1 Atomic chain

Consider an atomic chain with hopping matrix elements

$$t_{11}(R) = \begin{cases} t & \text{for } R = a \\ 0 & \text{else} \end{cases}$$

a) Calculate the dispersion relation $\varepsilon(k)$.

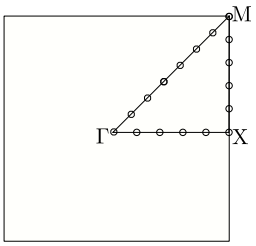
b) Calculate the bandstructure: Plot ε_k in the first Brillouin zone, e.g., $k = [-\pi/a, \pi/a]$

c) Calculate the DOS as histogram of ε_k.

2 Square lattice

Consider a square lattice with hopping matrix elements

$$t_{11}(\mathbf{R}) = \begin{cases} t & \text{for } |\mathbf{R}| = a \\ 0 & \text{else} \end{cases}$$



a) Calculate the dispersion relation $\varepsilon(k)$.

b) Calculate the bandstructure: plot $\varepsilon(k)$ along a path of high symmetry points: $\Gamma \to \mathrm{X} \to \mathrm{M} \to \Gamma$.

c) Calculate the DOS as histogram of ε_k for $\mathbf{k}$ in $k_x = [-\pi, \pi)$, $k_y = [-\pi, \pi)$. .

3 Square lattice with t' hopping

Consider a square lattice with hopping matrix elements

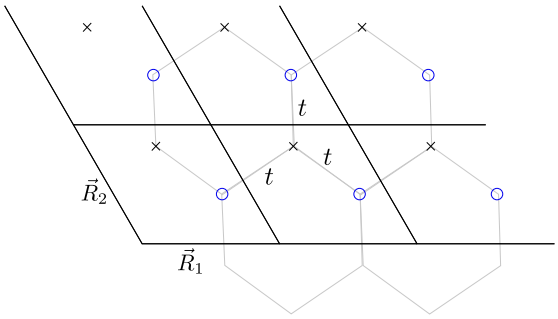
$$t_{11}(\mathbf{R}) = \begin{cases} t & \text{for } |\mathbf{R}| = a \\ t' & \text{for } \mathbf{R} = (a,a), (a,-a), (-a,a), (-a,-a) \\ 0 & \text{else} \end{cases}$$

a) Calculate the dispersion relation $\varepsilon(k)$.

b) Calculate the bandstructure: plot $\varepsilon(k)$ along a path of high symmetry points: $\Gamma \to \mathrm{X} \to \mathrm{M} \to \Gamma$.

c) Calculate the DOS.

d) Calculate the Fermi surface for $t = 0$, $t' = 0.1t$, and $t' = -0.1t$.

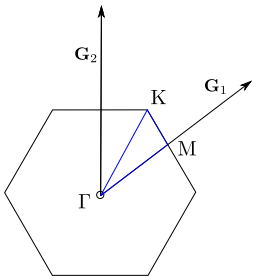


4 Honeycomb lattice

Consider a honeycomb lattice with hopping matrix elements

$$t_{12}(\mathbf{R}) = \begin{cases} t & \text{for } \mathbf{R} = \mathbf{0}, \mathbf{R}_1, -\mathbf{R}_2 \\ 0 & \text{else} \end{cases}$$

$$t_{21}(\mathbf{R}) = \begin{cases} t & \text{for } \mathbf{R} = \mathbf{0}, \mathbf{R}_2, -\mathbf{R}_1 \\ 0 & \text{else} \end{cases}$$



a) Calculate the dispersion relation $\varepsilon_{1,2}(\mathbf{k})$ in terms of k_1 and k_2 with $\mathbf{k} = k_1\mathbf{G}_1 + k_2\mathbf{G}_2$. Use $\mathbf{R}_i \cdot \mathbf{G}_j = 2\pi\delta_{ij}$ to simplify.

b) Calculate the bandstructure: plot $\varepsilon(k)$ along a path of high symmetry points: $\Gamma \to \mathrm{M} \to \mathrm{K} \to \Gamma$.

$$K = \frac{1}{3}(\mathbf{G}_1 + \mathbf{G}_2)$$
$$M = \frac{1}{2}\mathbf{G}_1$$

c) Calculate the DOS by calculating the dispersion in the primitive cell $k_1 = [0, 2\pi)$, $k_2 = [0, 2\pi)$.

d) From your DOS and bands: guess the shape of the Fermi surface for (close to) half filling.

5 Additional tasks

1) If you have time left consider optimizing your code:

- **a)** Start by identifying the heavy parts of your code!!!
- **b)** Consider replacing loops by `numpy` rountines.
- **c)** How could you use lattice symmetries to lessen the number of k-points in the calculation of the DOS?

2) Calculate the Fermi surface of graphene for a filling of 0.9, where a filling of 1.0 corresponds to half filling.