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Topological condensed matter physics
Problem set 3

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1. Ribbon spectra and edge states **9 Points**

a) **1 Point**

Let us consider the tight-binding chain we discussed in the very first lecture, governed by the Hamiltonian

$$H_1 = -t \sum_i c_i^\dagger c_{i+1} + \text{h.c.} \ ,$$

for which we computed the energy spectrum (*i.e.*, the bandstructure) using a Fourier transformation. The energy spectrum reads $E_1(k) = -2t\cos(k)$ where we set the lattice spacing to $a \equiv 1$. Now suppose the chain consists of $N = 7$ sites and open boundary conditions (OBC) are imposed (*i.e.*, the first and the last sites are *not* coupled by a hopping $-t$). Write down the real-space Hamiltonian for this system and determine the discrete eigenenergies by diagonalizing the real-space hopping matrix. While this can be done analytically you should use a computer program such as `mathematica`, `maple`, or a `python` implementation. Repeat the calculation for $N = 8$ and compare both spectra with E_1. Eventually add to the Hamiltonian the term $-t(c_1^\dagger c_N + c_N^\dagger c_1)$ in order to restore periodic boundary conditions (PBC). Now consider again the discrete energies for $N = 7$ and $N = 8$ and compare to E_1. What do you observe?

b) **2 Points**

We generalize H_1 to the two-dimensional square lattice case,

$$H_2 = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + \text{h.c.} \ ,$$

and $\langle ij \rangle$ denotes all combinations where j is a neighboring site of i (but each pair appears only once). For the case of PBC, perform a Fourier transformation of H_2 and calculate the energy–momentum relation $E_2(k_x, k_y)$. In the following, we consider a so-called nanoribbon (a cylinder) which exhibits OBC in the x–direction and PBC in the y-direction. We denote the position of a lattice site by (m, n) corresponding to $\vec{R}_{mn} = m\hat{\vec{e}}_x + n\hat{\vec{e}}_y$. Along the y–direction we can perform a Fourier-transformation while keeping the real-space representation along the x–direction:

$$c_{m,n}^\dagger = \frac{1}{N_y} \sum_{k_y} e^{ik_y n} c_{m,k_y}^\dagger \ .$$

Determine the Bloch matrix $h_2(k_y)$ in this hybrid representation for a ribbon with a width of eight sites. It is again possible to impose PBC. Compute the spectrum $\tilde{E}_2(k_y)$ of the ribbon. Check whether you recover the same energies you obtained for the case where you performed a full Fourier transformation. Do you observe a difference in the ribbon spectrum for OBC compared to PBC?

c) **2 Points**

We add to the previously considered square lattice ribbon a uniform magnetic field of strength $\alpha = 1/3$ piercing through the lattice (*i.e.*, the magnetic field is *locally* perpendicular to the ribbon). Using the knowledge you gained from the lecture about the Hofstadter butterfly determine the ribbon-Bloch matrix structure. Choose the Landau gauge such that the magnetic unit cell is increased in x-direction, the ribbon length must hence be a multiple of three. Do you observe a difference in the ribbon spectrum for OBC compared to PBC? *Hint:* a ribbon length of six magnetic unit cells is sufficient. It might be wise to think about an implementation where the ribbon width enters as a parameter.

d) **4 Points**

Eventually we consider the Hamiltonian H_2 (without magnetic field) on a honeycomb-lattice nanoribbon (aka "carbon nanotube") with zigzag edges. Now we have two atoms per unit cell, for a ribbon consisting of N unit cells along the x direction we have to deal with a $2N \times 2N$ matrix. Try to find the correct ribbon-Bloch matrix. Note that the "path" of k_y–independent hopping is not a straight line perpendicular to the edge (as it is the case for the square lattice), but a zigzag line instead. Diagonalize it as a function of k_y for different ribbon lengths for both PBC and OBC. Eventually add the Semenoff term,

$$H_S = M \sum_i (-1)^{\xi} c_i^\dagger c_i \tag{1}$$

where $\xi = 1$ on sublattice A and $\xi = 0$ on sublattice B. The Semenoff mass is nothing than a staggered sublattice potential term. How does H_S affect the OBC and PBC spectra?

Extra problem: **2 Points**

Usually a honeycomb ribbon has A–sites on one zigzag edge and B–sites on the other edge. What happens if you considered a ribbon which has B–sites on one edge and A–sites on the other edge? What happens, if both zigzag edges consist of A sites? Repeat these considerations with a finite Semenoff mass.

In case of questions or lack of clarity please write us an email for clarification or further advice.