Karlsruhe Institute of Technology WS 2012/1313
Institut for Theoretical Condensed Matter physics (TKM)
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http://www.tkm.kit.edu/english/teaching/ws2012_1437.php

Exercise Sheet No. 2
"Computational Condensed Matter Theory"

3 Hofstadter's butterfly on cubic lattices

Consider the tight-binding Hamiltonian

$$\hat{H} = -\sum_{\langle k,l \rangle} t_{kl} c_k^\dagger c_l \tag{1}$$

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

$$\hat{H} = -t \sum_{(x,y)\in\mathcal{L}} e^{i\phi^{\mathsf{v}}_{xy}}\ c^\dagger_{x,y+1} c_{x,y} + e^{i\phi^{\mathsf{h}}_{x,y}}\ c^\dagger_{x+1,y} c_{x,y} + \text{h.c.} \tag{2}$$

with phases as depicted in Fig. 1. In order to complement the model with a magnetic field, choose

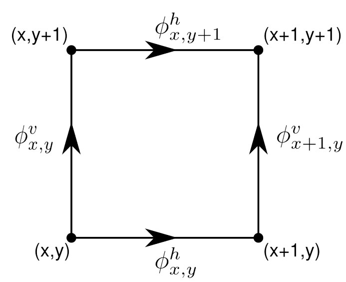

Figure 1: Arrangement of Peierls-phases in a cubic tight-binding lattice.

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 matlab function `eig()`. What is the reason for choosing the fractions that appear here?

c) Discuss your result.

4 Hofstadter's butterfly on the honeycombe lattice

Repeat the same exercise on the hexagonal tight binding lattice in toroidal geometry.

a) Construct the matrix representation of the hexagonal lattice with Peierls factors and double-periodic boundary conditions. To this end, recall exercise sheet 1: for the purpose of calculating a spectrum, the hexagonal lattice is equivalent to the brick-wall lattice which derives from the square lattice by eliminating bonds.

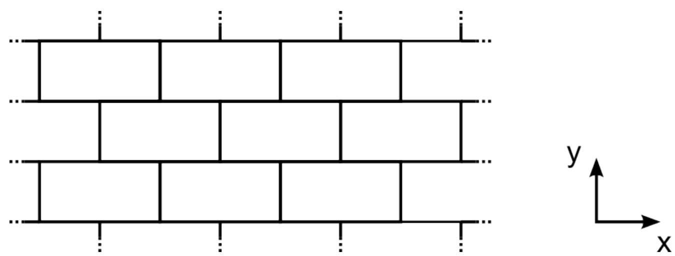

Figure 2: Brick wall-lattice with double periodic boundary conditions

b) Calculate the spectrum for zero flux and the corresponding density of states. Discuss how the Dirac-cone manifests here. Compare the results for $L = 24, 42, 72$.

c) Now choose $L = 42$ and add the same phases-factors as in the previous exercises. Compare your result with the Hofstadter butterfly in the 2-d cubic lattice and discuss it. How does the flux per plaquette relate to the Peierls factors?