Universität Regensburg
Institute for Theoretical Physics
Institute of Computational Condensed Matter Theory
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http://www.physik.uni-regensburg.de/forschung/evers/courses/cscn.phtml

Exercise Sheet No. 1
"Computational Condensed Matter Theory"

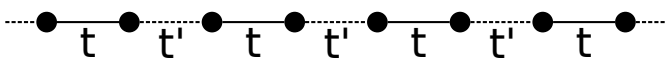
1 Band structures for tight-binding chains (1d)

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 Numpy, the function `numpy.fft.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 Numpy 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.py` function provided on the lecture website to achieve this.

Useful functions:

- numpy: `conjugate`, `eye`, `kron`, `linspace`, `real`, `sort`, `transpose`
- numpy.fft: `fftshift`
- numpy.linalg: `eigvals`

Please turn ...

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.

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 $L \geq 20$.

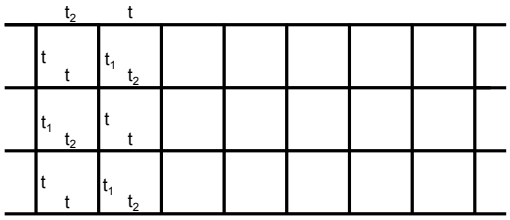


Figure 1: Ribbon from a square lattice with $M = 4$ constituting chains.

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. Also think of $t1$ and $t2$ as seperate hoppings and only set them equal to t in your calculation step.

For useful functions see problem 1