

The Brillouin zone of the bcc Bravais lattice

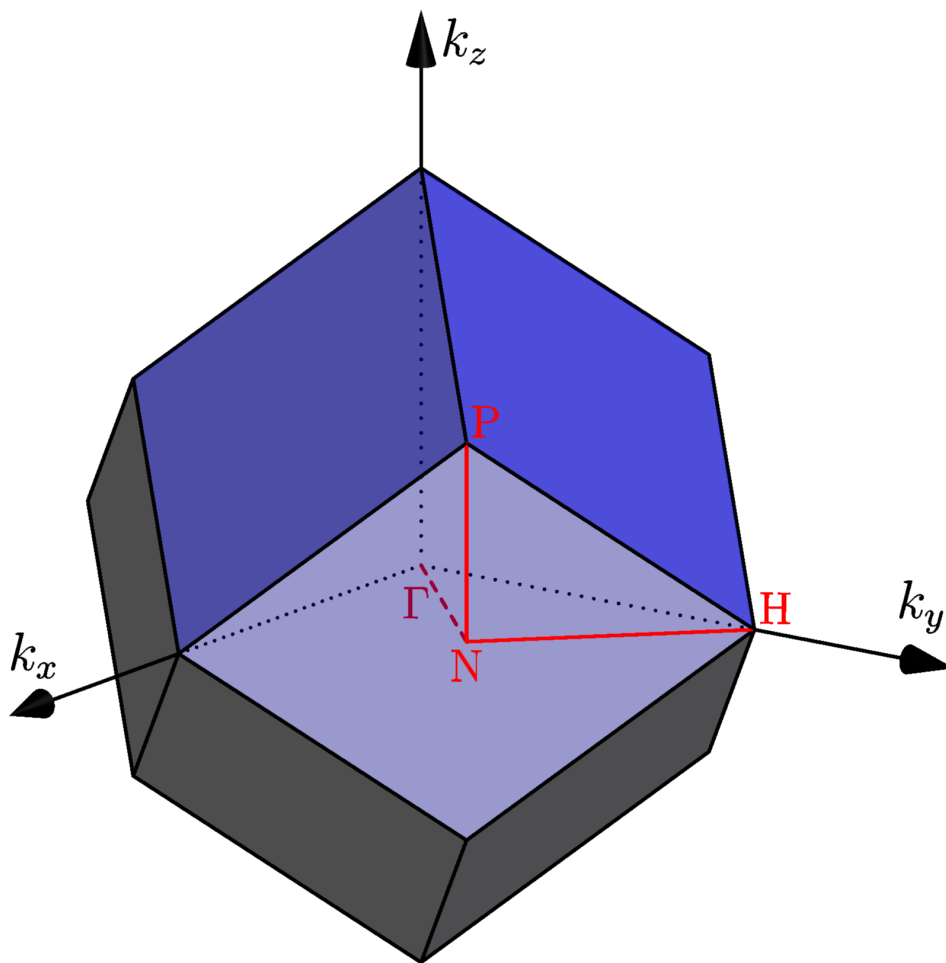
In this exercise we study some properties of the Brillouin zone of the bcc lattice. The bcc lattice can be described by three primitive vectors:

$$\mathbf{a}_1 = a/2 (-1, 1, 1),$$

$$\mathbf{a}_2 = a/2 (1, -1, 1),$$

$$\mathbf{a}_3 = a/2 (1, 1, -1).$$

1. Compute the primitive vectors of the bcc reciprocal lattice.



2. The Brillouin zone of the bcc lattice is shown in the figure. Plot the intersection of the bcc Brillouin zone with the plane $k_z = 0$.
3. Plot the intersection of the bcc Brillouin zone with the plane $k_x = k_y$.

4. In the plane given at point 3, let us consider the point \mathbf{k}' with coordinates $(1/2, 1/2, 1)$ in units $2\pi/a$. Show that this point is outside the first Brillouin zone.
5. Find a point \mathbf{k} in the first Brillouin zone such that $\mathbf{k}' = \mathbf{k} + \mathbf{G}$ where \mathbf{G} is a reciprocal lattice vector and find \mathbf{G} .
6. Using the program that plots the free electron energy bands, plot the bands for a bcc lattice along the line joining the point $\Gamma = (0, 0, 0)$ to the point \mathbf{k}' .
7. Find the cartesian coordinates of the point \mathbf{q}' in which the line given at previous point goes outside the first Brillouin zone.
8. The line that joins \mathbf{q}' to \mathbf{k}' is outside the first Brillouin zone. Find the point \mathbf{q} such that $\mathbf{q} = \mathbf{q}' - \mathbf{G}$. Plot the free-electron energy bands along the two lines $\Gamma \rightarrow \mathbf{q}'$ and $\mathbf{q} \rightarrow \mathbf{k}$ and show that they coincide with the bands found at point 6.