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. 2
"Computational Condensed Matter Theory"

4 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 square lattice with LxL sites and add a magnetic field via Peierls phases. As discussed in the lecture, for a square lattice we obtain

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

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

b) Discuss your result.

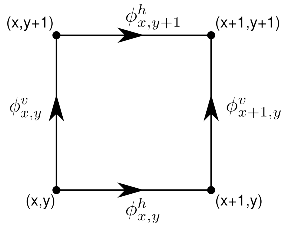


Figure 1: Arrangement of Peierls-phases in a square lattice.

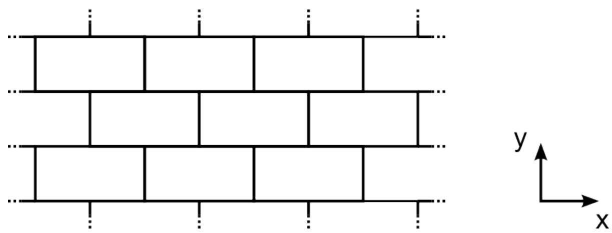


Figure 2: Brick-wall lattice with double periodic boundary conditions

5 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. (Fig. 2).

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

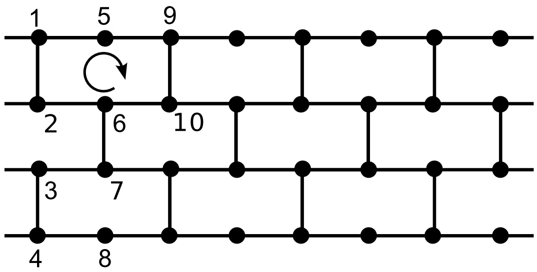
c) Now choose $L = 42$ and add the same phases-factors as in the previous exercises. Compare your result with the Hofstadter butterfly in the square lattice and discuss it. How does the flux per plaquette relate to the Peierls factors?

6* Quantum Spin Hall Effect in Graphene

Now consider a graphene ribbon with spin-orbit interactions. A model describing this system has been studied in Ref. [1] by Kane and Mele. Since the Hamiltonian of their model is diagonal in spin-space, for simplicity we consider only one spin component. As previously discussed in exercise 3 the lattice of graphene is again modelled by a brick-wall lattice. The Hamiltonian thus reads

$$H = -\sum_{\langle k,l \rangle} t c_k^\dagger c_l - \sum_{\langle\langle k,l \rangle\rangle} i t' \nu_{kl} c_k^\dagger c_l, \quad \nu_{kl} = -\nu_{lk} = \pm 1. \tag{2}$$

Here $\langle\langle k,l \rangle\rangle$ denotes pairs of next-nearest neighbors and $\nu_{kl} = +1$ if the electron encircles a plaquette clockwise to get to the second site (e.g. $\nu_{1,9} = \nu_{5,10} = \nu_{2,7} = \nu_{4,7} = \nu_{6,3} = +1$), and $\nu_{kl} = -1$ if it moves anti-clockwise (e.g., $\nu_{1,6} = \nu_{2,10} = \nu_{3,6} = \nu_{6,9} = \nu_{7,2} = -1$).



a) Construct the Hamiltonian Eq. 2 for a ribbon of size $M \times L$ with M=4 and L=64, and use a next-nearest neighbor hopping of $t' = 0.03t$. Assume periodic boundary condition in x- but not in y-direction.

b) Calculate and plot the dispersion relation $\varepsilon(k_x)$, and compare the band structure to the case without next-nearest neighbor hopping.

c) Visualize the probability density ($|\psi(x,y)|^2$) of a wavefunction with an energy eigenvalue of $\varepsilon(k_x) \approx 0$ and discuss its spatial structure.
Useful functions: `eig()`, `reshape()`, `imagesc()`.

References

[1] C.L. Kane and E.J. Mele, Phys. Rev. Lett. **95**, 226801 (2005), (arXiv:cond-mat/0411737)