SOLID STATE PHYSICS III **Solution session 1** September 18th 2025

(A.)

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

$$H_{\text{kin}} = \sum_{\substack{\boldsymbol{k},\boldsymbol{k}'\\ \sigma,\sigma'}} \langle \varphi_{\boldsymbol{k}',\sigma'}|\frac{\hat{p}^2}{2m}|\varphi_{\boldsymbol{k},\sigma}\rangle c^\dagger_{\boldsymbol{k}',\sigma'}c_{\boldsymbol{k},\sigma} \tag{1}$$

The matrix elements can be written as

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

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

$$H_{\text{kin}} = \sum_{\substack{\boldsymbol{k},\boldsymbol{k}'\\ \sigma,\sigma'}} \frac{\hbar^2k^2}{2m}\delta_{\boldsymbol{k}',\boldsymbol{k}}\delta_{\sigma',\sigma}c^\dagger_{\boldsymbol{k}',\sigma'}c_{\boldsymbol{k},\sigma} = \sum_{\boldsymbol{k},\sigma}\frac{\hbar^2k^2}{2m}c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k},\sigma} \tag{3}$$

Note that $c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k},\sigma}$ just gives the number of electrons in the $|\varphi_{\boldsymbol{k},\sigma}\rangle$ 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.

$$H_{\text{ext}} = \sum_{\substack{\boldsymbol{k},\boldsymbol{k}'\\ \sigma,\sigma'}} \langle \varphi_{\boldsymbol{k}',\sigma'}|U(\hat{\boldsymbol{r}})|\varphi_{\boldsymbol{k},\sigma}\rangle c^\dagger_{\boldsymbol{k}',\sigma'}c_{\boldsymbol{k},\sigma} \tag{4}$$

where

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

As a result we get

$$H_{\text{ext}} = \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} U(\boldsymbol{k}'-\boldsymbol{k})c^\dagger_{\boldsymbol{k}',\sigma}c_{\boldsymbol{k},\sigma}. \tag{6}$$

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

$$H_{\text{ext}} = \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} U(\boldsymbol{q}) c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma} \tag{7}$$

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

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

where

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

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

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

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

$$H_{\text{int}} = \frac{1}{2\Omega} \sum_{\substack{\boldsymbol{k}_1,\boldsymbol{k}_3,\boldsymbol{k}_4 \\ \sigma_3,\sigma_4}} \frac{4\pi e^2}{|\boldsymbol{k}_4 - \boldsymbol{k}_1|^2} c^{\dagger}_{\boldsymbol{k}_1,\sigma_4} c^{\dagger}_{\boldsymbol{k}_3+\boldsymbol{k}_4-\boldsymbol{k}_1,\sigma_3} c_{\boldsymbol{k}_3,\sigma_3} c_{\boldsymbol{k}_4,\sigma_4} \tag{11}$$

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

$$H_{\text{int}} = \frac{1}{2\Omega} \sum_{\substack{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}' \\ \sigma,\sigma'}} \frac{4\pi e^2}{|\boldsymbol{q}|^2} c^{\dagger}_{\boldsymbol{k}'+\boldsymbol{q},\sigma'} c^{\dagger}_{\boldsymbol{k}-\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma} c_{\boldsymbol{k}',\sigma'} \tag{12}$$

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 $\boldsymbol{r} - \boldsymbol{r}'$.

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

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

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

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

(B.)

A first approach : Let's start by noting that

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

So, from the definition of the spin operators we get

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

and thus

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

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

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

Another approach: We want to determine

$$\widehat{\boldsymbol{S}} = \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma_1,\sigma_2}\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\widehat{\boldsymbol{S}}_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle c^\dagger_{\boldsymbol{k}_1,\sigma_1}c_{\boldsymbol{k}_2,\sigma_2}$$

Therefore, it is necessary to evaluate

$$\begin{aligned}
\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\widehat{\boldsymbol{S}}_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle &= \int d^3\boldsymbol{r}\sum_{\sigma}\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\boldsymbol{r},\sigma\rangle\langle\boldsymbol{r},\sigma|\widehat{\boldsymbol{S}}_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle\\
&= \frac{1}{\Omega}\int d^3\boldsymbol{r}\sum_{\sigma}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}}\eta^*_{\sigma_1}(\sigma)\widehat{\boldsymbol{S}}_1e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}\eta_{\sigma_2}(\sigma)\\
&= \frac{1}{\Omega}\underbrace{\int d^3\boldsymbol{r}e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}}}_{=\Omega\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}}\sum_{\sigma}\eta^*_{\sigma_1}(\sigma)\widehat{\boldsymbol{S}}_1\eta_{\sigma_2}(\sigma)
\end{aligned}$$

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

$$\begin{aligned}
\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\hat{S}^x_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle &= \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_\sigma \frac{1}{2}\delta_{\sigma,\sigma_1}\delta_{\sigma,-\sigma_2} \\
&= \frac{1}{2}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\delta_{\sigma_1,-\sigma_2} \\
\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\hat{S}^y_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle &= \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_\sigma i\sigma_2\delta_{\sigma,\sigma_1}\delta_{\sigma,-\sigma_2} \\
&= i\sigma_2\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\delta_{\sigma_1,-\sigma_2} \\
\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\hat{S}^z_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle &= \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_\sigma \sigma_2\delta_{\sigma,\sigma_1}\delta_{\sigma,\sigma_2} \\
&= \sigma_2\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\delta_{\sigma_1,\sigma_2}
\end{aligned}$$

and finally

$$\begin{aligned}
\hat{S}^x &= \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma_1,\sigma_2}\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\hat{S}^x_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle c^\dagger_{\boldsymbol{k}_1,\sigma_1}c_{\boldsymbol{k}_2,\sigma_2} \\
&= \frac{1}{2}\sum_{\boldsymbol{k}}\sum_\sigma c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k},-\sigma} \\
&= \frac{1}{2}\sum_{\boldsymbol{k}}\left(c^\dagger_{\boldsymbol{k},\uparrow}c_{\boldsymbol{k},\downarrow}+c^\dagger_{\boldsymbol{k},\downarrow}c_{\boldsymbol{k},\uparrow}\right) \\
\hat{S}^y &= \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma_1,\sigma_2}\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\hat{S}^y_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle c^\dagger_{\boldsymbol{k}_1,\sigma_1}c_{\boldsymbol{k}_2,\sigma_2} \\
&= -i\sum_{\boldsymbol{k}}\sum_\sigma \sigma c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k},-\sigma} \\
&= \frac{i}{2}\sum_{\boldsymbol{k}}\left(c^\dagger_{\boldsymbol{k},\downarrow}c_{\boldsymbol{k},\uparrow}-c^\dagger_{\boldsymbol{k},\uparrow}c_{\boldsymbol{k},\downarrow}\right) \\
\hat{S}^z &= \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma_1,\sigma_2}\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\hat{S}^z_1|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle c^\dagger_{\boldsymbol{k}_1,\sigma_1}c_{\boldsymbol{k}_2,\sigma_2} \\
&= \sum_{\boldsymbol{k}}\sum_\sigma \sigma c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k},\sigma} \\
&= \frac{1}{2}\sum_{\boldsymbol{k}}\left(c^\dagger_{\boldsymbol{k},\uparrow}c_{\boldsymbol{k},\uparrow}-c^\dagger_{\boldsymbol{k},\downarrow}c_{\boldsymbol{k},\downarrow}\right)
\end{aligned}$$

(C.) We want to determine

$$\hat{n}(\boldsymbol{r})=\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma_1,\sigma_2}\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\hat{n}_1(\boldsymbol{r})|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle c^\dagger_{\boldsymbol{k}_1,\sigma_1}c_{\boldsymbol{k}_2,\sigma_2}$$

with

$$\hat{n}_1(\boldsymbol{r})=\sum_\sigma|\boldsymbol{r},\sigma\rangle\langle\boldsymbol{r},\sigma|$$

It is therefore necessary to evaluate

$$\begin{aligned}
\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\hat{n}_1(\boldsymbol{r})|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle &= \sum_\sigma\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\boldsymbol{r},\sigma\rangle\langle\boldsymbol{r},\sigma|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle \\
&= \sum_\sigma\varphi^*_{\boldsymbol{k}_1,\sigma_1}(\boldsymbol{r},\sigma)\varphi_{\boldsymbol{k}_2,\sigma_2}(\boldsymbol{r},\sigma)
\end{aligned}$$

and

$$\begin{aligned}\hat{n}(\boldsymbol{r}) &= \sum_{\sigma} \underbrace{\sum_{\boldsymbol{k}_1,\sigma_1} \varphi^*_{\boldsymbol{k}_1,\sigma_1}(\boldsymbol{r},\sigma) c^\dagger_{\boldsymbol{k}_1,\sigma_1}}_{=\Psi^\dagger(\boldsymbol{r},\sigma)} \underbrace{\sum_{\boldsymbol{k}_2,\sigma_2} \varphi_{\boldsymbol{k}_2,\sigma_2}(\boldsymbol{r},\sigma) c_{\boldsymbol{k}_2,\sigma_2}}_{=\Psi(\boldsymbol{r},\sigma)} \\ &= \sum_{\sigma} \Psi^\dagger(\boldsymbol{r},\sigma)\Psi(\boldsymbol{r},\sigma)\end{aligned}$$

(D.) We want to determine

$$\widehat{\boldsymbol{J}}(\boldsymbol{r}) = \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\sigma_1,\sigma_2} \langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \widehat{\boldsymbol{J}}_1(\boldsymbol{r}) | \varphi_{\boldsymbol{k}_2,\sigma_2} \rangle c^\dagger_{\boldsymbol{k}_1,\sigma_1} c_{\boldsymbol{k}_2,\sigma_2}$$

with

$$\begin{aligned}\widehat{\boldsymbol{J}}_1(\boldsymbol{r}) &= \frac{1}{2m} \sum_{\sigma} \Big(|\boldsymbol{r},\sigma\rangle\langle \boldsymbol{r},\sigma| \widehat{\boldsymbol{P}}_1 + \widehat{\boldsymbol{P}}_1 |\boldsymbol{r},\sigma\rangle\langle \boldsymbol{r},\sigma| \Big) \\ \langle \boldsymbol{r},\sigma| \widehat{\boldsymbol{P}}_1 |\psi\rangle &= \Big(-i\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big) \psi(\boldsymbol{r},\sigma)\end{aligned}$$

Therefore, it is necessary to evaluate

$$\begin{aligned}\langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \widehat{\boldsymbol{J}}(\boldsymbol{r}) | \varphi_{\boldsymbol{k}_2,\sigma_2} \rangle &= \frac{1}{2m} \sum_{\sigma} \Big(\langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \boldsymbol{r},\sigma\rangle\langle \boldsymbol{r},\sigma| \widehat{\boldsymbol{P}}_1 | \varphi_{\boldsymbol{k}_2,\sigma_2}\rangle + \langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \widehat{\boldsymbol{P}}_1 | \boldsymbol{r},\sigma\rangle\langle \boldsymbol{r},\sigma| \varphi_{\boldsymbol{k}_2,\sigma_2}\rangle \Big) \\ &= \frac{1}{2m} \sum_{\sigma} \Big(\langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \boldsymbol{r},\sigma\rangle\langle \boldsymbol{r},\sigma| \widehat{\boldsymbol{P}}_1 | \varphi_{\boldsymbol{k}_2,\sigma_2}\rangle + \langle \varphi_{\boldsymbol{k}_2,\sigma_2} | \boldsymbol{r},\sigma\rangle^*\langle \boldsymbol{r},\sigma| \widehat{\boldsymbol{P}}_1 | \varphi_{\boldsymbol{k}_1,\sigma_1}\rangle^* \Big)\end{aligned}$$

Consider

$$\begin{aligned}\langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \boldsymbol{r},\sigma\rangle\langle \boldsymbol{r},\sigma| \widehat{\boldsymbol{P}}_1 | \varphi_{\boldsymbol{k}_2,\sigma_2}\rangle &= \langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \boldsymbol{r},\sigma\rangle \Big(-i\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big) \langle \boldsymbol{r},\sigma | \varphi_{\boldsymbol{k}_2,\sigma_2}\rangle \\ &= \varphi^*_{\boldsymbol{k}_1,\sigma_1}(\boldsymbol{r},\sigma) \Big(-i\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big) \varphi_{\boldsymbol{k}_2,\sigma_2}(\boldsymbol{r},\sigma) \\ &= \frac{1}{\Omega} e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}} \eta^*_{\sigma_1}(\sigma) \Big(-i\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big) e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}} \eta_{\sigma_2}(\sigma) \\ &= \frac{1}{\Omega} \delta_{\sigma,\sigma_1}\delta_{\sigma,\sigma_2} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}} \Big(\boldsymbol{k}_2 - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big)\end{aligned}$$

so

$$\frac{1}{2m}\sum_{\sigma} \langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \boldsymbol{r},\sigma\rangle\langle \boldsymbol{r},\sigma| \widehat{\boldsymbol{P}}_1 | \varphi_{\boldsymbol{k}_2,\sigma_2}\rangle = \frac{1}{2m\Omega} \delta_{\sigma_1,\sigma_2} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}} \Big(\boldsymbol{k}_2 - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big)$$

and

$$\begin{aligned}\langle \varphi_{\boldsymbol{k}_1,\sigma_1} | \widehat{\boldsymbol{J}}_1(\boldsymbol{r}) | \varphi_{\boldsymbol{k}_2,\sigma_2} \rangle &= \frac{1}{2m\Omega} \delta_{\sigma_1,\sigma_2} \Big(e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}} \Big(\boldsymbol{k}_2 - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big) + e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}} \Big(\boldsymbol{k}_1 - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big) \Big) \\ &= \frac{1}{2m\Omega} \delta_{\sigma_1,\sigma_2} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}} \Big(\boldsymbol{k}_1 + \boldsymbol{k}_2 - 2\frac{e}{c}\boldsymbol{A}(\boldsymbol{r}) \Big)\end{aligned}$$

We draw from it

$$\begin{aligned}
\widehat{\boldsymbol{J}}(\boldsymbol{r}) &= \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma_1,\sigma_2}\langle\varphi_{\boldsymbol{k}_1,\sigma_1}|\widehat{\boldsymbol{J}}_1(\boldsymbol{r})|\varphi_{\boldsymbol{k}_2,\sigma_2}\rangle c^\dagger_{\boldsymbol{k}_1,\sigma_1}c_{\boldsymbol{k}_2,\sigma_2} \\
&= \frac{1}{2m\Omega}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma_1,\sigma_2}\delta_{\sigma_1,\sigma_2}e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}}\left(\boldsymbol{k}_1+\boldsymbol{k}_2-2\frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right)c^\dagger_{\boldsymbol{k}_1,\sigma_1}c_{\boldsymbol{k}_2,\sigma_2} \\
&= \underbrace{\frac{1}{2m\Omega}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma}e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}}\left(\boldsymbol{k}_1+\boldsymbol{k}_2\right)c^\dagger_{\boldsymbol{k}_1,\sigma}c_{\boldsymbol{k}_2,\sigma}}_{=\widehat{\boldsymbol{J}}_a(\boldsymbol{r})} \\
&\quad \underbrace{-\frac{e}{mc\Omega}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma}e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}}\boldsymbol{A}(\boldsymbol{r})c^\dagger_{\boldsymbol{k}_1,\sigma}c_{\boldsymbol{k}_2,\sigma}}_{=\widehat{\boldsymbol{J}}_b(\boldsymbol{r})}
\end{aligned}$$

The term $\widehat{\boldsymbol{J}}_a(\boldsymbol{r})$ writes

$$\begin{aligned}
\widehat{\boldsymbol{J}}_a(\boldsymbol{r}) &= \frac{1}{2m\Omega}\sum_{\sigma}\left(\sum_{\boldsymbol{k}_1}\boldsymbol{k}_1e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}}c^\dagger_{\boldsymbol{k}_1,\sigma}\right)\left(\sum_{\boldsymbol{k}_2}e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}c_{\boldsymbol{k}_2,\sigma}\right) \\
&\quad +\frac{1}{2m\Omega}\sum_{\sigma}\left(\sum_{\boldsymbol{k}_1}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}}c^\dagger_{\boldsymbol{k}_1,\sigma}\right)\left(\sum_{\boldsymbol{k}_2}\boldsymbol{k}_2e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}c_{\boldsymbol{k}_2,\sigma}\right) \\
&= \frac{i}{2m\Omega}\sum_{\sigma}\left\{\left(\nabla\sum_{\boldsymbol{k}_1}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}}c^\dagger_{\boldsymbol{k}_1,\sigma}\right)\left(\sum_{\boldsymbol{k}_2}e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}c_{\boldsymbol{k}_2,\sigma}\right)\right. \\
&\quad \left.-\left(\sum_{\boldsymbol{k}_1}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}}c^\dagger_{\boldsymbol{k}_1,\sigma}\right)\left(\nabla\sum_{\boldsymbol{k}_2}e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}c_{\boldsymbol{k}_2,\sigma}\right)\right\} \\
&= \frac{i}{2m}\sum_{\sigma}\left\{\left(\nabla\Psi^\dagger(\boldsymbol{r},\sigma)\right)\Psi(\boldsymbol{r},\sigma)-\Psi^\dagger(\boldsymbol{r},\sigma)\left(\nabla\Psi(\boldsymbol{r},\sigma)\right)\right\}
\end{aligned}$$

and the term $\widehat{\boldsymbol{J}}_b(\boldsymbol{r})$

$$\begin{aligned}
\widehat{\boldsymbol{J}}_b(\boldsymbol{r}) &= -\frac{e}{mc\Omega}\boldsymbol{A}(\boldsymbol{r})\sum_{\sigma}\underbrace{\left(\sum_{\boldsymbol{k}_1}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}}c^\dagger_{\boldsymbol{k}_1,\sigma}\right)}_{=\sqrt{\Omega}\Psi^\dagger(\boldsymbol{r},\sigma)}\underbrace{\left(\sum_{\boldsymbol{k}_2}e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}}c_{\boldsymbol{k}_2,\sigma}\right)}_{=\sqrt{\Omega}\Psi(\boldsymbol{r},\sigma)} \\
&= -\frac{e}{mc}\boldsymbol{A}(\boldsymbol{r})\hat{n}(\boldsymbol{r})
\end{aligned}$$

In particular, we note that

$$\begin{aligned}
\widehat{\boldsymbol{J}}(\boldsymbol{r}) &= \frac{1}{2m}\sum_{\sigma}\left\{\left(i\nabla\Psi^\dagger(\boldsymbol{r},\sigma)\right)\Psi(\boldsymbol{r},\sigma)-\Psi^\dagger(\boldsymbol{r},\sigma)\left(i\nabla\Psi(\boldsymbol{r},\sigma)\right)\right\} \\
&\quad -\frac{e}{mc}\boldsymbol{A}(\boldsymbol{r})\sum_{\sigma}\Psi^\dagger(\boldsymbol{r},\sigma)\Psi(\boldsymbol{r},\sigma) \\
&= \frac{1}{2m}\sum_{\sigma}\left\{\left[\left(i\nabla-\frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right)\Psi^\dagger(\boldsymbol{r},\sigma)\right]\Psi(\boldsymbol{r},\sigma)+\Psi^\dagger(\boldsymbol{r},\sigma)\left(-i\nabla-\frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right)\Psi(\boldsymbol{r},\sigma)\right\}
\end{aligned}$$

In order to determine the Fourier transform of $\widehat{\boldsymbol{J}}_a(\boldsymbol{r})$, let's take the result

$$\widehat{\boldsymbol{J}}_a(\boldsymbol{r}) = \frac{1}{2m\Omega}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma}e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}}\left(\boldsymbol{k}_1+\boldsymbol{k}_2\right)c^\dagger_{\boldsymbol{k}_1,\sigma}c_{\boldsymbol{k}_2,\sigma}$$

so

$$\begin{aligned}\widehat{\boldsymbol{J}}_a(\boldsymbol{q}) &= \int d^3\boldsymbol{r} e^{-i\boldsymbol{q}\boldsymbol{r}}\widehat{\boldsymbol{J}}_a(\boldsymbol{r}) \\ &= \frac{1}{2m\Omega}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\sigma}\underbrace{\int d\boldsymbol{r} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1-\boldsymbol{q})\cdot\boldsymbol{r}}}_{\Omega\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2-\boldsymbol{q}}}\left(\boldsymbol{k}_1+\boldsymbol{k}_2\right)c^{\dagger}_{\boldsymbol{k}_1,\sigma}c_{\boldsymbol{k}_2,\sigma} \\ &= \frac{1}{2m}\sum_{\boldsymbol{k}}\sum_{\sigma}(2\boldsymbol{k}-\boldsymbol{q})c^{\dagger}_{\boldsymbol{k}-\boldsymbol{q},\sigma}c_{\boldsymbol{k},\sigma}\end{aligned}$$

Finally, we can readily evaluate the current in the three proposed states. First, we can notice that the momentum is a good quantum number for all states, such that

$$\langle\widehat{\boldsymbol{J}}_a(\boldsymbol{q})\rangle = 0 \text{ for } \vec{q} \neq 0.$$

1. This state has all orbitals occupied, it should be an insulator. Indeed,

$$\langle\widehat{\boldsymbol{J}}_a(\boldsymbol{0})\rangle = \frac{1}{m}\sum_{\boldsymbol{k}\in\mathrm{BZ}}\boldsymbol{k} = 0$$

because the integral vanishes over the full Brillouin zone.

2. This state is a gapless metallic state, but no electric field has been applied to it: it is at rest. We therefore do not expect any spontaneous current. This is straightforward using that the integration domain is symmetric under $k \leftrightarrow -k$.

3. Now the Fermi sea has been shifted by $\boldsymbol{q}$: there should be a global movement of the electrons, and therefore a finite current. Each electron should contribute a momentum $\vec{q}$ in average.

$$\langle\widehat{\boldsymbol{J}}_a(\boldsymbol{0})\rangle = \frac{1}{m}\sum_{|\boldsymbol{k}|<k_F}\boldsymbol{k}+\boldsymbol{q} = 0$$

$$\langle\widehat{\boldsymbol{J}}_a(\boldsymbol{0})\rangle = \frac{N_e\boldsymbol{q}}{m}.$$