Graphene band structure and Density of states

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

- plot bands in the path $M \rightarrow \Gamma \rightarrow K$ (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 neighbour hopping integral is $t \sim 2.7 \text{eV}$ 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 contains 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

\[ \vec{a}_1 = a \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right) \]  
\[ \vec{a}_2 = a \left( \frac{\sqrt{3}}{2}, -\frac{1}{2} \right) \]  

The reciprocal lattice vectors then become

\[ \vec{b}_1 = \frac{4\pi}{a\sqrt{3}} \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \]  
\[ \vec{b}_2 = \frac{4\pi}{a\sqrt{3}} \left( -\frac{1}{2}, \frac{\sqrt{3}}{2} \right) \]  

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

\[ H = \begin{pmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{11} \end{pmatrix} \]  \hspace{1cm} (5)

where the hopping integrals are

\[ H_{11} = -t'(e^{i\vec{k}\vec{a}_1} + e^{i\vec{k}\vec{a}_2} + e^{i\vec{k}(\vec{a}_1-\vec{a}_2)} + e^{-i\vec{k}\vec{a}_1} + e^{-i\vec{k}\vec{a}_2}) \]  \hspace{1cm} (6)

\[ = -2t'[\cos(\vec{k}\vec{a}_1) + \cos(\vec{k}\vec{a}_2) + \cos(\vec{k}(\vec{a}_1 - \vec{a}_2))] \]  \hspace{1cm} (7)

\[ H_{12} = -t(1 + e^{i\vec{k}(\vec{a}_1-\vec{a}_2)} + e^{-i\vec{k}\vec{a}_2}) \]  \hspace{1cm} (8)

\[ |H_{12}|^2 = t^2[3 + 2\cos(\vec{k}\vec{a}_1) + 2\cos(\vec{k}\vec{a}_2) + 2\cos(\vec{k}(\vec{a}_1 - \vec{a}_2))] \]  \hspace{1cm} (9)

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

\[ \epsilon_{\vec{k}} = -t' \alpha(\vec{k}) \pm t \sqrt{3 + \alpha(\vec{k})} \]  \hspace{1cm} (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

$$\vec{k} = \frac{q_x}{2\pi} \vec{b}_1 + \frac{q_y}{2\pi} \vec{b}_2$$  \hspace{1cm} (11)

with $q_x \in [-\pi, \pi]$ 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

$$D(\omega) = \sum_{\vec{k} \in 1BZ} \delta(\omega - \epsilon_{\vec{k}}) = \sum_{q_i \in [-\pi, \pi]} \delta(\omega - \epsilon_q)$$  \hspace{1cm} (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 $\epsilon_q$ on a dense mesh $((q_x, q_y) = 200 \times 200$ or even $2000 \times 2000$) and add unity to the interval $D(\omega)$ for which $\omega - \frac{\Delta \omega}{2} < \epsilon_q < \omega + \frac{\Delta \omega}{2}$.

- Normalize the vector $D(\omega)$ such that $\int D(\omega) d\omega = 1$

- Print and plot $D(\omega)$