This exercise aims to familiarize you with second quantization by expressing physical operators and the Hamiltonian in this formalism, followed by solving the minimal tight-binding model.

(A.) The goal of this exercise is to write the Hamiltonian of an interacting electronic system in second quantization language. The Hamiltonian in coordinate representation reads as

$$H = H_{\text{kin}} + H_{\text{ext}} + H_{\text{int}} = \sum_i -\frac{\hbar^2 \Delta_i}{2m} + \sum_i U(\mathbf{r}_i) + \frac{1}{2}\sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) \tag{1}$$

where Δ_i stands for the laplacian in the ith coordinate, $U(\mathbf{r})$ is an external potential, and $V(\mathbf{r}_i, \mathbf{r}_j) = V(\mathbf{r}_i - \mathbf{r}_j) = \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$ is the Coulomb interaction between electrons.

1. Using the plane wave basis $\{|\varphi_{\boldsymbol{k},\sigma}\rangle\}$, write down the second quantized form of H_{kin}, and the expectation value should be calculated explicitly.
2. Find the second quantized form of H_{ext}. Simplify the final expression using the Fourier transform $U(\mathbf{q}) = \frac{1}{\Omega}\int d\mathbf{r} U(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}}$.
3. Write down the second quantized form of H_{int}. Explicitly calculate the matrix element using $\int d\mathbf{r} e^{i\mathbf{q}\mathbf{r}} \frac{1}{|\mathbf{r}|} = \frac{4\pi}{|\mathbf{q}|^2}$ (it is also helpful to do this integral by yourself if you do not remember how this was obtained). What do you observe about the wave vectors of the creation and annihilation operators? Can you explain why that is?

(B.) Let $\widehat{\boldsymbol{S}}_1$ be the spin-1/2 operator acting on $\mathcal{H}^{(1)}$

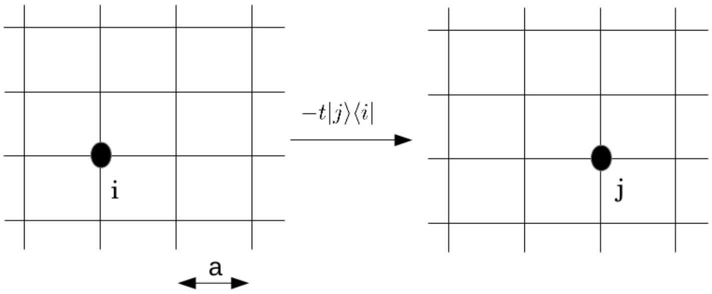
$$\begin{cases} \hat{S}_1^x |\varphi_{\boldsymbol{k},\sigma}\rangle = \frac{1}{2}|\varphi_{\boldsymbol{k},-\sigma}\rangle \\ \hat{S}_1^y |\varphi_{\boldsymbol{k},\sigma}\rangle = i\sigma|\varphi_{\boldsymbol{k},-\sigma}\rangle \\ \hat{S}_1^z |\varphi_{\boldsymbol{k},\sigma}\rangle = \sigma|\varphi_{\boldsymbol{k},\sigma}\rangle \end{cases}$$

Show that the total spin operator $\widehat{\boldsymbol{S}}$ acting on the Fock space is given by

$$\begin{aligned} \hat{S}^x &= \frac{1}{2}\sum_{\boldsymbol{k}} \left(c^\dagger_{\boldsymbol{k},\uparrow} c_{\boldsymbol{k},\downarrow} + c^\dagger_{\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} \right) \\ \hat{S}^y &= \frac{i}{2}\sum_{\boldsymbol{k}} \left(c^\dagger_{\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} - c^\dagger_{\boldsymbol{k},\uparrow} c_{\boldsymbol{k},\downarrow} \right) \\ \hat{S}^z &= \frac{1}{2}\sum_{\boldsymbol{k}} \left(c^\dagger_{\boldsymbol{k},\uparrow} c_{\boldsymbol{k},\uparrow} - c^\dagger_{\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\downarrow} \right) \end{aligned}$$

Tight-binding model

(C.) 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?