Exercise for Computational Materials Sciences

Exercise 1, October 22nd, 2024. Discussion on November 5th, 2024

1) Atomic chain

Consider a nearest-neighbour one-dimensional tight-binding chain with periodic boundary conditions:

$$\hat{H} = t \sum_{i=1}^{N-1} \left(\hat{c}_i^\dagger \hat{c}_{i+1} + h.c. \right) + t \left(\hat{c}_N^\dagger \hat{c}_1 + h.c. \right)$$

A compact way to represent this Hamiltonian is to write that we have a 1D chain with lattice constant a where the hopping term between two sites separated by distance R is given by:

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

a) Use the Fourier transform to calculate the dispersion relation $\varepsilon(k)$ for $t = -1$.

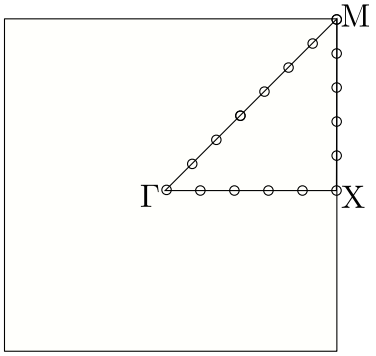
b) Calculate the bandstructure: Plot ε_k in the first Brillouin zone, e.g., $k = [-\pi/a, \pi/a]$

c) Calculate the density of states (DOS). Recall that the density of states $\rho(\varepsilon)$ is give by $\rho(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k)$. You may approximate this with a histogram of ε_k.

2) Square lattice

Consider a nearest neighbour square lattice with lattice constant a. The hopping matrix elements between sites separated by vector $\mathbf{R}$ are given by:

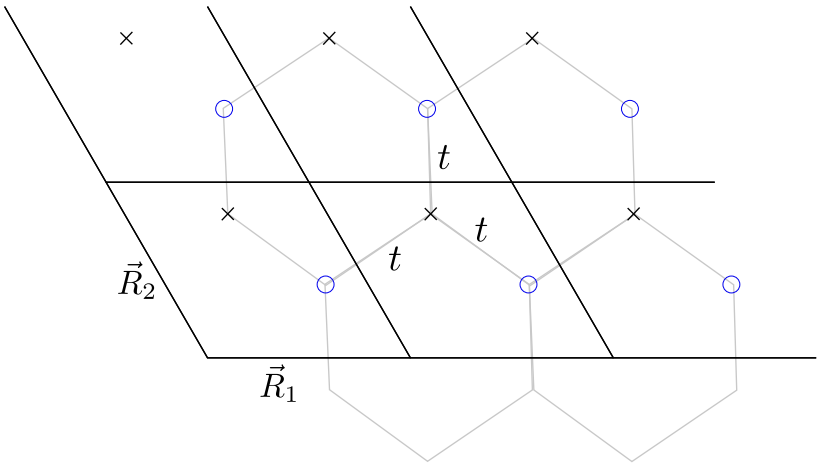
$$t(\mathbf{R}) = \begin{cases} t & \text{for } |\mathbf{R}| = a \\ 0 & \text{else} \end{cases}$$



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 density of states as a histogram of ε_k for $\mathbf{k}$ in $k_x = [-\pi, \pi)$, $k_y = [-\pi, \pi)$.



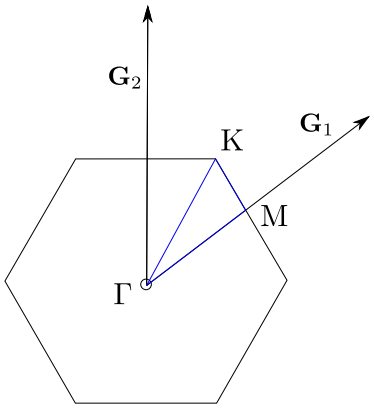
3) Honeycomb lattice

Consider a honeycomb lattice with hopping matrix elements

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

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

where t_{12} refers to the hopping process from sublattice 1 (blue circle) to sublattice 2 (black cross) and vice versa.



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.

4) Nearly free electrons—cosine potential

Consider the following periodic potential

$$V(x) = v_0 \cos\left(2\pi\frac{x}{a}\right).$$

a) Calculate the corresponding Fourier-transformed Potential V_G.

b) Write down the corresponding Hamilton operator in the Bloch representation.

c) Numerically diagonalize the Hamilton operator and plot the band structure for sufficiently small v_0. What is the band gap at the Brillouin zone edge?

d) Above which value of v_0 does the approximation of small v_0 break down? Confirm your answer with numerically obtained band structures for various values of v_0.

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 `python/numpy` routines.
- **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.