Karlsruhe Institute of Technology WS 2013/2014
Institute for Theoretical Condensed Matter physics (TKM)
Institute of Nanotechnology (INT)
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http://www.tkm.kit.edu/lehre/ws2013_ccmt_ueb.php

Exercise Sheet No. 1
"Computational Condensed Matter Theory"

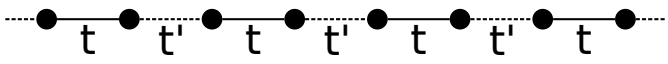
1 Band structures for tight-binding chains (1d)

Consider the tight-binding Hamiltonian

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

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 ussed 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

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

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

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

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 $\eta \to 0$, 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 $L \geq 20$.

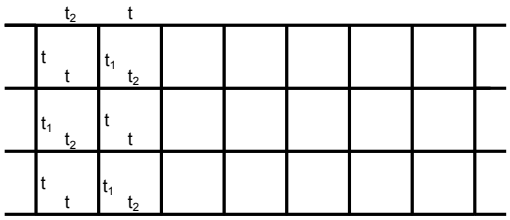


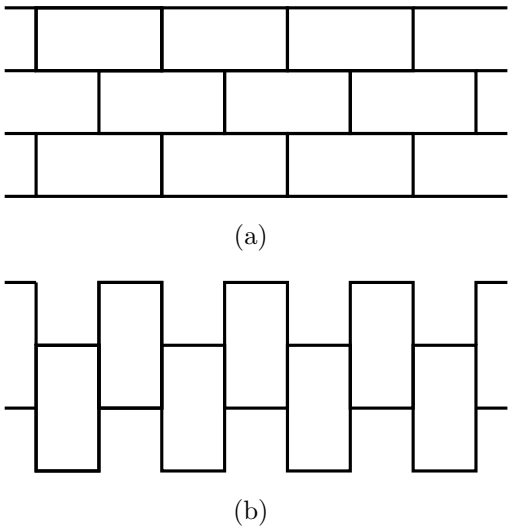
Figure 1: Ribbon from a square lattice with $M = 4$ constituting chains.

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.



(a)

(b)

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

a) 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.

b) 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.

c) 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`