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http://www.tkm.kit.edu/english/teaching/ws2012_1437.php

# Exercise Sheet No. 1
# "Computational Condensed Matter Theory"

## 1 Bandstructures 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, so $t_{lj} = t$ and apply periodic boundary conditions (PBC) $\Psi(x+M) = \Psi(x)$, so the chain turns into a ring. Choose the lattice constant $a$ as unit of length and $t$ as unit of the energy. Perform a numerical Fourier transformation and plot your result for L=512 lattice sites. Verify your dispersion relation by comparing it with the analytical answer $\epsilon(k) = -2t\cos k$.
[In Matlab the function `fft()` performs a discrete Fourier transformation (FT) of a vector or all columns of a matrix. Think how you can use this function to do the (unitary) FT of the Hamiltonian. Beware: The implementation of matlab uses a different normalization!]

**b)** Next consider a doubling of the unit cell to describe a situation where the hopping matrix element takes alternating values $t$ and $t+\delta t$. Calculate numerically the resulting band structure for $\delta t/t = 0.1$ and L=512 and discuss your result. In the calculation make sure, that all elements belonging to the same unit cell are Fourier transformed with the same wave vector and diagonalize the remaining subblocks.

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

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

where $\delta(\epsilon)$ denotes the $\delta$-function. Use the Lorentzian representation of the $\delta$-function

$$\delta(\epsilon) = \lim_{\eta \to 0} \frac{1}{\pi} \frac{\eta}{\epsilon^2 + \eta^2}$$

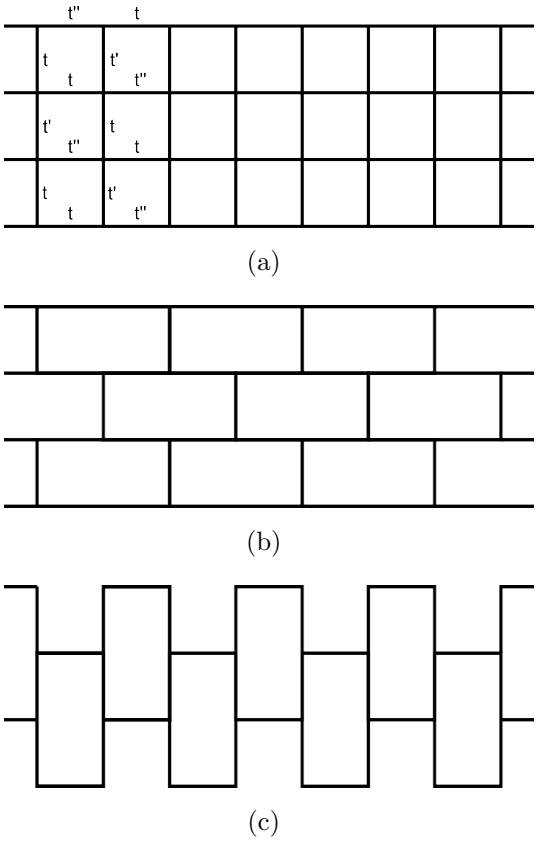
where $\eta > 0$ represents the broadening energy scale, in order to numerically calculate the DOS $\varrho_\eta(\epsilon)$ of the tight binding chain (1a), and discuss your results.

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

**Please turn ...**

**2(*)** **Bandstructures of quasi-1d-lattices: graphene ribbons**

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 $L \geq 20$.




(a)

(b)

(c)

Figure 1: Up: Ribbon from a square lattice with $M = 4$ constituting chains. Center: zigzag-graphene ribbon. Bottom: Armchair-ribbon.

**a)** Calculate the bandstructure for a ribbon that realizes a piece of a square lattice, see Fig. 1a, with $M = 4$

**b)** Eliminate bonds from the previous ribbon to obtain an zig-zag ribbon (Fig. 1b, $t' = 0, t = t''$). Again determine the bandstructure and plot the density of states.

**c)** Eliminate bonds from the first ribbon so as to realize an armchair-nanoribbon (Fig. 1c, $t'' = 0, t = t'$) and repeat your bandstructure-calculation.

() d) Investigate the crossover between a) and b)

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`