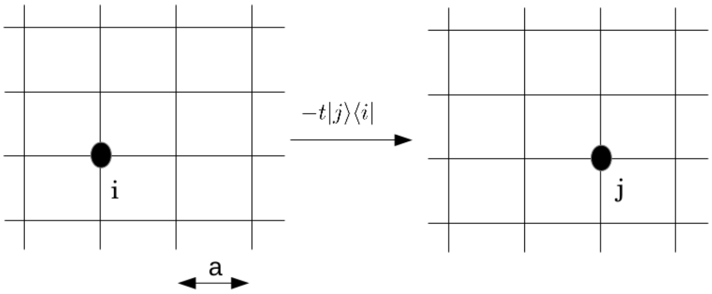
SOLID STATE PHYSICS III

Exercise session 2

September 25th 2025

(A.) We want to calculate the dispersion relation $\mathcal{E}_{\mathbf{k}} = f(\mathbf{k})$ for a *tight-binding* model on the square lattice.



1. With $|i\rangle$ being the physical state where the particle is on site i, the tight-binding Hamiltonian reads as:
$$H = -t \sum_{\langle i,j\rangle} \big(|i\rangle\langle j| + |j\rangle\langle i|\big),$$
where t is the hopping amplitude, and $\langle i, j\rangle$ denotes the summation over nearest neighbor interactions on a square lattice of N sites. By introducing the states $|\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k}\cdot\mathbf{r_i}}|i\rangle$, where the sum is taken on all sites of the lattice and $\mathbf{k}$ belongs to the first Brillouin zone, show that we can rewrite the Hamiltonian in the form:
$$H = \sum_{\mathbf{k}} \mathcal{E}_{\mathbf{k}} |\mathbf{k}\rangle\langle\mathbf{k}|.$$
What is the expression for $\mathcal{E}_{\mathbf{k}}$?
2. In second quantization, the tight-binding Hamiltonian is written:
$$H = -t \sum_{\langle i,j\rangle,\sigma} \big(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}\big),$$
where $c^\dagger_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator of an electron on site i with spin σ. What transformation is needed to diagonalize the Hamiltonian?

(B.) 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 electron 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. (**??**) 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. (**??**) explicitly. Show that $D(E = 0)$ diverges. (The integral can be carried out exactly, but the divergence can be shown without that as well.)

(C.) The purpose of this exercise is to determine an effective Hamiltonian for the Hubbard model on N sites,

$$H = \sum_{\langle i,j\rangle} H_{(i,j)} = \underbrace{-t\sum_{\langle i,j\rangle,\sigma}\left(c^\dagger_{i,\sigma}c_{j,\sigma} + c^\dagger_{j,\sigma}c_{i,\sigma}\right)}_{=H_t} + \underbrace{U\sum_i n_{i\uparrow}n_{i\downarrow}}_{=H_U},$$

at half-filling (N electrons) using the degenerate perturbation theory (limit $U \gg t$). At second order in H_t, the effective Hamiltonian is given by

$$H_{\text{eff}} \;=\; \underbrace{P_0 H_U P_0}_{H^{(0)}_{\text{eff}}} + \underbrace{P_0 H_t P_0}_{H^{(1)}_{\text{eff}}} + \underbrace{\sum_{n\neq 0}\frac{P_0 H_t P_n H_t P_0}{E_0 - E_n}}_{H^{(2)}_{\text{eff}}}$$

with P_n being the projector on the eigensubspace of H_U with energy E_n.

1. What are the configurations that consist the eigensubspace of H_U with zero energy?

2. Show that the matrix elements of $H_{\text{eff}}^{(0)}$ and $H_{\text{eff}}^{(1)}$ are zero ($\Rightarrow H_{\text{eff}} = H_{\text{eff}}^{(2)}$).

3. Show that
$$\sum_{n\neq 0} \frac{P_0 H_t P_n H_t P_0}{E_0 - E_n} = \sum_{\langle i,j\rangle} \frac{P_0 H^t_{(i,j)} P_1 H^t_{(i,j)} P_0}{E_0 - E_1},$$
with $H^t_{(i,j)} = -t(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma})$.

   In the following we will focus on on the case of the Hubbard model on two sites
$$H = \underbrace{-t(c^\dagger_{1\uparrow} c_{2\uparrow} + c^\dagger_{2\uparrow} c_{1\uparrow} + c^\dagger_{1\downarrow} c_{2\downarrow} + c^\dagger_{2\downarrow} c_{1\downarrow})}_{=H_t} + \underbrace{U\,(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})}_{=H_U}$$

4. The 2-particle Fock space is build up of 6 states $|1\rangle = c^\dagger_{1\uparrow} c^\dagger_{2\uparrow}|0\rangle$, $|2\rangle = c^\dagger_{1\downarrow} c^\dagger_{2\downarrow}|0\rangle$, $|3\rangle = c^\dagger_{1\uparrow} c^\dagger_{2\downarrow}|0\rangle$, $|4\rangle = c^\dagger_{1\downarrow} c^\dagger_{2\uparrow}|0\rangle$, $|5\rangle = c^\dagger_{1\uparrow} c^\dagger_{1\downarrow}|0\rangle$ et $|6\rangle = c^\dagger_{2\uparrow} c^\dagger_{2\downarrow}|0\rangle$. Check that $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$ are eigenstates of H_U with eigenvalue 0 and that $\{|5\rangle, |6\rangle\}$ are eigenstates of H_U with eigenvalue U. We then have
$$\begin{aligned} P_0 &= \sum_{m=1}^{4} |m\rangle\langle m| \\ P_1 &= \sum_{m=5}^{6} |m\rangle\langle m| \end{aligned}$$

5. Determine the matrix elements of $H_{\text{eff}}^{(2)}$, then diagonalize $H_{\text{eff}}^{(2)}$.

6. The fundamental subspace of H_U is build up of 4 states with one electron per site, we can define $|\sigma_1, \sigma_2\rangle = c^\dagger_{1\sigma_1} c^\dagger_{2\sigma_2}|0\rangle$. By using this notation, show that the eigenstates of H_{eff} are the triplets (with energy 0)
$$|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle \text{ and } \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle)$$
and the singlet (with energy $-4t^2/U$)
$$\frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle)$$

(D.) The two-site Hubbard model with two electrons (half-filling) contains only 6 states. It is therefore possible to obtain an exact formula for the eigenspectrum (page 13 of lecture notes).

$$\begin{cases} E_\pm &= \frac{U \pm \sqrt{U^2 + 16t^2}}{2} \\ E_0 &= 0 \end{cases}$$

Show that by expanding this energy in second order, we find the same energies as obtained in the previous exercise.