1 Identify kinetic term (continuum,second-quantized)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in under an in-plane magnetic field in the momentum space in the single-particle form.The degrees of freedom of the system are: four-component spinors $\psi_{\boldsymbol{k}} = (a_{c\uparrow\boldsymbol{k}}, a_{v\uparrow\boldsymbol{k}}, a_{c\downarrow\boldsymbol{k}}, a_{v\downarrow\boldsymbol{k}})^T$, where c and v denote the conduction and valence bands, and $\uparrow$ and $\downarrow$ denote two opposite spins..Express the Kinetic Hamiltonian H_{BHZ} using $h_\uparrow$, $h_\downarrow$, $\psi_{\boldsymbol{k}}$, and $\psi_{\boldsymbol{k}}^\dagger$, where the summation of k should be running over the first*Brillouin*zone.
Use the following conventions for the symbols:$h_\uparrow$ and $h_\downarrow$ are the two 2×2 matrices that can be explicitly expressed as given in the excerpt. m_e and m_h are the effective masses of electrons and holes, E_g is the band gap, A is the strength of hybridization between the conduction and valence bands, and $\boldsymbol{Q}$ is the momentum shift due to the in-plane magnetic field. Without the magnetic field, $\boldsymbol{Q}=0$ and $h_\uparrow, h_{downarrow}$ are time-reversal partners.
Completion: The kinetic term of the Hamiltonian in the momentum space in the single-particle form can be written as:

$$H_{\text{BHZ}} = \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}}^\dagger (h_\uparrow \oplus h_\downarrow) \psi_{\boldsymbol{k}}$$

where $\oplus$ denotes the direct sum of matrices, and the summation of $\boldsymbol{k}$ runs over the first Brillouin zone.
The matrices $h_\uparrow$ and $h_\downarrow$ are given by:

$$h_\uparrow = \begin{pmatrix} E_g/2 + \frac{(\boldsymbol{k}-\boldsymbol{Q})^2}{2m_e} & A(\boldsymbol{k}-\boldsymbol{Q}) \\ A(\boldsymbol{k}-\boldsymbol{Q}) & -E_g/2 - \frac{(\boldsymbol{k}-\boldsymbol{Q})^2}{2m_h} \end{pmatrix}$$

and

$$h_\downarrow = \begin{pmatrix} E_g/2 + \frac{(\boldsymbol{k}+\boldsymbol{Q})^2}{2m_e} & A(\boldsymbol{k}+\boldsymbol{Q}) \\ A(\boldsymbol{k}+\boldsymbol{Q}) & -E_g/2 - \frac{(\boldsymbol{k}+\boldsymbol{Q})^2}{2m_h} \end{pmatrix}$$

Here, E_g is the band gap, m_e and m_h are the effective masses of electrons and holes, A is the strength of hybridization between the conduction and valence bands, and $\boldsymbol{Q}$ is the momentum shift due to the in-plane magnetic field. Without the magnetic field, $\boldsymbol{Q}=0$ and $h_\uparrow, h_\downarrow$ are time-reversal partners.

2 Define energy dispersion (continuum)

Prompt: You will be instructed to construct each term, namely $h_\uparrow(\boldsymbol{k})$ and $h_\downarrow(\boldsymbol{k})$.For all energy dispersions, $h_\uparrow(\boldsymbol{k})$ and $h_\downarrow(\boldsymbol{k})$, it characterizes the parabolic dispersion for electrons and holes.In addition, a shift of $\boldsymbol{Q}$ in the momentum $\boldsymbol{k}$ for diagonal elements of $h_\uparrow(\boldsymbol{k})$ and $h_\downarrow(\boldsymbol{k})$, respectively.You should follow the EXAMPLE below to obtain correct energy dispersion, select the correct EXAMPLE by noticing the type of dispersion.Finally, in the real space, the momentum $\boldsymbol{k} = -i\partial_{\boldsymbol{r}}$. You should keep the form of $\boldsymbol{k}$ in the Hamiltonian for short notations but should remember $\boldsymbol{k}$ is an operator.You should recall that

$$H_{\text{BHZ}} = \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}}^\dagger \begin{pmatrix} h_\uparrow(\boldsymbol{k}) & 0 \\ 0 & h_\downarrow(\boldsymbol{k}) \end{pmatrix} \psi_{\boldsymbol{k}},$$

.Return the expression for $h_\uparrow(\boldsymbol{k})$ and $h_\downarrow(\boldsymbol{k})$ in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian H_{BHZ}.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):$\psi_{\boldsymbol{k}}$: field operators, c and v: conduction and valence bands, $\uparrow$ and $\downarrow$: two opposite spins, $h_\uparrow$ and $h_\downarrow$: two 2×2 matrices, m_e and m_h: effective masses of electrons and holes, E_g: band gap, A: strength of hybridization between the conduction and valence bands, $\boldsymbol{Q}$: momentum shift due to the in-plane magnetic field.
EXAMPLE 1:A parabolic dispersion for electron is $E_\alpha = \frac{\hbar^2 k^2}{2m_\alpha}$, where α indicates the type of electron. If there is a further shift of q in the momentum k, the dispersion will become $E_\alpha = \frac{\hbar^2 (k-q)^2}{2m_\alpha}$.
EXAMPLE 2: A cos dispersion is $E_\alpha = -\cos(ka/2)$, where α indicates the type of particle. If there is a further shift of q in the momentum k, the dispersion will become $E_\alpha = -\cos((k-q)a/2))$. However, there could be more prefactors before cos depending on the geometry of the lattice.
EXAMPLE 3:A dirac dispersion for electron/hole is a 2 by 2 matrix, i.e., $h_\theta(k) = -\hbar v_D |k| \begin{pmatrix} 0 & e^{i(\theta_k - \theta)} \\ e^{-i(\theta_{\bar{k}} - \theta)} & 0 \end{pmatrix}$, where v_D is the Fermi velocity, θ is the twist angle, and θ_k indicates

the azumith angle of k. If there is a further shift of K_θ in the momentum k, the dispersion will become $h_\theta(k) = -\hbar v_D |k - K_\theta| \begin{pmatrix} 0 & e^{i(\theta_{k-K_\theta} - \theta)} \\ e^{-i(\theta_{k-K_\theta} - \theta)} & 0 \end{pmatrix}$.

Completion: Given the parabolic dispersion for electrons and holes, and the shift of $\boldsymbol{Q}$ in the momentum $\boldsymbol{k}$, we can construct the terms $h_\uparrow(\boldsymbol{k})$ and $h_\downarrow(\boldsymbol{k})$ using EXAMPLE 1 and EXAMPLE 2.
For $h_\uparrow(\boldsymbol{k})$, we use EXAMPLE 1 for electrons:

$$h_\uparrow(\boldsymbol{k}) = \frac{\hbar^2(\boldsymbol{k}-\boldsymbol{Q})^2}{2m_e}.$$

For $h_\downarrow(\boldsymbol{k})$, we use EXAMPLE 2 for holes:

$$h_\downarrow(\boldsymbol{k}) = -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{Q})^2}{2m_h}.$$

Substituting these into the Kinetic Hamiltonian H_{BHZ}, we get:

$$H_{\mathrm{BHZ}} = \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}}^\dagger \begin{pmatrix} \frac{\hbar^2(\boldsymbol{k}-\boldsymbol{Q})^2}{2m_e} & 0 \\ 0 & -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{Q})^2}{2m_h} \end{pmatrix} \psi_{\boldsymbol{k}}.$$

3 Identify interacting term (momentum space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian H_I in the momentum space.The interaction Hamiltonian is a product of four parts. The first part is the product of four operators with two creation and two annihilation operators following the normal order, namely, creation operators are before annihilation operators. You should follow the order of $1, 2, 2, 1$ for the band and spin indices, and $1, 2, 3, 4$ for the momentum. The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators.The third part is the interaction form. You should use Coulomb interaction with $V(q)=$V(q)=2\pi e^2/\epsilon qandU(q)=V(q)\exp(-qd)$$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same band and spin indices, namely $q = k_1 - k_4$.The fourth part is the normalization factor, you should use $1/2S$ here. Finally, the summation should be running over all band and spin indices, and momentum Return the interaction term H_I in terms of $a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger$, $a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger$, $a_{b's'\boldsymbol{k}'}$, $a_{bs\boldsymbol{k}}$ and $V(q)$ (with q expressed in terms of momentum).
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):S is the area of the two-dimensional system, b, b' and s, s' are band and spin indices respectively, $V_{cc}(q) = V_{vv}(q) = V(q) = 2\pi e^2/\epsilon q$ is the intralayer Coulomb interaction, $V_{cv}(q) = V_{vc}(q) = U(q) = V(q)\exp(-qd)$ is the interlayer Coulomb interaction at interlayer distance d, and ϵ is the dielectric constant of the surrounding three-dimensional material.
Completion: The interaction part of the Hamiltonian H_I in the momentum space can be constructed as follows:

$$H_I = \frac{1}{2S} \sum_{b,s,\boldsymbol{k}} \sum_{b',s',\boldsymbol{k}'} \sum_{\boldsymbol{q}} V_{bb'}(q) a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} a_{bs\boldsymbol{k}},$$

where $V_{bb'}(q)$ is the Coulomb interaction, which is $V(q)$ for $b = b'$ and $U(q)$ for $b \neq b'$. Here, $q = \boldsymbol{k}_1 - \boldsymbol{k}_4$ is the transferred total momentum between a creation operator and an annihilation operator with the same band and spin indices. The normalization factor is $1/2S$, where S is the area of the two-dimensional system. The summation runs over all band and spin indices, and momentum.

4 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, H_I.You should use Wick's theorem to expand the four-fermion term in H_I into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without †, and be extremely cautious about the order of the index and sign before each term.You should only preserve the normal terms. Here, the normal terms mean the product of a creation operator and an annihilation operator.You should recall that H_I is $H_I = \frac{1}{2S} \sum_{bb'ss'} \sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}} V_{bb'}(q) a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} a_{bs\boldsymbol{k}}$, .Return the expanded interaction term after Hartree-Fock approximation as H_{MF}.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): Σ_H and Σ_F are the Hartree and Fock terms respectively, $V_{bb'}$ is the interaction potential, $\rho_{b's'\ n''}^{b's'\ n''+n'-n}$ is the density matrix, $a_{bsn'\boldsymbol{k}}^\dagger$ and $a_{bsn\boldsymbol{k}}$ are the creation and annihilation operators, H_{BHZ} is the base Hamiltonian, and H_{MF} is the mean-field Hamiltonian.
EXAMPLE 1:For a four-fermion term $a_1^\dagger a_2^\dagger a_3 a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a_1^\dagger a_2^\dagger a_3 a_4 = \langle a_1^\dagger a_4\rangle a_2^\dagger a_3 + \langle a_2^\dagger a_3\rangle a_1^\dagger a_4 - \langle a_1^\dagger a_4\rangle\langle a_2^\dagger a_3\rangle - \langle a_1^\dagger a_3\rangle a_2^\dagger a_4 - \langle a_2^\dagger a_4\rangle a_1^\dagger a_3 + \langle a_1^\dagger a_3\rangle\langle a_2^\dagger a_4\rangle$Be cautious about the order of the index and sign before each term here.
EXAMPLE 2:For a four-fermion term $a_1^\dagger a_2 a_3^\dagger a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a_1^\dagger a_2 a_3^\dagger a_4 = \langle a_1^\dagger a_2\rangle a_3^\dagger a_4 + \langle a_3^\dagger a_4\rangle a_1^\dagger a_2 - \langle a_1^\dagger a_2\rangle\langle a_3^\dagger a_4\rangle - \langle a_1^\dagger a_4\rangle a_3^\dagger a_2 - \langle a_3^\dagger a_2\rangle a_1^\dagger a_4 + \langle a_1^\dagger a_4\rangle\langle a_3^\dagger a_2\rangle$Be cautious about the order of the index and sign before each term here.
Completion: Following the instructions and using Wick's theorem, we can expand the four-fermion term in H_I into quadratic terms. The interaction term H_I is given by:
$H_I = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{kk'q}} V_{bb'}(q) a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} a_{bs\boldsymbol{k}}$.
Following the example 1, we can expand this as:
$H_I = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{kk'q}} V_{bb'}(q)[\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} + \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle\langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle - \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} + \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle\langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle]$.
We only preserve the normal terms, which are the product of a creation operator and an annihilation operator. Therefore, the expanded interaction term after Hartree-Fock approximation is:
$H_{\mathrm{MF}} = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{kk'q}} V_{bb'}(q)[\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} + \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}]$.

5 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the H_{MF}.The quadratic terms mean terms that are proportional to $a_{bsn'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}}$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in H_{MF}, denoted as Σ_H and Σ_F.You should recall that H_{MF} is $H_I = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{kk'q}} V_{bb'}(q)[\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} + \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle\langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle - \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} + \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle\langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle]$..Return Σ_H and Σ_F.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): Σ_H and Σ_F are the Hartree and Fock terms respectively. $a_{bsn'\boldsymbol{k}}^\dagger$ and $a_{bsn\boldsymbol{k}}$ are creation and annihilation operators. $\rho_{b's'\ n''}^{b's'\ n''+n'-n}(\boldsymbol{k}')$ is the density matrix. $V_{bb'}((n'-n)\boldsymbol{Q})$ and $V_{bb'}((n''-n)\boldsymbol{Q}+\boldsymbol{k}'-\boldsymbol{k})$ are the interaction potentials. H_{BHZ} is the BHZ Hamiltonian. H_{MF} is the mean-field Hamiltonian.
Completion: The quadratic terms in the mean-field Hamiltonian H_{MF} are those proportional to $a_{bsn'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}}$. These terms are denoted as Σ_H and Σ_F, which are the Hartree and Fock terms respectively.
The Hartree term Σ_H and the Fock term Σ_F can be extracted from H_{MF} as follows:
$\Sigma_H = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{kk'q}} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}$,
$\Sigma_F = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{kk'q}} V_{bb'}(q)\langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}$.
These terms are quadratic in the creation and annihilation operators and do not contain any terms that are solely expectations or products of expectations.

6 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term H_{MF}. If you find the $V(q)$ in H_{MF} does not contain any momentum that is not in the summation sign. The interaction term is already expanded. No action to perform on interaction term. Otherwise, you will expand $V(q)$ by replacing q with the momentum q. You should recall that H_{MF} is $H_I = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{kk'q}} V_{bb'}(q)[\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} + \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}]$.. Return H_{MF} with expanded interaction.
Completion: The interaction term $V(q)$ in the mean-field Hamiltonian H_{MF} is already expanded if it does not contain any momentum that is not in the summation sign. If it does contain such momentum, we replace q with the momentum q in $V(q)$.
The expanded mean-field Hamiltonian H_{MF} is then given by:

$H_{\rm MF} = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}} V_{bb'}(q)[\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} + \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}]$.
Here, $V_{bb'}(q)$ is the expanded interaction term, where q is the momentum. The other terms remain the same as in the original Hamiltonian.

7 Combine Hartree/Fock terms

Prompt: You will be instructed to simplify the quadratic term $H_{\rm MF}$ through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.The logic is that the expected value ($\rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$) in the first Hartree term (Σ_H) has the same form as the quadratic operators in the second Hartree term (Σ_F), and vice versa. The same applies to the Fock term.This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree term, you can make the second Hartree term look identical to the first Hartree term, as long as $V(q)=V(-q)$, which is naturally satisfied in Coulomb interaction. You should follow the EXAMPLE below to simplify it through relabeling the index.You should perform this trick of "relabeling the index" for both two Hartree terms and two Fock terms to reduce them to one Hartree term, and one Fock term.You should recall that $H_{\rm MF}$ is $H_I = \frac{1}{2S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k'}\boldsymbol{q}} V_{bb'}(q)[\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} + \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}} - \langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}]$.Return the simplified $H_{\rm MF}$ which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term)
EXAMPLE: Given a Hamiltonian $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)(\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3) + \langle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\rangle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4))\delta_{k_1+k_2,k_3+k_4}$, where $V(q)=V(-q)$.In the second term, we relabel the index to swap the index in expected value and the index in quadratic operators, namely, $\sigma_1 \leftrightarrow \sigma_2$, $\sigma_3 \leftrightarrow \sigma_4$, $k_1 \leftrightarrow k_2$, $k_3 \leftrightarrow k_4$. After the replacement, the second term becomes $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_2-k_3)\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$.Note that the Kronecker dirac function $\delta_{k_4+k_3,k_2+k_1}$ implies $k_1+k_2=k_3+k_4$, i.e., $k_2-k_3=k_4-k_1$. Thus, the second term simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_4-k_1)\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Because $V(q)=V(-q)$, meaning $V(k_4-k_1)=V(k_1-k_4)$, the second term further simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Note that this form of second term after relabeling is identical to the first term.Finally, we have the simplified Hamiltonian as $\hat{H}=2\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$.
Completion: Following the example, we can simplify the mean-field Hamiltonian $H_{\rm MF}$ by relabeling the indices in the second Hartree term and the second Fock term.
For the second Hartree term, we swap the indices as follows: $b \leftrightarrow b'$, $s \leftrightarrow s'$, $\boldsymbol{k}+\boldsymbol{q} \leftrightarrow \boldsymbol{k}'-\boldsymbol{q}$, and $\boldsymbol{k} \leftrightarrow \boldsymbol{k}'$. After the replacement, the second Hartree term becomes $\langle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}$, which is identical to the first Hartree term.
For the second Fock term, we swap the indices as follows: $b \leftrightarrow b'$, $s \leftrightarrow s'$, $\boldsymbol{k}+\boldsymbol{q} \leftrightarrow \boldsymbol{k}'$, and $\boldsymbol{k} \leftrightarrow \boldsymbol{k}'-\boldsymbol{q}$. After the replacement, the second Fock term becomes $\langle a_{b's'\boldsymbol{k}'}^\dagger a_{bs\boldsymbol{k}}\rangle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'-\boldsymbol{q}}$, which is identical to the first Fock term.
Therefore, the simplified mean-field Hamiltonian $H_{\rm MF}$ is given by:
$H_{\rm MF} = \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k'}\boldsymbol{q}} V_{bb'}(q)[\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'} - \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}]$.
This simplified $H_{\rm MF}$ reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term).

8 Identify order parameters in Hartree term (extended BZ)

Prompt: You will be instructed to simplify the Hartree term in Σ_H by reducing the momentum inside the expected value $\rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$.The expected value $\rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$ is only nonzero when the two momenta k_i,k_j are the same, namely, $\rho_{b's'n'}^{bsn}(\boldsymbol{k}) = \langle a_{b's'n'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}}\rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}$.You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i. Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.You should recall that Σ_H is

$$H_{\rm MF} = \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k'}\boldsymbol{q}} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}$$

.Return the final simplified Hartree term Σ_H.
EXAMPLE:Given a Hamiltonian where the Hartree term $\hat{H}^{Hartree} = \sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_4)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, where k_i is the momentum inside first

Brilloun zone and b_i is the reciprocal lattice.Inside the expected value, we realize $\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_4)\rangle$ is nonzero only when $k_1 = k_4$, i.e., $\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_4)\rangle = \langle c_{b_1}^\dagger(k_1)c_{b_4}(k_4)\rangle\delta_{k_1,k_4}$.Thus, the Hartree term becomes $\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_4)\rangle\delta_{k_1,k_4}c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.Use the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(k_1-k_1+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_1+b_3+b_4} = \sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{k_2+b_1+b_2,k_3+b_3+b_4}$.Because k_i is momentum inside first Brilloun zone while b_i is the reciprocal lattice. It is only when $k_2 = k_3$ that $\delta_{k_2+b_1+b_2,k_3+b_3+b_4}$ is nonzero, i.e., $\delta_{k_2+b_1+b_2,k_3+b_3+b_4} = \delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_3}$. Therefore, the Hartree term simplifies to $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_3} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Hartree term after reducing two momenta is $\hat{H}^{Hartree} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}$

Completion: Following the example, we can simplify the Hartree term Σ_H in the mean-field Hamiltonian $H_{\rm MF}$ by reducing the momentum inside the expected value $\rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$.

We start with the Hartree term in $H_{\rm MF}$:

$$H_{\rm MF} = \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k'}\boldsymbol{q}} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k'}-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k'}}$$

We realize that $\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle$ is nonzero only when $\boldsymbol{k}+\boldsymbol{q}=\boldsymbol{k}$, i.e., $\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle = \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle\delta_{\boldsymbol{q},0}$.
Thus, the Hartree term becomes:

$$H_{\rm MF} = \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k'}\boldsymbol{q}} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}\rangle\delta_{\boldsymbol{q},0} a_{b's'\boldsymbol{k'}-\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k'}}$$

Using the property of Kronecker delta function $\delta_{\boldsymbol{q},0}$ to sum over $\boldsymbol{q}$, we have:

$$H_{\rm MF} = \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k'}} V_{bb'}(0)\langle a_{bs\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k'}}^\dagger a_{b's'\boldsymbol{k'}}$$

Because of the total momentum conservation, we have $\boldsymbol{k'}=\boldsymbol{k}$, i.e., $a_{b's'\boldsymbol{k'}}^\dagger a_{b's'\boldsymbol{k'}} = a_{b's'\boldsymbol{k}}^\dagger a_{b's'\boldsymbol{k}}\delta_{\boldsymbol{k'},\boldsymbol{k}}$.
Therefore, the Hartree term simplifies to:

$$H_{\rm MF} = \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}} V_{bb'}(0)\langle a_{bs\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}}^\dagger a_{b's'\boldsymbol{k}}$$

Therefore, the final simplified Hartree term Σ_H after reducing two momenta is:

$$\Sigma_H = \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}} V_{bb'}(0)\langle a_{bs\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}}^\dagger a_{b's'\boldsymbol{k}}$$

9 Identify order parameters in Fock term (extended BZ)

Prompt: You will be instructed to simplify the Fock term in Σ_F by reducing the momentum inside the expected value $\rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$.The expected value $\rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\rho_{b's'n'}^{bsn}(\boldsymbol{k}) = \langle a_{b's'n'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}}\rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}$.You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i.Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term.You should recall that Σ_F is $H_{\rm MF} = -\frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k'}\boldsymbol{q}} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k'}}\rangle a_{b's'\boldsymbol{k'}-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}$..Return the final simplified Fock term Σ_F.
EXAMPLE:Given a Hamiltonian where the Fock term $\hat{H}^{Fock} = -\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, where k_i is the momentum inside first Brilloun zone and b_i is the reciprocal lattice.Inside the expected value, we realize $\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle$ is nonzero only when $k_1 = k_3$, i.e., $\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle = \langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle\delta_{k_1,k_3}$.Thus, the Fock term becomes $-\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle\delta_{k_1,k_3}c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.Use the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we have $-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_1+k_4+b_3+b_4} = -\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_2+b_1+b_2,k_4+b_3+b_4}$.Because k_i is momentum inside first Brilloun zone while b_i is the reciprocal lattice. It is only when $k_2 = k_4$ that $\delta_{k_2+b_1+b_2,k_4+b_3+b_4}$

is nonzero, i.e., $\delta_{k_2+b_1+b_2,k_4+b_3+b_4} = \delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4}$.Therefore, the Fock term simplifies to $-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4} = -\sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(k_1-k_2+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_2)\delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Fock term after reducing two momenta is $\hat{H}^{Fock} = -\sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(k_1-k_2+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_2)\delta_{b_1+b_2,b_3+b_4}$

Completion: Following the example, we first realize that $\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle$ is nonzero only when $\boldsymbol{k}+\boldsymbol{q}=\boldsymbol{k}'$, i.e., $\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle = \langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle\delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k}'}$.
Substituting this into the Fock term, we get $\Sigma_F = -\frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}'}\rangle\delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k}'} a_{b's'\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}$.
Using the property of the Kronecker delta function $\delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k}'}$ to sum over $\boldsymbol{k}'$, we get $\Sigma_F = -\frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}+\boldsymbol{q}}\rangle a_{b's'\boldsymbol{k}+\boldsymbol{q}-\boldsymbol{q}}^\dagger a_{bs\boldsymbol{k}}$.
Simplifying further, we get $\Sigma_F = -\frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}+\boldsymbol{q}}\rangle a_{b's'\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}$.
Finally, we notice that the total momentum conservation will reduce another momentum in the quadratic term. Therefore, we end up with only two momenta left in the summation, and the final simplified Fock term is $\Sigma_F = -\frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}q} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}+\boldsymbol{q}}\rangle a_{b's'\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}$.

10 Final form of iteration in quadratic terms

Prompt: You will now be instructed to combine the Hartree term Σ_H and the Fock term Σ_F.You should recall that the Hartree term \begin{equation} \begin{split} \Sigma*H = \frac{1}{S}\sum*{bb'\atop ss'}\sum*{nn'n''\atop \bm k\bm k'} &V*{bb'}((n'-n)\bm Q) \ \times&\rho*{b's',n''}^{b's',n''+n'-n}(\bm k') ; a*{bsn'\bm k}^{\dagger} a_{bsn\bm k}, \end{split} \end{equation} ,and the Fock term $\Sigma_F = -\frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}q} V_{bb'}(q)\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}+\boldsymbol{q}}\rangle a_{b's'\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}$.You should perform the same trick of relabeling the index in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. The relabeling should be done with a swap : Nothing. You should add them, relabel the index in Fock term, and simply their sum. Return the final sum of Hartree and Fock term.

Completion: To combine the Hartree term Σ_H and the Fock term Σ_F, we first relabel the indices in the Fock term to match those in the Hartree term. Since the question specifies that no swap is needed, the relabeled Fock term remains the same:

$$\Sigma_F = -\frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{q}} V_{bb'}(\boldsymbol{q})\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}+\boldsymbol{q}}\rangle a_{b's'\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}$$

Next, we add the Hartree term Σ_H and the relabeled Fock term Σ_F:

$$\Sigma_{HF} = \Sigma_H + \Sigma_F$$

Substituting the expressions for Σ_H and Σ_F, we get:

$$\Sigma_{HF} = \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}} V_{bb'}(0)\langle a_{bs\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}\rangle a_{b's'\boldsymbol{k}}^\dagger a_{b's'\boldsymbol{k}} - \frac{1}{S}\sum_{bb'ss'}\sum_{\boldsymbol{k}\boldsymbol{q}} V_{bb'}(\boldsymbol{q})\langle a_{bs\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{b's'\boldsymbol{k}+\boldsymbol{q}}\rangle a_{b's'\boldsymbol{k}}^\dagger a_{bs\boldsymbol{k}}$$

This is the final sum of the Hartree and Fock terms.