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. 2
"Computational Condensed Matter Theory"

1 Band structures of graphene ribbons

Consider cases where certain bonds are eliminated from the previous square lattice ribbon (recall **Sheet 1.2**) to simulate a hexagonal lattice, as it is representative, e.g., for graphene.

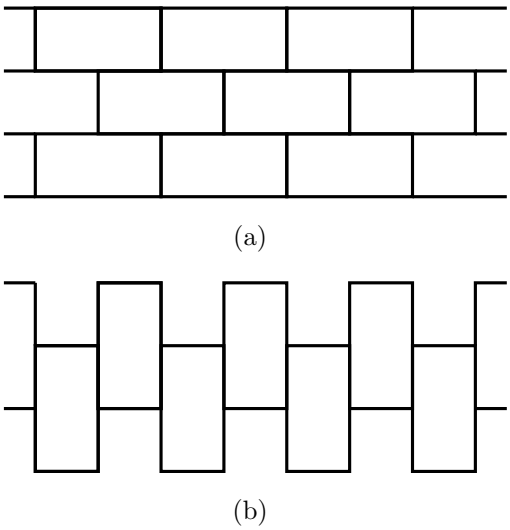

Figure 1: (a) zigzag graphene ribbon. (b) armchair graphene ribbon.

a) Eliminate bonds to obtain a zig-zag ribbon (Fig. 1a, $t_1 = 0, t_2 = t$). Determine the band structure and plot the density of states (As in **Sheet 1** use a Gaussian & Lorentzian curve to achieve this).

b) Eliminate bonds to realize an armchair-nanoribbon (Fig. 1b, $t_2 = 0, t_1 = t$). Again, determine the band structure and the density of states.

c) Discuss your results by investigating the crossover between the zig-zag & armchair case. Also think about the implications for a transport experiment.

Hint: Consider what the unit cell of this problem is and use that information to generate the matrix blocks for the full hamiltonian.

Useful functions:

- numpy: `conjugate`, `diag`, `eye`, `hstack`, `kron`, `linspace`, `transpose`, `vstack`, `zeros`
- numpy.fft: `fftshift`
- numpy.linalg: `eigvalsh`

2 Hofstadter's butterfly on cubic lattices

Consider the tight-binding Hamiltonian $\hat{H} = -\sum_{\langle k,l \rangle} t_{kl} c_k^\dagger c_l$ with double-periodic boundary conditions (torus geometry); $c_k^\dagger, c_k$ denote fermionic creation and annihilation operators. The hopping matrix t_{kl} connects nearest neighbors, only.

a) Let (x, y) be a site in a two dimensional cubic lattice with LxL sites and add a magnetic field via Peierls phases. As discussed in the lecture, we get for the cubic lattice

$$\hat{H} = -t \sum_{(x,y)\in\mathcal{L}} e^{i\phi^{\mathsf{v}}_{xy}}\ c^\dagger_{x,y+1} c_{x,y} + e^{i\phi^{\mathsf{h}}_{x,y}}\ c^\dagger_{x+1,y} c_{x,y} + \text{h.c.} \tag{1}$$

with phases as depicted in Fig. 2. In order to complement the model with a magnetic field, choose a gauge where $\phi^{\mathsf{h}}_{x,y} = \Phi \cdot (y-1)$ and $\phi^{\mathsf{v}}_{x,y} = 0$ otherwise. Calculate the spectrum for a linear system size $L = 42$ nodes at $\Phi/2\pi = 1/42, 1/21, 1/7, 4/21, 8/21, 2/7, 1/2$ via exact diagonalization of a full matrix using the Numpy function `eigvals()`. What is the reason for choosing the fractions that appear here?

b) Now disregard the fractions mentioned in **a)** and calculate the spectrum for a whole range of fluxes. Consider what the maximum flux should be to obtain a picture without repeating the spectrum pattern. Discuss your result.

Hint: Omit lines in your final spectrum plot to see individual points. Also do not calculate the spectrum for more than, e.g., 100 fluxes as this calculation will take a long time.

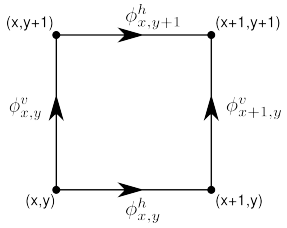

Figure 2: Arrangement of Peierls-phases in a cubic lattice.