## Free electrons and the hexagonal Bravais lattice

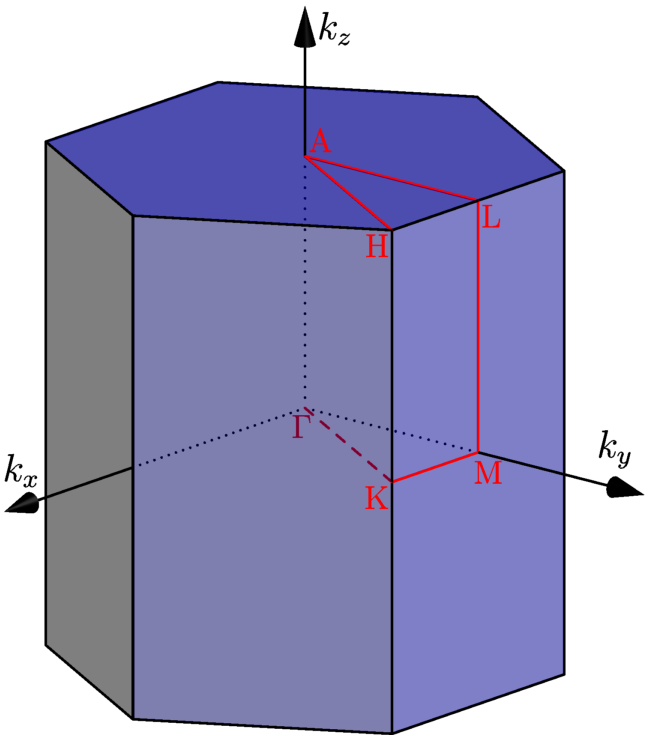
The hexagonal Bravais lattice can be described with three primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a\ (1,0,0), \\ \mathbf{a}_2 &= a\ (-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0), \\ \mathbf{a}_3 &= (0,0,c) \end{aligned}$$

that depend on two parameters $a$ and $c$.

1. Find the primitive vectors of the reciprocal lattice.

2. Find the volume of the first Brillouin zone of the hexagonal Bravais lattice.




3. The first Brillouin zone of the hexagonal Bravais lattice and a few high symmetry points, $\Gamma$, $A$, $H$, $K$, $M$, $L$, are shown in the figure. Find the cartesian coordinates of these points.

4. Let us consider the path $\Gamma \to M \to L \to A \to \Gamma \to K \to H \to A$. Find the length of each line of this path.

5. Modify the program that plots the free electron bands so that an hexagonal Bravais lattice can be required in input. The $c/a$ ratio should be a new input variable.

6. Compute the energy of the band described by the reciprocal lattice vector $\mathbf{G} = 0$ in the high symmetry points shown in the figure (You can use the $\mathrm{Ry}/(2\pi/a)^2$ units for the energy).

7. Plot the free electron energy bands for the path described at point 4, using the program modified at point 5. Discuss the three cases $c/a = 1$, $c/a = 2$, $c/a = 1/2$.