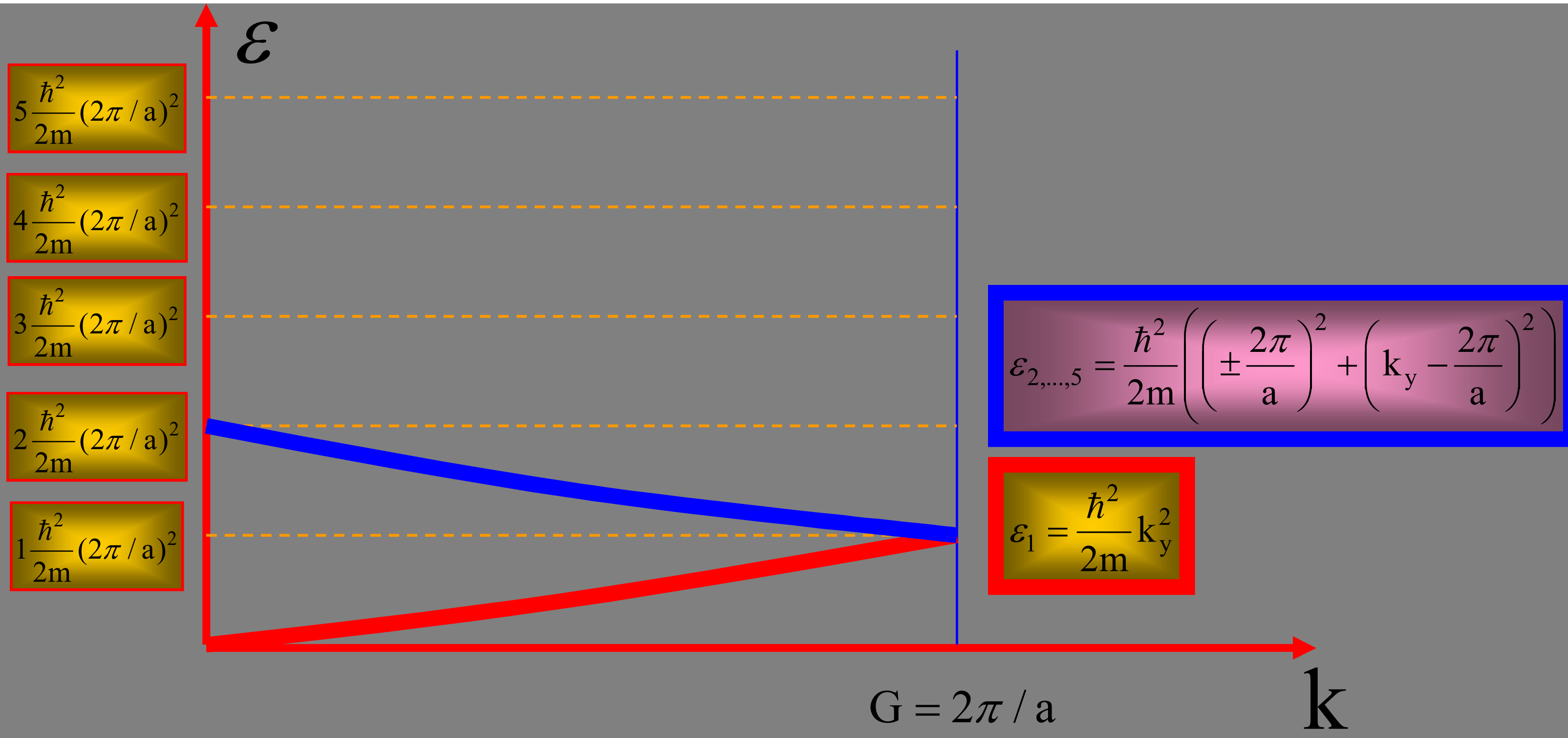
If $\mathbf{G} = 0 \Rightarrow G_x = G_y = G_z = 0 \Rightarrow \boxed{\varepsilon_1 = \frac{\hbar^2}{2m}k_y^2}$



If

$$\mathbf{G} = \frac{2\pi}{a}(000)$$

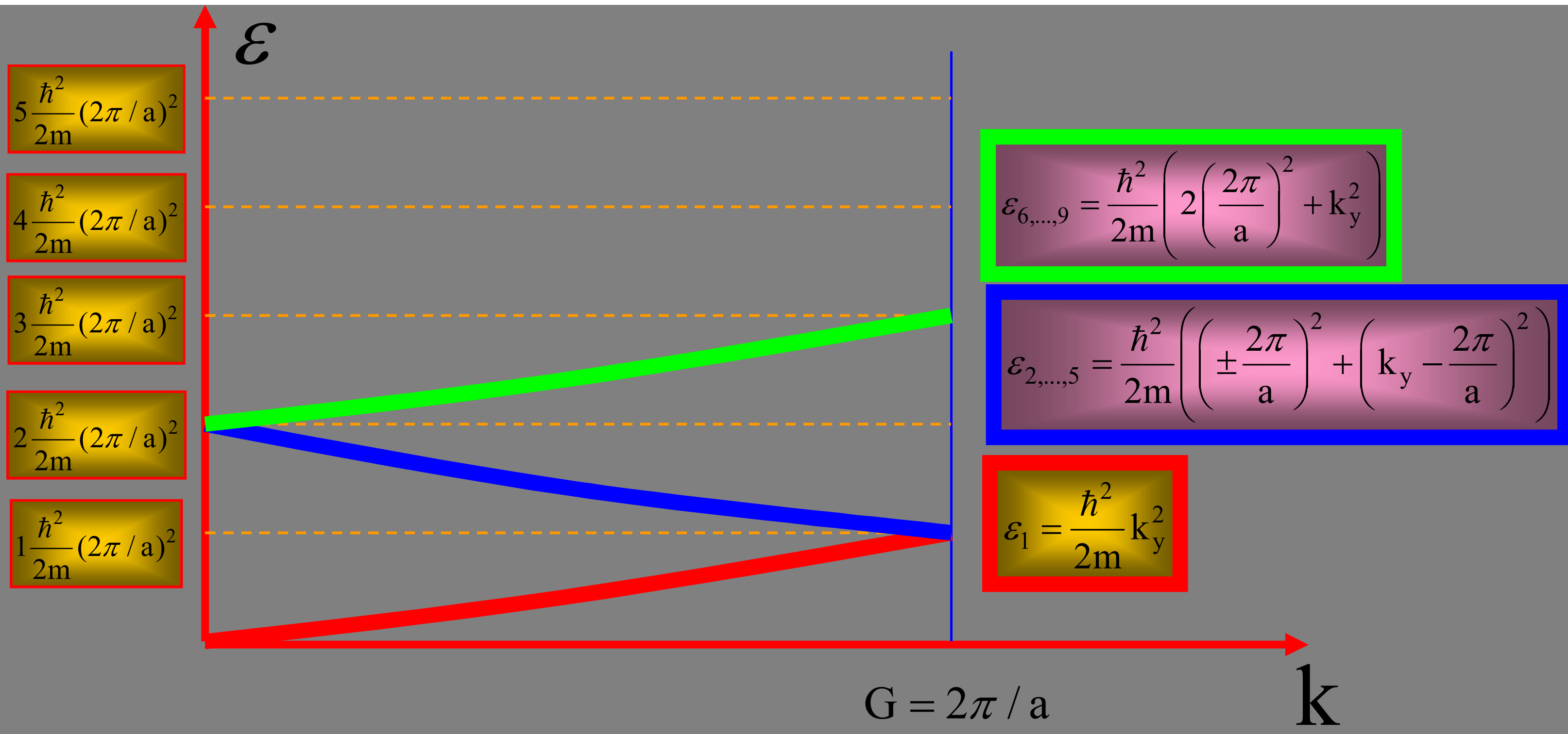
$$\boxed{\varepsilon_1 = \frac{\hbar^2}{2m}k_y^2}$$



If

$$\mathbf{G} = \frac{2\pi}{a}\left(1\,\bar{1}\,0, \bar{1}\,\bar{1}\,0, 0\,\bar{1}\,1, 0\,\bar{1}\,\bar{1}\right)$$

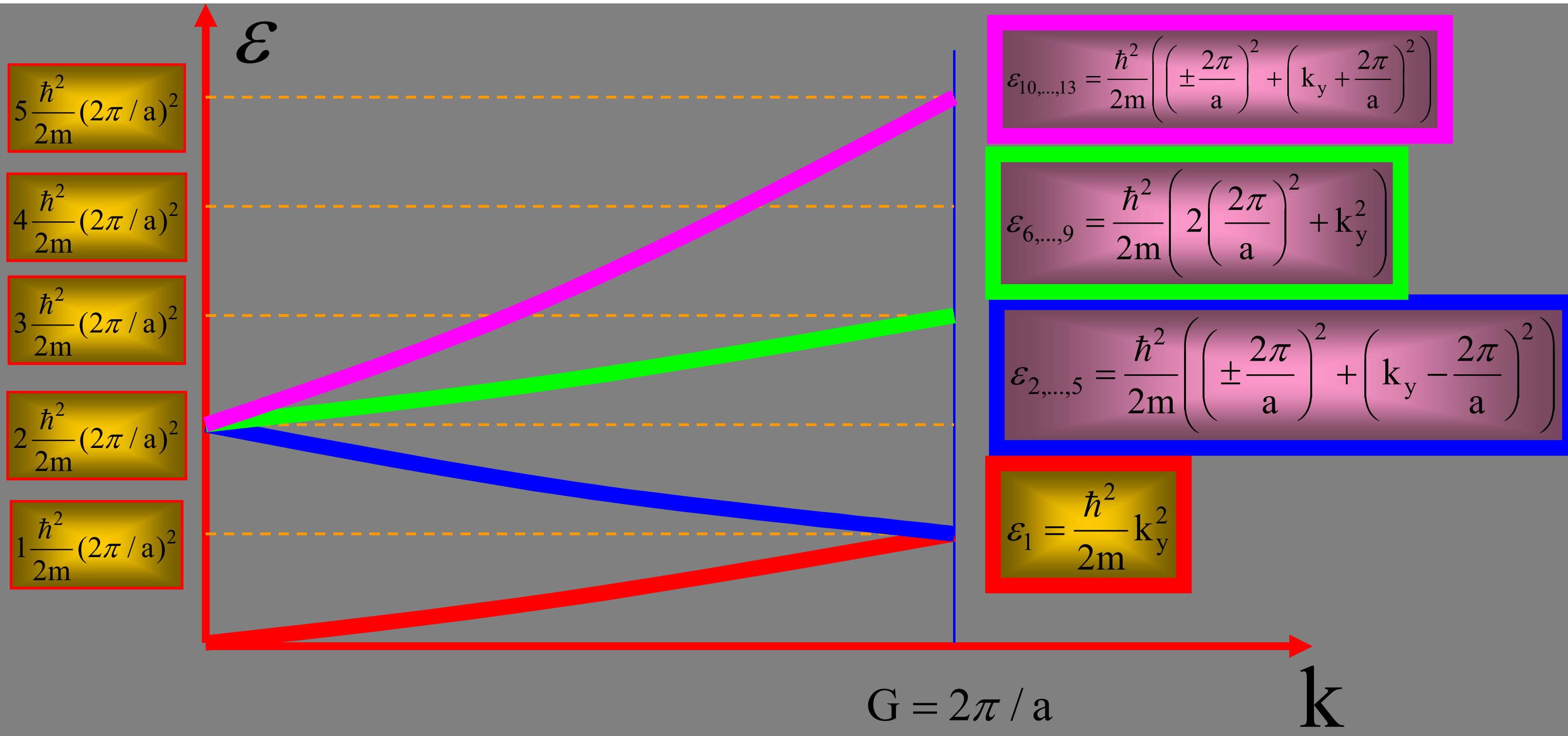
$$\varepsilon_{2,\ldots,5} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y - \frac{2\pi}{a}\right)^2\right)$$



If

$$\mathbf{G} = \frac{2\pi}{a}\left(101, \bar{1}01, 10\bar{1}, \bar{1}0\bar{1}\right)$$

$$\varepsilon_{6,\ldots,9} = \frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}\right)^2 + k_y^2 + \left(\frac{2\pi}{a}\right)^2\right)$$

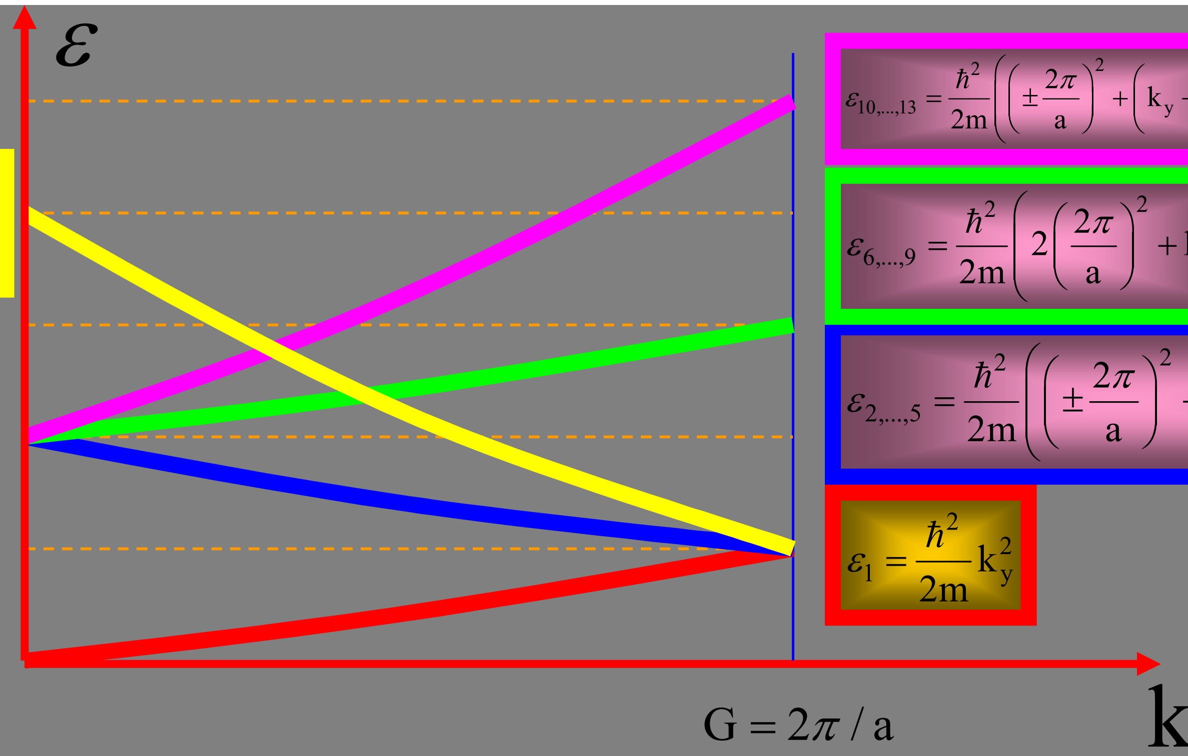


If

$$\mathbf{G} = \frac{2\pi}{a}\left(110, \bar{1}10, 011, 01\bar{1}\right)$$

$$\varepsilon_{10,\dots,13} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y + \frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{14} = \frac{\hbar^2}{2m}\left(\left(k_y - 2\frac{2\pi}{a}\right)^2\right)$$



$$\varepsilon_{10,\ldots,13} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y + \frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{6,\ldots,9} = \frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{2,\ldots,5} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y - \frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_1 = \frac{\hbar^2}{2m}k_y^2$$

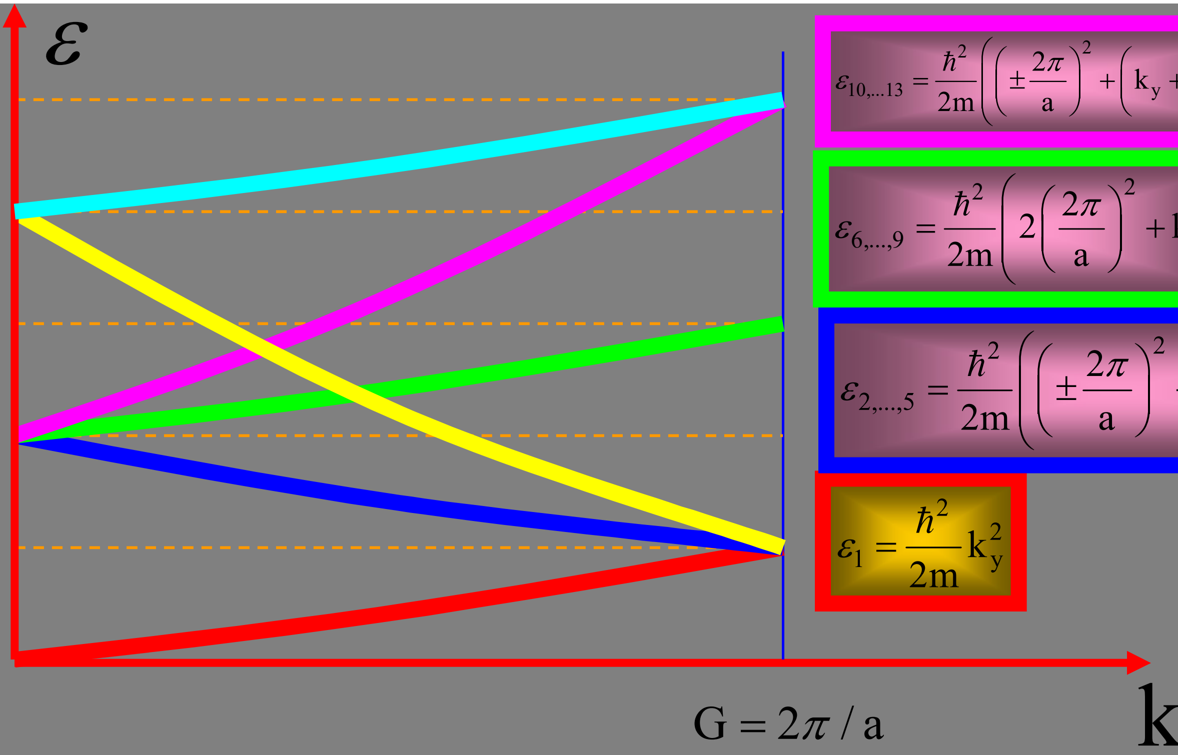
If

$$\mathbf{G} = \frac{2\pi}{a}\left(0\bar{2}0\right)$$

$$\varepsilon_{14} = \frac{\hbar^2}{2m}\left(\left(k_y - 2\frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{15,\ldots,18} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{14} = \frac{\hbar^2}{2m}\left(\left(k_y - 2\frac{2\pi}{a}\right)^2\right)$$



$$\varepsilon_{10,\ldots,13} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y + \frac{2\pi}{a}\right)^2\right)$$

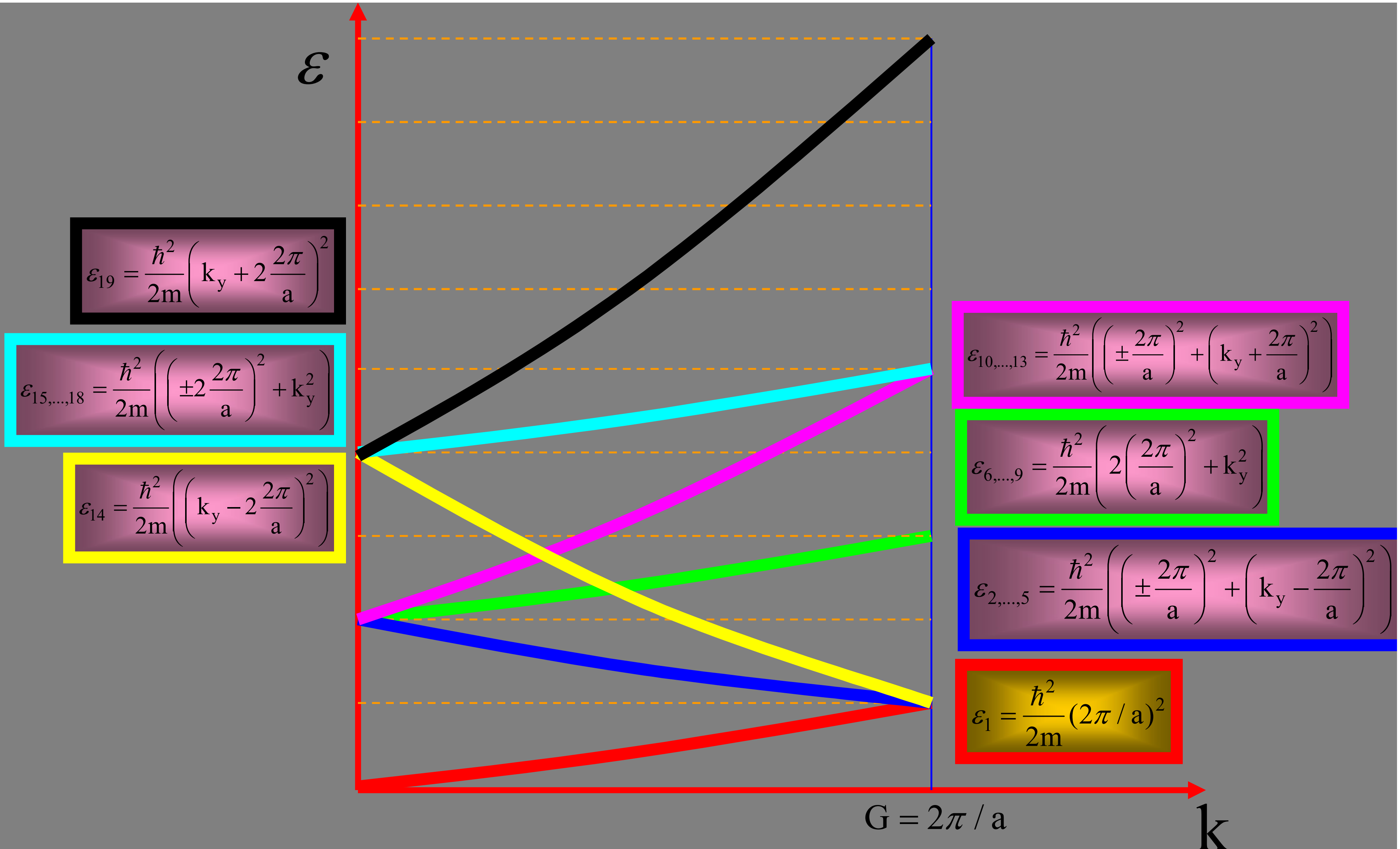
$$\varepsilon_{6,\ldots,9} = \frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{2,\ldots,5} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y - \frac{2\pi}{a}\right)^2\right)$$

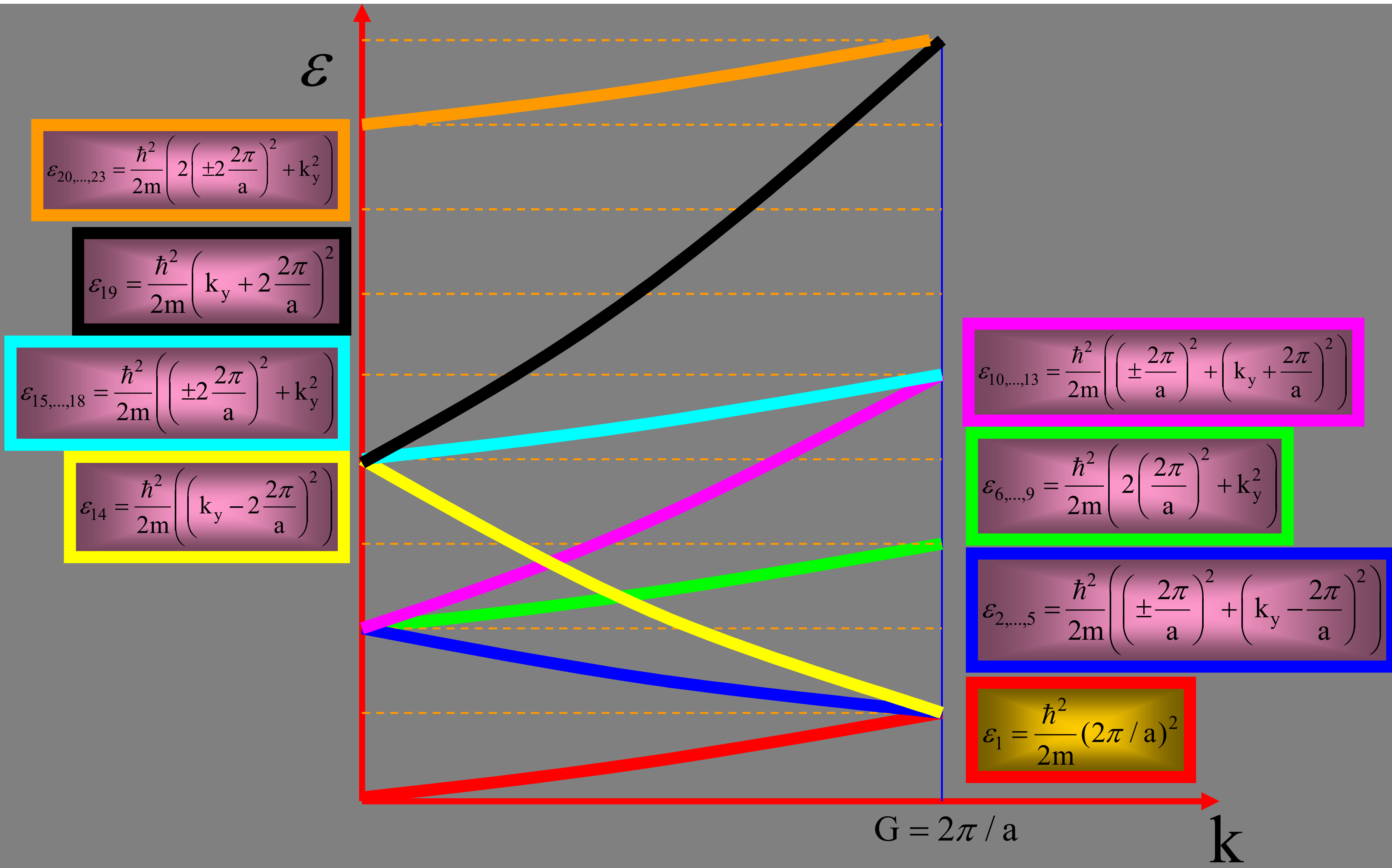
$$\varepsilon_1 = \frac{\hbar^2}{2m}k_y^2$$

$$\mathbf{G} = \frac{2\pi}{a}\left(200, \bar{2}00, 002, 00\bar{2}\right)$$

$$\varepsilon_{15,\ldots,18} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

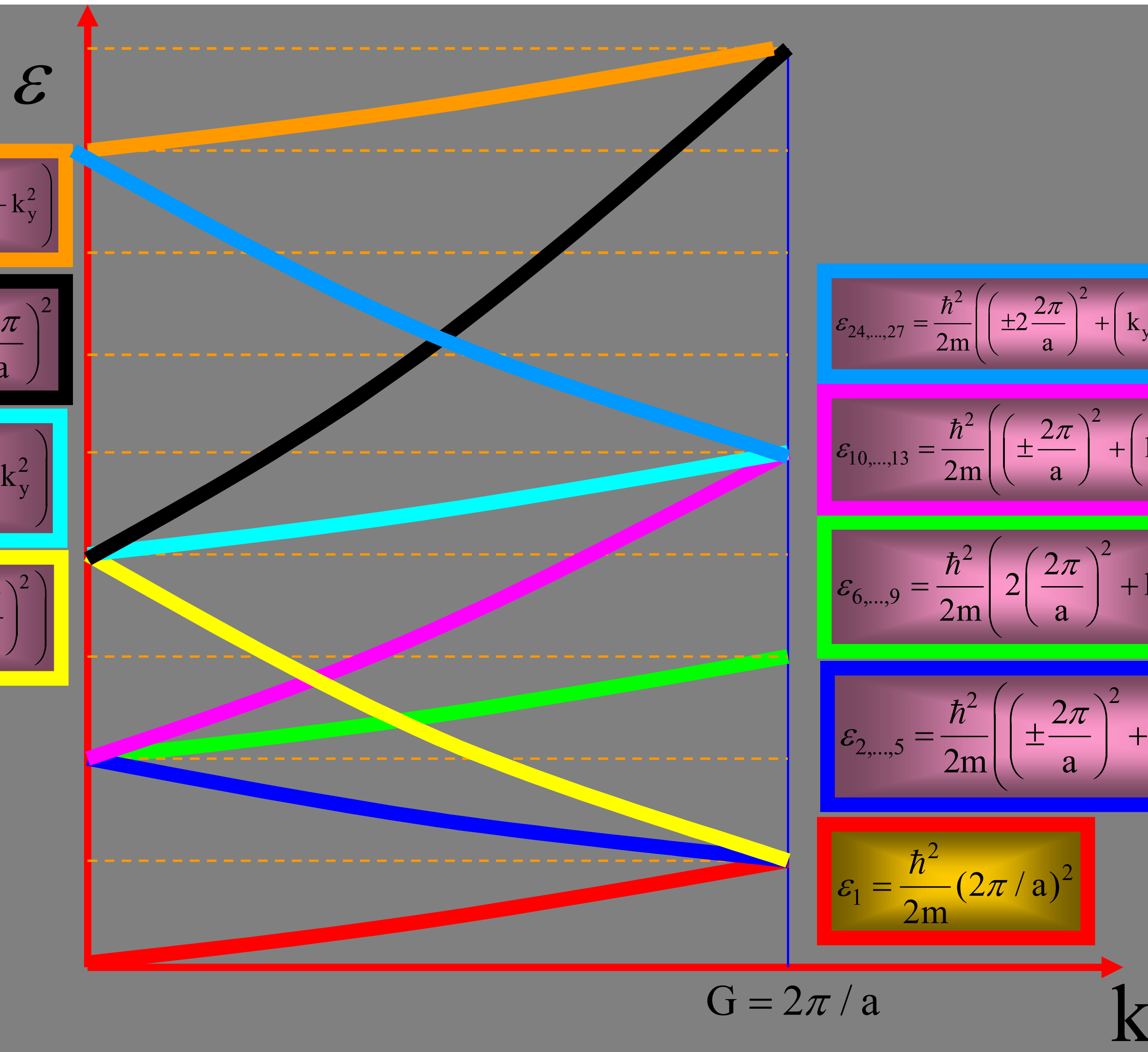


$$\mathbf{G} = \frac{2\pi}{a}(020) \Rightarrow \varepsilon_{19} = \frac{\hbar^2}{2m}\left(k_y + 2\frac{2\pi}{a}\right)^2$$



$$\mathbf{G} = \frac{2\pi}{a}\left(202, \bar{2}02, 20\bar{2}, \bar{2}0\bar{2}\right)$$

$$\varepsilon_{20,\dots,23} = \frac{\hbar^2}{2m}\left(2\left(\pm 2\frac{2\pi}{a}\right)^2 + k_y^2\right)$$



$$\varepsilon_{20,\dots,23} = \frac{\hbar^2}{2m}\left(2\left(\pm 2\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{19} = \frac{\hbar^2}{2m}\left(k_y + 2\frac{2\pi}{a}\right)^2$$

$$\varepsilon_{15,\dots,18} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{14} = \frac{\hbar^2}{2m}\left(\left(k_y - 2\frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{24,\dots,27} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + \left(k_y - 2\frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{10,\dots,13} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y + \frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{6,\dots,9} = \frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{2,\dots,5} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y - \frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_1 = \frac{\hbar^2}{2m}(2\pi / a)^2$$

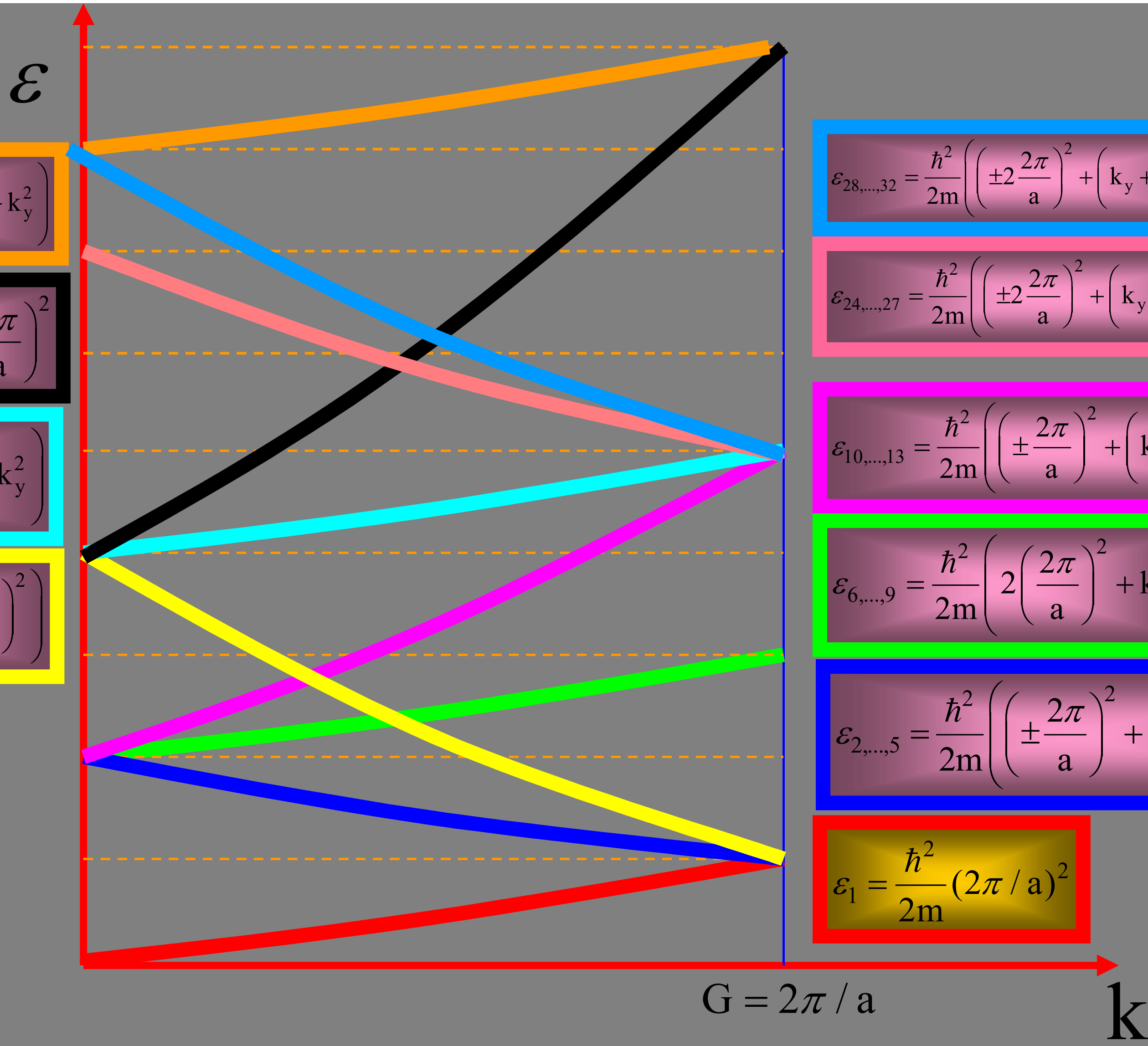
$$\mathbf{G} = \frac{2\pi}{a}\left(2\bar{2}0, \bar{2}\bar{2}0, 0\bar{2}2, 0\bar{2}\bar{2}\right) \Rightarrow \varepsilon_{24,\dots,27} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + \left(k_y - 2\frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{20,\dots,23} = \frac{\hbar^2}{2m}\left(2\left(\pm 2\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{19} = \frac{\hbar^2}{2m}\left(k_y + 2\frac{2\pi}{a}\right)^2$$

$$\varepsilon_{15,\dots,18} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{14} = \frac{\hbar^2}{2m}\left(\left(k_y - 2\frac{2\pi}{a}\right)^2\right)$$



$$\varepsilon_{28,\dots,32} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + \left(k_y + 2\frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{24,\dots,27} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + \left(k_y - 2\frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{10,\dots,13} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y + \frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_{6,\dots,9} = \frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}\right)^2 + k_y^2\right)$$

$$\varepsilon_{2,\dots,5} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y - \frac{2\pi}{a}\right)^2\right)$$

$$\varepsilon_1 = \frac{\hbar^2}{2m}(2\pi / a)^2$$

$$\mathbf{G} = \frac{2\pi}{a}\left(220, \bar{2}20, 022, 02\bar{2}\right) \longrightarrow \varepsilon_{28,\dots,32} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + \left(k_y + 2\frac{2\pi}{a}\right)^2\right)$$

PRACTICE

Find the following empty fcc lattice band structure.

Miller indexes are even or odd.

$$X = \left(0, \frac{2\pi}{a}, 0\right) \qquad w = \left(\frac{\pi}{a}, \frac{2\pi}{a}, 0\right)$$

$$L = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right) \qquad K = \left(\frac{3\pi}{2a}, \frac{3\pi}{2a}, 0\right)$$