Graphene band structure and Density of states

Compute and plot the graphene band-structure and its density of states.

- plot bands in the path $M \to \Gamma \to K$ (see Fig.2 for details)
- plot Density of states for $t = 1$ and
  - $t' = 0$
  - $t' = -1/12$
  - $t' = 1/12$

Graphene is a single layer of graphite and is arranged in honeycomb lattice structure (See figure below).

In a tight-binding approximation, the nearest neighbout hopping integral is $t \sim 2.7eV$ and next nearest neighbour $t' \ll t$.

The honeycomb lattice structure is not a Bravais lattice, but needs to be treated as lattice with a two atoms in the basis (The smallest unit cell containes two atoms).

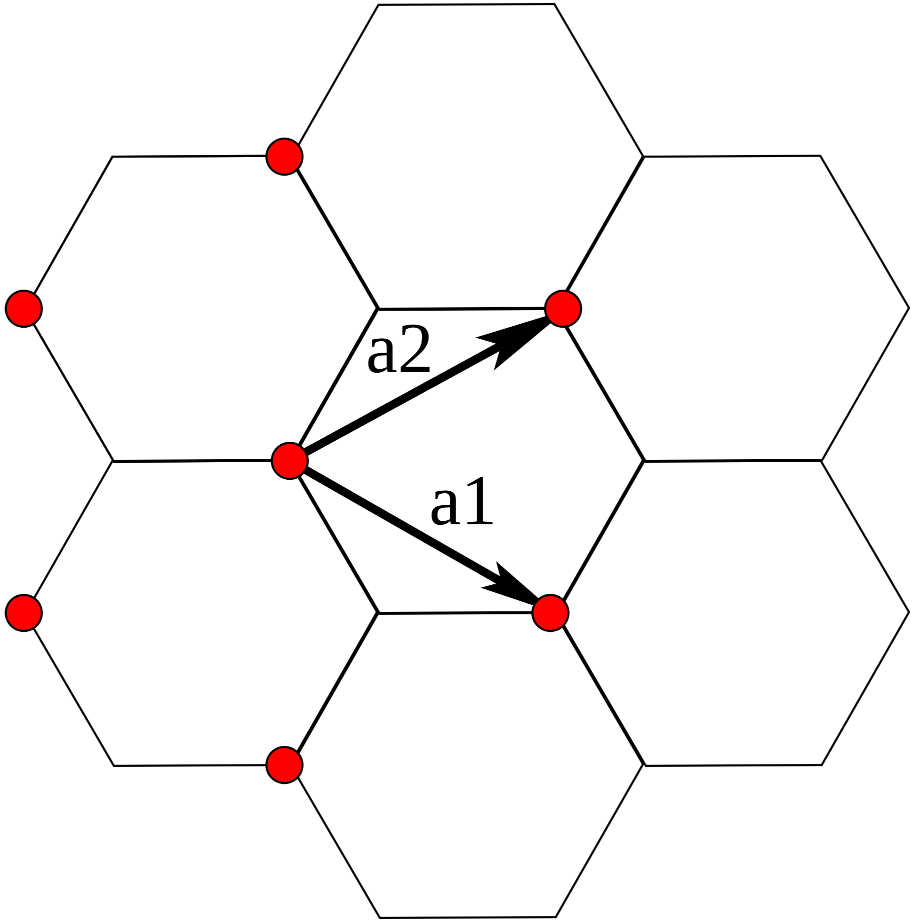

Figure 1: The lattice structure of graphene is a honeycomb lattice.

Possible choice of the Bravais unite vectors is shown in Figure 1

$$\vec{a}_1 = a(\frac{\sqrt{3}}{2}, \frac{1}{2}) \tag{1}$$

$$\vec{a}_2 = a(\frac{\sqrt{3}}{2}, -\frac{1}{2}) \tag{2}$$

The reciprocal lattice vectors then become

$$\vec{b}_1 = \frac{4\pi}{a\sqrt{3}}(\frac{1}{2}, \frac{\sqrt{3}}{2}) \tag{3}$$

$$\vec{b}_2 = \frac{4\pi}{a\sqrt{3}}(-\frac{1}{2}, \frac{\sqrt{3}}{2}) \tag{4}$$

The reciprocal lattice is again honeycomb lattice but is rotated for 90 degrees with respect to the direct lattice.

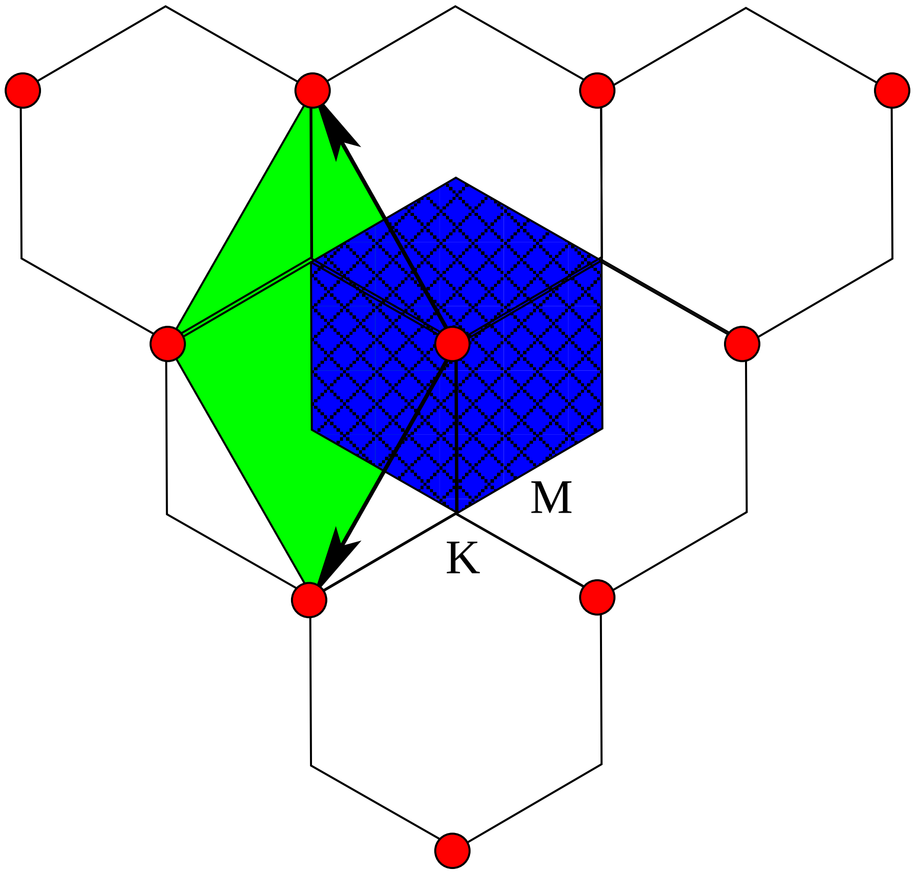

Figure 2: The reciprocal lattice and possible choice for the first Brillouin zone.

In the tight-binding approximation, the hopping Hamiltonian takes the form

$$H = \left(\begin{array}{cc} H_{11} & H_{12} \\ H_{12}^* & H_{11} \end{array} \right) \tag{5}$$

where the hopping integrals are

$$\begin{aligned} H_{11} &= -t'(e^{i\vec{k}\vec{a}_1} + e^{i\vec{k}\vec{a}_2} + e^{i\vec{k}(\vec{a}_1-\vec{a}_2)} + e^{i\vec{k}(\vec{a}_2-\vec{a}_1)} + e^{-i\vec{k}\vec{a}_1} + e^{-i\vec{k}\vec{a}_2}) && (6)\\ &= -2t'[\cos(\vec{k}\vec{a}_1) + \cos(\vec{k}\vec{a}_2) + \cos(\vec{k}(\vec{a}_1 - \vec{a}_2))] && (7)\\ H_{12} &= -t(1 + e^{i\vec{k}(\vec{a}_1-\vec{a}_2)} + e^{-i\vec{k}\vec{a}_2}) && (8)\\ |H_{12}|^2 &= t^2[3 + 2\cos(\vec{k}\vec{a}_1) + 2\cos(\vec{k}\vec{a}_2) + 2\cos(\vec{k}(\vec{a}_1 - \vec{a}_2))] && (9) \end{aligned}$$

The eigenvalues of the Hamiltonian matrix $\epsilon_{\vec{k}}$ are

$$\epsilon_{\vec{k}} = -t'\alpha(\vec{k}) \pm t\sqrt{3 + \alpha(\vec{k})} \tag{10}$$

where

$$\alpha(\vec{k}) = 2\cos(\vec{k}\vec{a}_1) + 2\cos(\vec{k}\vec{a}_2) + 2\cos(\vec{k}(\vec{a}_1 - \vec{a}_2))$$

To compute Density of states, we can take the Brillouin zone marked with green in Fig. 2.

The momentum $\vec{k}$ is then

$$\vec{k} = \frac{q_x}{2\pi}\vec{b}_1 + \frac{q_y}{2\pi}\vec{b}_2 \tag{11}$$

whith $q_x \in [-\pi, \pi]$ and $q_y \in [-\pi, \pi]$.

The dispersion becomes

$$\epsilon(q) = -t'\alpha(q) \pm t\sqrt{3 + \alpha(q)}$$

$$\alpha(q_x, q_y) = 2\cos(q_x) + 2\cos(q_y) + 2\cos(q_x - q_y)$$

The density of states is defined by

$$D(\omega) = \sum_{\vec{k}\in 1BZ} \delta(\omega - \epsilon_{\vec{k}}) = \sum_{q_i\in[-\pi,\pi]} \delta(\omega - \epsilon_q) \tag{12}$$

The algorithm might proceed as follows

- prepare vector $D(\omega)$ of size $N_{bin} \sim 100$ which will store the number of points with the energy in certain small interval $[\omega - \frac{\Delta\omega}{2}, \omega + \frac{\Delta\omega}{2}]$.
- Initialized the vector $D(\omega)$ to zero.
- compute energies ϵ_q on a dense mesh ($(q_x, q_y) = 200 \times 200$ or even 2000×2000) and add add unity to the interval $D(\omega)$ for which $\omega - \frac{\Delta\omega}{2} < \epsilon_q < \omega + \frac{\Delta\omega}{2}$.
- Normlize the vector $D(\omega)$ such that $\int D(\omega) d\omega = 1$
- Print and plot $D(\omega)$