Continue with tight binding model

(A.) In this exercise we will explore the dispersion relation and the density of states of the tight binding model on the one dimensional chain and on the square lattice. The density of states for an electronic system can defined be as,

$$D_n(E) = \frac{2}{V} \sum_k \delta(E - E_n(k)) \tag{1}$$

where $\sum_k$ is a sum over the first Brillouin zone and $E_n(k)$ is the dispersion energy of n^{th} band.

1. Show that the density of states can also be written as the surface integral

$$D_n(E) = \frac{2}{(2\pi)^d} \int\limits_{E_n(k)=E} \frac{dS}{|\nabla E_n(k)|} \tag{2}$$

where the integral is over a constant energy surface.

2. Write down the dispersion relation of the one dimensional nearest neighbour tight binding model,

$$H = -t \sum_{i,\sigma} \left(c^\dagger_{i,\sigma} c_{i+1,\sigma} + c^\dagger_{i+1,\sigma} c_{i,\sigma} \right).$$

What are the constant energy 'surfaces'? Write down the density of states explicitly. At what energies can we find singularities (divergences)?

3. Consider the tight binding model on the square lattice discussed in the previous exercise. At what energies can we expect divergences in the density of states?
Draw the constant energy surface close to empty filling, at half filling and close to complete filling.

4. Consider energies close to the bottom of the spectrum and approximate Eq. (2) by assuming that k_x, k_y are small in this case. Evaluate the integral in this limit.

5. Contemplate on the form of the density of states for energies close to the top of the spectrum. How is it connected to the previous case?

6. Calculate the density of states at $E = 0$. Identify the constant energy surface for $E = 0$, and write down Eq. (2) explicitly. Show that $D(E = 0)$ diverges. (The integral can be carried out exactly, but the divergence can be shown without that as well.)

Topological Invariants of Bands

(B.) Consider the simple two-band model in one dimension with (single-particle) Hamiltonian:

$$H(k) = \mathbf{E}(k) \cdot \boldsymbol{\sigma} \tag{3}$$

with the vector of Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$.

If you start with a linear chain tight binding model with a *two*-site unit cell, the single-particle Hamiltonian can be brought into this form after a Fourier transform. It is the two-site unit cell which leads to a two by two matrix of the Hamiltonian in momentum space. As you know any two-by-two Hermitian matrix can be written as a linear combination of the identity matrix and the three Pauli matrices. The precise real-space form of the Hamiltonian is not so important for this exercise. This will be addressed in more detail in the second problem in this sheet.

(a) Show that the eigenvalues of the system are given by

$$\epsilon(k) = \pm|\mathbf{E}(k)| \, . \tag{4}$$

(b) From now on let us consider the special case with $\mathbf{E}(k) = (0, -t\sin(k), -t\cos(k) + \mu)$ with $t > 0$. Compute the parameters where the energy gap between the two bands vanishes. Plot the energy bands for the different typical situations.

(c) The winding number for this special setup is given by

$$\nu = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}k \; \hat{\mathbf{e}}_{\mathbf{x}} \cdot \left(\mathbf{n}(k) \times \frac{\partial \mathbf{n}(k)}{\partial k} \right) \tag{5}$$

with $\mathbf{n}(k) = \mathbf{E}(k)/|\mathbf{E}(k)|$. Compute the winding number for the cases $\mu = 0$, $\mu \to \pm\infty$! The winding number has to be an integer and can only change when bands are crossing. What does this imply for the phase diagram of this model?

(d) **(optional)** Let us now consider a two-dimensional system with the Hamiltonian

$$H(\mathbf{k}) = \mathbf{E}(\mathbf{k}) \cdot \boldsymbol{\sigma} \tag{6}$$

and $\mathbf{E}(\mathbf{k}) = (\sin(k_x), \sin(k_y), \cos(k_x) + \cos(k_y) + m)$. The momenta are restricted to the first Brillouinzone $\mathbf{k} \in (-\pi, \pi] \times (-\pi, \pi]$. Redo task (b) for this system and compute the Chern number

$$C = \frac{1}{4\pi} \int_{-\pi}^{\pi} \mathrm{d}k_x \int_{-\pi}^{\pi} \mathrm{d}k_y \; \mathbf{n} \cdot \left(\frac{\partial \mathbf{n}}{\partial k_x} \times \frac{\partial \mathbf{n}}{\partial k_x} \right) \tag{7}$$

for values of m where the band gap does not close. Use a mathematical computation program to do so.