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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 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. 1.

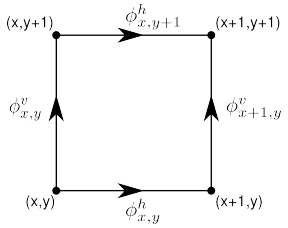


Figure 1: Arrangement of Peierls-phases in a cubic lattice.

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

b) Discuss your result.

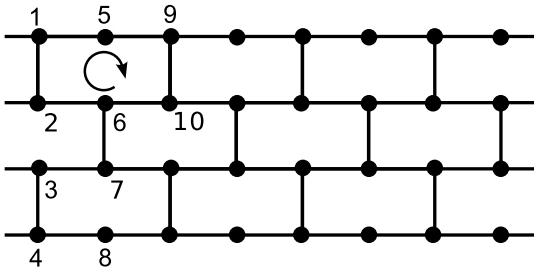
5 Quantum Spin Hall Effect in Graphene

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()`.

6* **Bound states of the resonant level model**

The resonant level model consists of a single impurity, i.e. a single site, coupled to a non-interacting conduction band (lead). In the following we study a fermionic system and represent the lead by a one dimensional tight binding chain of M sites

$$\hat{H}_{\mathrm{L}} = -t \sum_{x=2}^{M} \hat{c}_{x-1}^\dagger \hat{c}_x + \hat{c}_x^\dagger \hat{c}_{x-1} \tag{3}$$

and the impurity, labelled by d, couples to the lead at site x_0 with a coupling strength V

$$\hat{H} = \hat{H}_{\mathrm{L}} + \epsilon^{\mathrm{d}} \hat{d}^\dagger \hat{d} + V \left(\hat{d}^\dagger \hat{c}_{x_0} + \hat{c}_{x_0}^\dagger \hat{d} \right) \tag{4}$$

Calculate the energy eigen levels ε_ℓ for

a) the resonant level coupled to the end of the chain, $x_0 = 1$,

b) the resonant level coupled to the bulk, i.e. x_0 somewhere in the middle of the chain.

Use a bath size of at least $M = 100$ sites, set $\epsilon^{\mathrm{d}} = 0.3$, $t = 1$, and $V = 0.9$.

c) Visualize the probability density ($|\psi_\ell|^2$) of the eigenfunctions with maximal/minimal energy ε_ℓ.

References

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