

Second quantization for observables

(A.)

1. Using the form given in the exercise we can write

$$H_{\text{kin}} = \sum_{\substack{\mathbf{k}, \mathbf{k}' \\ \sigma, \sigma'}} \langle \varphi_{\mathbf{k}', \sigma'} | \frac{\hat{p}^2}{2m} | \varphi_{\mathbf{k}, \sigma} \rangle c_{\mathbf{k}', \sigma'}^\dagger c_{\mathbf{k}, \sigma} \quad (1)$$

The matrix elements can be written as

$$\begin{aligned} \langle \varphi_{\mathbf{k}', \sigma'} | \hat{p}^2 | \varphi_{\mathbf{k}, \sigma} \rangle &= -\hbar^2 \sum_s \int d\mathbf{r} \varphi_{\mathbf{k}', \sigma'}^*(\mathbf{r}, s) \Delta \varphi_{\mathbf{k}, \sigma}(\mathbf{r}, s) \\ &= -\frac{\hbar^2}{\Omega} \sum_s \int d\mathbf{r} e^{-i\mathbf{k}'\mathbf{r}} \Delta e^{i\mathbf{k}\mathbf{r}} \delta_{\sigma', s} \delta_{\sigma, s} \\ &= \frac{\hbar^2}{\Omega} k^2 \sum_s \int d\mathbf{r} e^{-i\mathbf{k}'\mathbf{r}} e^{i\mathbf{k}\mathbf{r}} \delta_{\sigma', s} \delta_{\sigma, s} = \frac{\hbar^2}{\Omega} k^2 \Omega \delta_{\mathbf{k}', \mathbf{k}} \delta_{\sigma', \sigma} \end{aligned} \quad (2)$$

where we used that the plane waves states are orthogonal to each other ($\int d\mathbf{r} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}} = \Omega \delta_{\mathbf{k}, \mathbf{k}'}$).

$$H_{\text{kin}} = \sum_{\substack{\mathbf{k}, \mathbf{k}' \\ \sigma, \sigma'}} \frac{\hbar^2 k^2}{2m} \delta_{\mathbf{k}', \mathbf{k}} \delta_{\sigma', \sigma} c_{\mathbf{k}', \sigma'}^\dagger c_{\mathbf{k}, \sigma} = \sum_{\mathbf{k}, \sigma} \frac{\hbar^2 k^2}{2m} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \quad (3)$$

Note that $c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma}$ just gives the number of electrons in the $|\varphi_{\mathbf{k}, \sigma}\rangle$ state. We see that in the plane wave basis H_{kin} is diagonal, or in other words it doesn't change the electron state. This is because the plane waves are eigenstates of the momentum operator.

- 2.

$$H_{\text{ext}} = \sum_{\substack{\mathbf{k}, \mathbf{k}' \\ \sigma, \sigma'}} \langle \varphi_{\mathbf{k}', \sigma'} | U(\hat{\mathbf{r}}) | \varphi_{\mathbf{k}, \sigma} \rangle c_{\mathbf{k}', \sigma'}^\dagger c_{\mathbf{k}, \sigma} \quad (4)$$

where

$$\begin{aligned} \langle \varphi_{\mathbf{k}', \sigma'} | U(\hat{\mathbf{r}}) | \varphi_{\mathbf{k}, \sigma} \rangle &= \frac{1}{\Omega} \sum_s \int d\mathbf{r} e^{-i\mathbf{k}'\mathbf{r}} U(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} \delta_{\sigma', s} \delta_{\sigma, s} \\ &= \frac{1}{\Omega} \delta_{\sigma, \sigma'} \int d\mathbf{r} U(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}} = \delta_{\sigma, \sigma'} U(\mathbf{k}' - \mathbf{k}). \end{aligned} \quad (5)$$

As a result we get

$$H_{\text{ext}} = \sum_{\mathbf{k}, \mathbf{k}', \sigma} U(\mathbf{k}' - \mathbf{k}) c_{\mathbf{k}', \sigma}^\dagger c_{\mathbf{k}, \sigma}. \quad (6)$$

With a change of variables $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ we get

$$H_{\text{ext}} = \sum_{\mathbf{k}, \mathbf{q}, \sigma} U(\mathbf{q}) c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \quad (7)$$

We see that the external potential can change the momentum of an electron, but the possible values of the momentum change are related to nonzero Fourier components of the external potential. Recall from your studies about Bragg scattering on the periodic potential of the localized positive ions. There the potential had nonzero Fourier components only for reciprocal lattice vectors, therefore the momentum of the electrons could be changed by a reciprocal lattice vector.

3. The second quantized form of H_{int} reads as

$$H_{\text{int}} = \frac{1}{2} \sum_{\substack{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4 \\ \sigma_1, \sigma_2, \sigma_3, \sigma_4}} \langle \varphi_{\mathbf{k}_1, \sigma_1} \otimes \varphi_{\mathbf{k}_2, \sigma_2} | V(\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2) | \varphi_{\mathbf{k}_4, \sigma_4} \otimes \varphi_{\mathbf{k}_3, \sigma_3} \rangle c_{\mathbf{k}_1, \sigma_1}^\dagger c_{\mathbf{k}_2, \sigma_2}^\dagger c_{\mathbf{k}_3, \sigma_3} c_{\mathbf{k}_4, \sigma_4} \quad (8)$$

where

$$\begin{aligned} & \langle \varphi_{\mathbf{k}_1, \sigma_1} \otimes \varphi_{\mathbf{k}_2, \sigma_2} | V(\hat{\mathbf{r}} - \hat{\mathbf{r}}') | \varphi_{\mathbf{k}_4, \sigma_4} \otimes \varphi_{\mathbf{k}_3, \sigma_3} \rangle \\ &= \sum_s \sum_{s'} \frac{1}{\Omega^2} \int d\mathbf{r} \int d\mathbf{r}' e^{-i\mathbf{k}_1 \mathbf{r}} e^{-i\mathbf{k}_2 \mathbf{r}'} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} e^{i\mathbf{k}_4 \mathbf{r}} e^{i\mathbf{k}_3 \mathbf{r}'} \delta_{\sigma_1, s} \delta_{\sigma_2, s'} \delta_{\sigma_4, s} \delta_{\sigma_3, s'} \end{aligned} \quad (9)$$

Here we change the $\mathbf{r}$ integral variable to $\mathbf{R} = \mathbf{r} - \mathbf{r}'$. The integral in the $\mathbf{R}, \mathbf{r}'$ variables read as

$$\begin{aligned} & \langle \varphi_{\mathbf{k}_1, \sigma_1} \otimes \varphi_{\mathbf{k}_2, \sigma_2} | V(\hat{\mathbf{r}} - \hat{\mathbf{r}}') | \varphi_{\mathbf{k}_4, \sigma_4} \otimes \varphi_{\mathbf{k}_3, \sigma_3} \rangle \\ &= \frac{1}{\Omega^2} \int d\mathbf{R} \int d\mathbf{r}' e^{i(\mathbf{k}_4 - \mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_2) \mathbf{r}'} e^{i(\mathbf{k}_4 - \mathbf{k}_1) \mathbf{R}} \frac{e^2}{|\mathbf{R}|} \delta_{\sigma_1, \sigma_4} \delta_{\sigma_2, \sigma_3} \\ &= \frac{1}{\Omega} \delta_{\sigma_1, \sigma_4} \delta_{\sigma_2, \sigma_3} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \frac{4\pi e^2}{|\mathbf{k}_4 - \mathbf{k}_1|^2} \end{aligned} \quad (10)$$

Putting this back to the expression of H_{int} we get

$$H_{\text{int}} = \frac{1}{2\Omega} \sum_{\substack{\mathbf{k}_1, \mathbf{k}_3, \mathbf{k}_4 \\ \sigma_3, \sigma_4}} \frac{4\pi e^2}{|\mathbf{k}_4 - \mathbf{k}_1|^2} c_{\mathbf{k}_1, \sigma_4}^\dagger c_{\mathbf{k}_3 + \mathbf{k}_4 - \mathbf{k}_1, \sigma_3}^\dagger c_{\mathbf{k}_3, \sigma_3} c_{\mathbf{k}_4, \sigma_4} \quad (11)$$

By introducing a new variable $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_4$ instead of $\mathbf{k}_1$, and renaming the variables $\mathbf{k}_3$ and $\mathbf{k}_4$ we get

$$H_{\text{int}} = \frac{1}{2\Omega} \sum_{\substack{\mathbf{q}, \mathbf{k}, \mathbf{k}' \\ \sigma, \sigma'}} \frac{4\pi e^2}{|\mathbf{q}|^2} c_{\mathbf{k}'+\mathbf{q}, \sigma'}^\dagger c_{\mathbf{k}-\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}, \sigma} c_{\mathbf{k}', \sigma'} \quad (12)$$

We see that the total momentum is conserved by H_{int} , the total momentum of the annihilated electrons is equal to the total momentum of the created electrons. This is because the Coulomb interaction is translational invariant, it only depends on $\mathbf{r} - \mathbf{r}'$.

One term in the expression of H_{int} describes the scattering process where two electrons with momenta $\mathbf{k}$ and $\mathbf{k}'$ interact and exchange some momentum $\mathbf{q}$, so after the interaction they will have $\mathbf{k} + \mathbf{q}$ and $\mathbf{k}' - \mathbf{q}$ momenta. The electron spins are untouched during the process.

Bonus: The integral $\int d\mathbf{r} e^{i\mathbf{q}\mathbf{r}} \frac{1}{r}$ cannot be carried out immediately, as it is not absolute convergent. One needs to introduce a regularization term. So we have

$$I(\mathbf{q}, \varepsilon) = \int d\mathbf{r} e^{i\mathbf{q}\mathbf{r} - \varepsilon|\mathbf{r}|} \frac{1}{|\mathbf{r}|} \quad (13)$$

This can be calculated in spherical coordinates choosing the $\mathbf{q}$ vector to be in the z direction. The value of the integral we are interested is then given by $\lim_{\varepsilon \rightarrow 0} I(\mathbf{q}, \varepsilon)$.

(B.)

A first approach : Let's start by noting that

$$\begin{aligned} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \varphi_{\mathbf{k}_2, \sigma_2} \rangle &= \int d^3\mathbf{r} \sum_{\sigma} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \mathbf{r}, \sigma \rangle \langle \mathbf{r}, \sigma | \varphi_{\mathbf{k}_2, \sigma_2} \rangle \\ &= \frac{1}{\Omega} \int d^3\mathbf{r} \sum_{\sigma} e^{-i\mathbf{k}_1 \cdot \mathbf{r}} \eta_{\sigma_1}^*(\sigma) e^{i\mathbf{k}_2 \cdot \mathbf{r}} \eta_{\sigma_2}(\sigma) \\ &= \frac{1}{\Omega} \int d^3\mathbf{r} \underbrace{e^{i(\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{r}}}_{=\Omega \delta_{\mathbf{k}_1, \mathbf{k}_2}} \sum_{\sigma} \underbrace{\eta_{\sigma_1}^*(\sigma) \eta_{\sigma_2}(\sigma)}_{=\delta_{\sigma, \sigma_1} \delta_{\sigma, \sigma_2}} \\ &= \delta_{\mathbf{k}_1, \mathbf{k}_2} \delta_{\sigma_1, \sigma_2} \end{aligned}$$

So, from the definition of the spin operators we get

$$\begin{aligned} \langle \varphi_{\mathbf{k}_1, \sigma_1} | S_1^x | \varphi_{\mathbf{k}_2, \sigma_2} \rangle &= \frac{1}{2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \varphi_{\mathbf{k}_2, -\sigma_2} \rangle \\ &= \frac{1}{2} \delta_{\mathbf{k}_1, \mathbf{k}_2} \delta_{\sigma_1, -\sigma_2} \\ \langle \varphi_{\mathbf{k}_1, \sigma_1} | S_1^y | \varphi_{\mathbf{k}_2, \sigma_2} \rangle &= i\sigma_2 \langle \varphi_{\mathbf{k}_1, \sigma_1} | \varphi_{\mathbf{k}_2, -\sigma_2} \rangle \\ &= i\sigma_2 \delta_{\mathbf{k}_1, \mathbf{k}_2} \delta_{\sigma_1, -\sigma_2} \\ \langle \varphi_{\mathbf{k}_1, \sigma_1} | S_1^z | \varphi_{\mathbf{k}_2, \sigma_2} \rangle &= \sigma_2 \langle \varphi_{\mathbf{k}_1, \sigma_1} | \varphi_{\mathbf{k}_2, \sigma_2} \rangle \\ &= \sigma_2 \delta_{\mathbf{k}_1, \mathbf{k}_2} \delta_{\sigma_1, \sigma_2} \end{aligned}$$

and thus

$$\begin{aligned} \hat{S}^x &= \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma_1, \sigma_2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^x | \varphi_{\mathbf{k}_2, \sigma_2} \rangle c_{\mathbf{k}_1, \sigma_1}^\dagger c_{\mathbf{k}_2, \sigma_2} \\ &= \frac{1}{2} \sum_{\mathbf{k}} \sum_{\sigma} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, -\sigma} \\ &= \frac{1}{2} \sum_{\mathbf{k}} \left(c_{\mathbf{k}, \uparrow}^\dagger c_{\mathbf{k}, \downarrow} + c_{\mathbf{k}, \downarrow}^\dagger c_{\mathbf{k}, \uparrow} \right) \end{aligned}$$

$$\begin{aligned}
\hat{S}^y &= \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma_1, \sigma_2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^y | \varphi_{\mathbf{k}_2, \sigma_2} \rangle c_{\mathbf{k}_1, \sigma_1}^\dagger c_{\mathbf{k}_2, \sigma_2} \\
&= -i \sum_{\mathbf{k}} \sum_{\sigma} \sigma c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, -\sigma} \\
&= \frac{i}{2} \sum_{\mathbf{k}} \left(c_{\mathbf{k}, \downarrow}^\dagger c_{\mathbf{k}, \uparrow} - c_{\mathbf{k}, \uparrow}^\dagger c_{\mathbf{k}, \downarrow} \right)
\end{aligned}$$

$$\begin{aligned}
\hat{S}^z &= \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma_1, \sigma_2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^z | \varphi_{\mathbf{k}_2, \sigma_2} \rangle c_{\mathbf{k}_1, \sigma_1}^\dagger c_{\mathbf{k}_2, \sigma_2} \\
&= \sum_{\mathbf{k}} \sum_{\sigma} \sigma c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \\
&= \frac{1}{2} \sum_{\mathbf{k}} \left(c_{\mathbf{k}, \uparrow}^\dagger c_{\mathbf{k}, \uparrow} - c_{\mathbf{k}, \downarrow}^\dagger c_{\mathbf{k}, \downarrow} \right)
\end{aligned}$$

Another approach: We want to determine

$$\hat{S} = \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma_1, \sigma_2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1 | \varphi_{\mathbf{k}_2, \sigma_2} \rangle c_{\mathbf{k}_1, \sigma_1}^\dagger c_{\mathbf{k}_2, \sigma_2}$$

Therefore, it is necessary to evaluate

$$\begin{aligned}
\langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1 | \varphi_{\mathbf{k}_2, \sigma_2} \rangle &= \int d^3 \mathbf{r} \sum_{\sigma} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \mathbf{r}, \sigma \rangle \langle \mathbf{r}, \sigma | \hat{S}_1 | \varphi_{\mathbf{k}_2, \sigma_2} \rangle \\
&= \frac{1}{\Omega} \int d^3 \mathbf{r} \sum_{\sigma} e^{-i \mathbf{k}_1 \cdot \mathbf{r}} \eta_{\sigma_1}^*(\sigma) \hat{S}_1 e^{i \mathbf{k}_2 \cdot \mathbf{r}} \eta_{\sigma_2}(\sigma) \\
&= \frac{1}{\Omega} \underbrace{\int d^3 \mathbf{r} e^{i(\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{r}}}_{= \Omega \delta_{\mathbf{k}_1, \mathbf{k}_2}} \sum_{\sigma} \eta_{\sigma_1}^*(\sigma) \hat{S}_1 \eta_{\sigma_2}(\sigma)
\end{aligned}$$

Consider the spin part

$$\begin{aligned}
\eta_{\sigma_1}^*(\sigma) \hat{S}_1^x \eta_{\sigma_2}(\sigma) &= \frac{1}{2} \eta_{\sigma_1}^*(\sigma) \eta_{-\sigma_2}(\sigma) \\
&= \frac{1}{2} \delta_{\sigma, \sigma_1} \delta_{\sigma, -\sigma_2} \\
\eta_{\sigma_1}^*(\sigma) \hat{S}_1^y \eta_{\sigma_2}(\sigma) &= i \sigma_2 \eta_{\sigma_1}^*(\sigma) \eta_{-\sigma_2}(\sigma) \\
&= i \sigma_2 \delta_{\sigma, \sigma_1} \delta_{\sigma, -\sigma_2} \\
\eta_{\sigma_1}^*(\sigma) \hat{S}_1^z \eta_{\sigma_2}(\sigma) &= \sigma_2 \eta_{\sigma_1}^*(\sigma) \eta_{\sigma_2}(\sigma) \\
&= \sigma_2 \delta_{\sigma, \sigma_1} \delta_{\sigma, \sigma_2}
\end{aligned}$$

so

$$\begin{aligned}
\langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^x | \varphi_{\mathbf{k}_2, \sigma_2} \rangle &= \delta_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma} \frac{1}{2} \delta_{\sigma, \sigma_1} \delta_{\sigma, -\sigma_2} \\
&= \frac{1}{2} \delta_{\mathbf{k}_1, \mathbf{k}_2} \delta_{\sigma_1, -\sigma_2} \\
\langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^y | \varphi_{\mathbf{k}_2, \sigma_2} \rangle &= \delta_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma} i \sigma_2 \delta_{\sigma, \sigma_1} \delta_{\sigma, -\sigma_2} \\
&= i \sigma_2 \delta_{\mathbf{k}_1, \mathbf{k}_2} \delta_{\sigma_1, -\sigma_2} \\
\langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^z | \varphi_{\mathbf{k}_2, \sigma_2} \rangle &= \delta_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma} \sigma_2 \delta_{\sigma, \sigma_1} \delta_{\sigma, \sigma_2} \\
&= \sigma_2 \delta_{\mathbf{k}_1, \mathbf{k}_2} \delta_{\sigma_1, \sigma_2}
\end{aligned}$$

and finally

$$\begin{aligned}
\hat{S}^x &= \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma_1, \sigma_2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^x | \varphi_{\mathbf{k}_2, \sigma_2} \rangle c_{\mathbf{k}_1, \sigma_1}^{\dagger} c_{\mathbf{k}_2, \sigma_2} \\
&= \frac{1}{2} \sum_{\mathbf{k}} \sum_{\sigma} c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, -\sigma} \\
&= \frac{1}{2} \sum_{\mathbf{k}} \left(c_{\mathbf{k}, \uparrow}^{\dagger} c_{\mathbf{k}, \downarrow} + c_{\mathbf{k}, \downarrow}^{\dagger} c_{\mathbf{k}, \uparrow} \right) \\
\hat{S}^y &= \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma_1, \sigma_2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^y | \varphi_{\mathbf{k}_2, \sigma_2} \rangle c_{\mathbf{k}_1, \sigma_1}^{\dagger} c_{\mathbf{k}_2, \sigma_2} \\
&= -i \sum_{\mathbf{k}} \sum_{\sigma} \sigma c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, -\sigma} \\
&= \frac{i}{2} \sum_{\mathbf{k}} \left(c_{\mathbf{k}, \downarrow}^{\dagger} c_{\mathbf{k}, \uparrow} - c_{\mathbf{k}, \uparrow}^{\dagger} c_{\mathbf{k}, \downarrow} \right) \\
\hat{S}^z &= \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\sigma_1, \sigma_2} \langle \varphi_{\mathbf{k}_1, \sigma_1} | \hat{S}_1^z | \varphi_{\mathbf{k}_2, \sigma_2} \rangle c_{\mathbf{k}_1, \sigma_1}^{\dagger} c_{\mathbf{k}_2, \sigma_2} \\
&= \sum_{\mathbf{k}} \sum_{\sigma} \sigma c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} \\
&= \frac{1}{2} \sum_{\mathbf{k}} \left(c_{\mathbf{k}, \uparrow}^{\dagger} c_{\mathbf{k}, \uparrow} - c_{\mathbf{k}, \downarrow}^{\dagger} c_{\mathbf{k}, \downarrow} \right)
\end{aligned}$$

Tight-binding

(C.) *The tight-binding model on a square lattice.*

1. The simplest way is to start by reversing the relationship, that is, writing the N states $|j\rangle$ according to the N states $|\mathbf{k}\rangle$. Let's not forget that $\mathbf{k}$ belongs to the first Brillouin zone, that is, $\mathbf{k} = \left(-\frac{\pi}{a} + \frac{2\pi}{L}n_x\right)\mathbf{e}_x + \left(-\frac{\pi}{a} + \frac{2\pi}{L}n_y\right)\mathbf{e}_y$, with $n_x = 1 \dots \frac{L}{a}$ et $n_y = 1 \dots \frac{L}{a}$, where L is the length of the lattice so that $L^2 = Na^2$. We have (simple inversion of Fourier transform):

$$|i\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} |\mathbf{k}\rangle \quad (14)$$

It is verified that:

$$\begin{aligned}
 |\mathbf{k}\rangle &= \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} \left(\frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{r}_i} |\mathbf{k}'\rangle \right) \\
 &= \frac{1}{N} \sum_{\mathbf{k}'} \underbrace{\left(\sum_i e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} \right)}_{=N\delta_{\mathbf{k},\mathbf{k}'}} |\mathbf{k}'\rangle = |\mathbf{k}\rangle.
 \end{aligned} \tag{15}$$

Let's use Eq. (14) to rewrite the Hamiltonian.

$$\begin{aligned}
 H &= -t \sum_{\langle i,j \rangle} (|i\rangle\langle j| + |j\rangle\langle i|) \\
 &= -t \sum_i \left(\sum_{j, \text{ neighbours of } i} |i\rangle\langle j| \right) \\
 &= -\frac{t}{N} \sum_{\mathbf{k}', \mathbf{k}} \sum_i \left(\sum_{j, \text{ neighbours of } i} e^{i(\mathbf{k}\cdot\mathbf{r}_i - \mathbf{k}'\cdot\mathbf{r}_j)} \right) |\mathbf{k}\rangle\langle\mathbf{k}'| \\
 &= -\frac{t}{N} \sum_{\mathbf{k}', \mathbf{k}} \eta(\mathbf{k}') \underbrace{\left(\sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} \right)}_{=N\delta_{\mathbf{k},\mathbf{k}'}} |\mathbf{k}\rangle\langle\mathbf{k}'|,
 \end{aligned} \tag{16}$$

where $\eta(\mathbf{k}') = e^{ia\mathbf{k}'\cdot\mathbf{e}_x} + e^{-ia\mathbf{k}'\cdot\mathbf{e}_x} + e^{ia\mathbf{k}'\cdot\mathbf{e}_y} + e^{-ia\mathbf{k}'\cdot\mathbf{e}_y} = 2(\cos(k'_x a) + \cos(k'_y a))$.

We then obtain:

$$H = \sum_{\mathbf{k}} \mathcal{E}_{\mathbf{k}} |\mathbf{k}\rangle\langle\mathbf{k}|,$$

with $\mathcal{E}_{\mathbf{k}} = -2t(\cos(k_x a) + \cos(k_y a))$.

2. Taking inspiration from the previous question, we can introduce the creation operator:

$$c_{\mathbf{k},\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{i,\sigma}^\dagger. \tag{17}$$

By taking the hermitian conjugate, one must necessarily have

$$c_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{i,\sigma}. \tag{18}$$

To be acceptable, these operators must follow the fermionic anti-commutations relations:

$$\{c_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}^\dagger\} = \frac{1}{N} \sum_{i,j} e^{i(\mathbf{k}\cdot\mathbf{r}_i - \mathbf{k}'\cdot\mathbf{r}_j)} \underbrace{\{c_{i,\sigma}, c_{j,\sigma'}^\dagger\}}_{=\delta_{i,j}\delta_{\sigma,\sigma'}} = \frac{1}{N} \underbrace{\sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i}}_{=N\delta_{\mathbf{k},\mathbf{k}'}} \delta_{\sigma,\sigma'} = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'}. \tag{19}$$

And also, $\{c_{\mathbf{k}',\sigma'}^\dagger, c_{\mathbf{k},\sigma}^\dagger\} = \{c_{\mathbf{k}',\sigma'}, c_{\mathbf{k},\sigma}\} = 0$.

We then repeat the same calculations as in Eq. (16) to get:

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}) = \sum_{\mathbf{k}, \sigma} \mathcal{E}_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}.$$