

Exercise Sheet No. 1 “Computational Condensed Matter Theory”

1 Band structures for tight-binding chains (1d)

Consider the tight-binding Hamiltonian

$$\hat{H} = \sum_{\langle l,j \rangle} t_{lj} c_l^\dagger c_j \quad (1)$$

where c_l^\dagger, c_l denote fermionic creation and annihilation operators acting at the site l of a one-dimensional (1d) tight-binding chain. The hopping matrix t_{lj} connects nearest neighbors, only.

- a) Let the chain be translationally invariant consisting of a two-site unit cell with hopping t within the cell and hopping $t' = t + \delta t$ between the cells, such that t and t' are alternating:



Assume periodic boundary conditions. Choose the lattice constant a as the unit of length and the hopping amplitude t as the unit of energy. Perform a numerical Fourier transformation of the Hamiltonian and then block-wise diagonalize the resulting matrix to obtain the band structure. Plot your result for a system with $L = 512$ lattice sites and different δt values of 0, 0.01, 0.1 and 1. Discuss your result.

Hint 1: In Matlab, the function `fft()` can be used to perform a Fourier transformation (FT) of a discrete function represented as a column vector. If applied to a matrix, the Fourier transformation will be applied to all column vectors independently. Think how you can use this function to do the (unitary) FT of the Hamiltonian. Beware: The implementation of matlab uses a different normalization!

Hint 2: Since the unit cell contains more than one site, the same Fourier wave vector has to be used for each element of the unit cell. Use the `mfft.m` function provided on the lecture website to achieve this.

- b) The density of states, $\varrho(\epsilon)$, (DOS) is related to the dispersion relation via

$$\varrho(\epsilon) = \frac{1}{M} \sum_k^{\text{B. Z.}} \delta(\epsilon - \epsilon(k)) \quad M: \text{Number of sites}, \quad (2)$$

where $\delta(\epsilon)$ denotes the δ -function. The Lorentzian and Gaussian representations of the δ -function with a finite broadening are given by

$$\delta_\eta^L(\epsilon) = \frac{1}{\pi} \frac{\eta}{\epsilon^2 + \eta^2}, \quad \delta_\eta^G(\epsilon) = \frac{1}{\eta\sqrt{\pi}} e^{-\epsilon^2/\eta^2}.$$

Numerically calculate the density of states for the tight-binding chain for the system in (1a).

Examine the dependence of $\varrho_\eta(\epsilon)$ on the artificial broadening η for different numbers of lattice sites $M = 128, 256, 512$ both for the Lorentzian and the Gaussian representations. Discuss the relevant energy scales and show, that your result $\varrho_\eta(\epsilon)$ becomes independent of η in the limit $\eta \rightarrow 0$, provided the system size M goes to infinity first.

Please turn ...

2 Band structures of quasi-1d-lattices

Consider the Hamiltonian (1), but now with sites l, j that are situated on a quasi-1d-strip (ribbon) realized by M chains coupled in parallel. Consider rings with sizes $M \times L$ with $L \geq 20$.

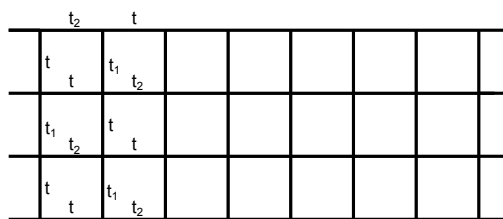


Figure 1: Ribbon from a square lattice with $M = 4$ constituting chains.

Calculate the band structure for a ribbon that realizes a piece of a square lattice, see Fig. 1, with $M = 4$ and $t_1 = t_2 = t$. Assume periodic boundary conditions in x - but not in y -direction. Also plot the density of states. Discuss your results.

Hint: Consider what the unit cell of this problem is and how to use that knowledge to simplify the construction of the Hamiltonian matrix.

3(*) Band structures of graphene ribbons

Now consider the case when certain bonds are eliminated from the previous ribbon to simulate graphene.

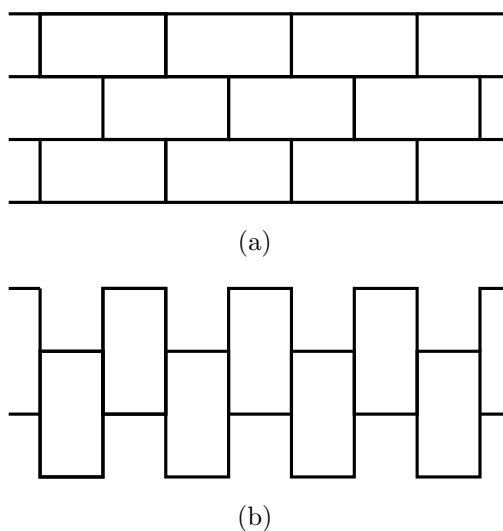


Figure 2: (a) zigzag graphene ribbon. (b) armchair graphene ribbon.

- Eliminate bonds from the previous ribbon to obtain an zig-zag ribbon (Fig. 2a, $t_1 = 0, t_2 = t$). Again determine the band structure and plot the density of states.
- Eliminate bonds from the first ribbon so as to realize an armchair-nanoribbon (Fig. 2b, $t_2 = 0, t_1 = t$) and repeat your band structure calculation.
- Investigate the crossover between 2) and 3a).

Think about what kind of unit cell you need for this problem. Discuss your results. What implications do you see for a transport experiment?

Hint Useful commands to solve the problems in Matlab:

`doc, zeros, ones, diag, eye, toeplitz, kron, fft, fftshift, eig, figure, plot`

Useful Matlab functions provided on the lecture website:

`mfft, strip`