1 Identify kinetic term (lattice)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in twisted homobilayer WSe$_2$ (tWSe$_2$) in the real space in the second-quantized form.The degrees of freedom of the system are: the position of site i in a triangular lattice formed in the moir'e pattern, and the spin index sThe kinetic term is a tight-binding model composed of the following hopping process: site i and site j with the amplitude $t_s (\boldsymbol{R}_i - \boldsymbol{R}_j)$
The summation should be taken over all the position of site i in a triangular lattice formed in the moir'e pattern, and the spin index s and all real space positions.Return the Kinetic Hamiltonian H. Use the following conventions for the symbols:R_i represents the position of site i in a triangular lattice formed in the moir'e pattern, s is the spin index, and t and U are, respectively, the hopping parameter and the interaction strength. $c_{i,s}^\dagger$ is used to represent the hole operator, and $s =\uparrow$ and $\downarrow$ are locked to $+K$ and $-K$ valleys, respectively. A filling factor ν is defined as $(1/\mathcal{N}) \sum_{i,s} c_{i,s}^\dagger c_{i,s}$, which counts the number of holes per moir'e cell ($\mathcal{N}$ is the total number of moir'e sites in the system).
Completion: The kinetic term of the Hamiltonian in the second-quantized form for the twisted homobilayer WSe$_2$ (tWSe$_2$) system can be written as:

$$H = -\sum_{i,j,s} t_s (\boldsymbol{R}_i - \boldsymbol{R}_j) c_{i,s}^\dagger c_{j,s}$$

Here, $c_{i,s}^\dagger$ and $c_{j,s}$ are the creation and annihilation operators for a hole at site i and j with spin s, respectively. The sum is taken over all sites i and j in the triangular lattice formed in the moiré pattern and over all spin indices s. The term $t_s (\boldsymbol{R}_i - \boldsymbol{R}_j)$ represents the hopping amplitude between site i and site j with spin s. The negative sign in front of the sum indicates that the energy of the system decreases when a hole hops from one site to another.

2 Identify interacting term (real space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian, H_{Coulomb} in the real space in the second-quantized form.The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian H.The interaction is a density-density interaction composed of the following process: site i and site j with the interaction strength $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$. The summation should be taken over all spins s and s' and all real space positions.Return the interaction term H_{Coulomb} in terms of $n_{i,s}$.
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): R_i represents the position of site i in a triangular lattice formed in the moir'e pattern, s is the spin index, $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is the interaction strength, $n_{i,s}$ is the binary occupancy number of site i, and $c_{i,s}^\dagger$ represents the hole operator.
Completion: The interaction part of the Hamiltonian, H_{Coulomb}, in the real space in the second-quantized form can be constructed as follows:
$H_{\text{Coulomb}} = \frac{1}{2} \sum_{i,j,s,s'} U(\boldsymbol{R}_i - \boldsymbol{R}_j) n_{i,s} n_{j,s'}$
Here, $n_{i,s} = c_{i,s}^\dagger c_{i,s}$ is the number operator, representing the occupancy number of site i with spin s. The factor of 1/2 is included to avoid double counting of interactions. The summation is taken over all spins s and s' and all real space positions i and j. The interaction strength between site i and site j is given by $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$.

3 Fourier transform noninteracting term to momentum space (lattice)

Prompt: You will be instructed to convert the noninteracting Hamiltonian H_0 in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to $c_{R_i,s}^\dagger$ in the real space to the $c_{\boldsymbol{k},s}^\dagger$ in the momentum space, which is defined as $c_{\boldsymbol{k},s}^\dagger = \frac{1}{\sqrt{N}} \sum_i c_{R_i,s}^\dagger e^{ik \cdot R_i}$, where R_{\bm{i}} is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. You should recall that $H = \sum_s \sum_{i,j} t_s (\boldsymbol{R}_i - \boldsymbol{R}_j) c_{i,s}^\dagger c_{j,s}$ Express the total noninteracting Hamiltonian H_0 in terms of $c_{\boldsymbol{k},s}^\dagger$. Simplify any summation index if possible.
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): H0 is the noninteracting Hamiltonian,

$\bm{k}$ is the momentum, $\varepsilon_s(\bm{k})$ is the non-interacting band energy dispersion, and $c_{\bm{k},s}^\dagger$ is the creation operator in momentum space.

EXAMPLE: Write a Kinetic Hamiltonian $\hat{H}$ in the second quantized form in the real space, $\hat{H} = \sum_{i,j} t(R_i - R_j)c^\dagger(R_i)c(R_j)$, where i,j are summed over the entire real space. Define the Fourier transformation $c^\dagger(k) = \frac{1}{\sqrt{N}}\sum_i c^\dagger(R_i)e^{ik\cdot R_i}$, where i is integrated over the entire real space containing N unit cells, N is the number of unit cells. This leads to the inverse Fourier transformation $c^\dagger(R_i) = \frac{1}{\sqrt{N}}\sum_k c^\dagger(k)e^{-ik\cdot R_i}$, where k is first Brillouin zone. Thus, substitute $c^\dagger(R_i)$ and $c(R_j)$ into $\hat{H}$, we get

$$\hat{H} = \sum_{i,j} t(R_i - R_j)\frac{1}{\sqrt{N}}\sum_{k_1} c^\dagger(k_1)e^{-ik_1\cdot R_i}\frac{1}{\sqrt{N}}\sum_{k_2} c(k_2)e^{ik_2\cdot R_j}$$

$$= \frac{1}{N}\sum_{i,j}\sum_{k_1,k_2} c^\dagger(k_1)c(k_2)e^{-ik_1\cdot R_i}e^{ik_2\cdot R_j}t(R_i - R_j)$$

Now make a replacement by defining $n = R_i - R_j$ The Hamiltonian become

$$\hat{H} = \frac{1}{N}\sum_{i,n}\sum_{k_1,k_2} c^\dagger(k_1)c(k_2)t(n)e^{-i(k_1-k_2)\cdot R_i}e^{-ik_2\cdot n}$$

Because $\frac{1}{N}\sum_i e^{-i(k_1-k_2)\cdot R_i} = \delta(k_1,k_2)$, where $\delta(k_1,k_2)$ is the Kronecker delta function. therefore

$$\hat{H} = \sum_{k_1,k_2}\sum_n t(n)e^{-ik_2\cdot n}c^\dagger(k_1)c(k_2)\delta(k_1,k_2)$$

Using the property of Kronecker delta function and sum over k_2, we obtain

$$\hat{H} = \sum_{k_1}\sum_n t(n)e^{-ik_1\cdot n}c^\dagger(k_1)c(k_1)$$

For simplicity, we replace k_1 with k, we obtain

$$\hat{H} = \sum_k\sum_n t(n)e^{-ik\cdot n}c^\dagger(k)c(k)$$

If we define energy dispersion $E(k) = \sum_n t(n)e^{-ik\cdot n}$, where n is the summation of all hopping pairs, the Hamiltonian in the momentum space is

$$\hat{H} = \sum_k E(k)c^\dagger(k)c(k)$$

Completion: Following the example, we first apply the Fourier transformation to the creation and annihilation operators in the noninteracting Hamiltonian H_0. The Fourier transformation is defined as $c_{\bm{k},s}^\dagger = \frac{1}{\sqrt{N}}\sum_i c_{R_i,s}^\dagger e^{ik\cdot R_i}$ and its inverse is $c_{R_i,s}^\dagger = \frac{1}{\sqrt{N}}\sum_k c_{\bm{k},s}^\dagger e^{-i\bm{k}\cdot R_i}$.

Substituting these into the Hamiltonian H_0, we get:

$$H_0 = -\sum_s\sum_{i,j} t_s\left(\bm{R}_i - \bm{R}_j\right)\frac{1}{\sqrt{N}}\sum_{\bm{k}_1} c_{\bm{k}_1,s}^\dagger e^{-i\bm{k}_1\cdot R_i}\frac{1}{\sqrt{N}}\sum_{\bm{k}_2} c_{\bm{k}_2,s}e^{i\bm{k}_2\cdot R_j}$$

Simplifying, we get:

$$H_0 = -\frac{1}{N}\sum_s\sum_{i,j}\sum_{\bm{k}_1,\bm{k}_2} t_s\left(\bm{R}_i - \bm{R}_j\right)c_{\bm{k}_1,s}^\dagger c_{\bm{k}_2,s}e^{-i\bm{k}_1\cdot R_i}e^{i\bm{k}_2\cdot R_j}$$

Now, we make a replacement by defining $\bm{n} = \bm{R}_i - \bm{R}_j$, and the Hamiltonian becomes:

$$H_0 = -\frac{1}{N}\sum_s\sum_{i,n}\sum_{\bm{k}_1,\bm{k}_2} t_s(\bm{n})c_{\bm{k}_1,s}^\dagger c_{\bm{k}_2,s}e^{-i(\bm{k}_1-\bm{k}_2)\cdot R_i}e^{-i\bm{k}_2\cdot\bm{n}}$$

Because $\frac{1}{N}\sum_i e^{-i(\bm{k}_1-\bm{k}_2)\cdot R_i} = \delta(\bm{k}_1,\bm{k}_2)$, where $\delta(\bm{k}_1,\bm{k}_2)$ is the Kronecker delta function, we have:

$$H_0 = -\sum_s\sum_{\bm{k}_1,\bm{k}_2}\sum_n t_s(\bm{n})e^{-i\bm{k}_2\cdot\bm{n}}c_{\bm{k}_1,s}^\dagger c_{\bm{k}_2,s}\delta(\bm{k}_1,\bm{k}_2)$$

Using the property of the Kronecker delta function and summing over $\bm{k}_2$, we obtain:

$$H_0 = -\sum_s\sum_{\bm{k}_1}\sum_n t_s(\bm{n})e^{-i\bm{k}_1\cdot\bm{n}}c_{\bm{k}_1,s}^\dagger c_{\bm{k}_1,s}$$

For simplicity, we replace k_1 with k, and we obtain:

$$H_0 = -\sum_s \sum_{\bm{k}} \sum_{\bm{n}} t_s(\bm{n}) e^{-i\bm{k}\cdot\bm{n}} c_{\bm{k},s}^\dagger c_{\bm{k},s}$$

If we define the non-interacting band energy dispersion $\varepsilon_s(\bm{k}) = -\sum_{\bm{n}} t_s(\bm{n}) e^{-i\bm{k}\cdot\bm{n}}$, where $\bm{n}$ is the summation of all hopping pairs, the noninteracting Hamiltonian H_0 in the momentum space is:

$$H_0 = \sum_s \sum_{\bm{k}} \varepsilon_s(\bm{k}) c_{\bm{k},s}^\dagger c_{\bm{k},s}$$

4 Fourier transform interacting term to momentum space (lattice)

Prompt: You will be instructed to convert the interacting Hamiltonian, H_{Coulomb}, in the second-quantized form the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to $c_{R_i,s}^\dagger$ in the real space to the $c_{k_\alpha,s}^\dagger$ in the momentum space, which is defined as $c_{\bm{k},s}^\dagger = \frac{1}{\sqrt{N}} \sum_i c_{R_i,s}^\dagger e^{ik\cdot R_i}$, where \bm{R} is integrated over all sites in the entire real space, and \bm{q} is defined within the first Brillouin zone. You should follow the EXAMPLE below to apply the Fourier transformation.You should recall that H_{Coulomb} is $H_{\text{Coulomb}} = \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\bm{R}_i - \bm{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s}$. Express H_{Coulomb} in terms of $c_{k_\alpha,s}^\dagger$. Simplify any summation index if possible.

EXAMPLE:Write an interacting Hamiltonian $\hat{H}^{int}$ in the second quantized form in the real space, $\hat{H}^{int} = \sum_{s,s'} \sum_{i,j} U(R_i - R_j) c_s^\dagger(R_i) c_{s'}^\dagger(R_j) c_{s'}(R_j) c_s(R_i)$, where i,j are summed over the entire real space.Define the Fourier transformation $c_s^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_s^\dagger(R_i) e^{ik\cdot R_i}$, where i is integrated over the entire real space containing N unit cells, N is the number of unit cells.This leads to the inverse Fourier transformation $c_s^\dagger(R_i) = \frac{1}{\sqrt{N}} \sum_k c_s^\dagger(k) e^{-ik\cdot R_i}$, where k is summed over the first Brillouin zone.Thus, substitute $c^\dagger(R_i)$ and $c(R_j)$ into $\hat{H}^{int}$, we get

$$\hat{H}^{int} = \sum_{s,s'} \sum_{i,j} U(R_i - R_j) \frac{1}{\sqrt{N}} \sum_{k_1} c_s^\dagger(k_1) e^{-ik_1\cdot R_i} \frac{1}{\sqrt{N}} \sum_{k_2} c_{s'}^\dagger(k_2) e^{-ik_2\cdot R_j} \frac{1}{\sqrt{N}} \sum_{k_3} c_{s'}(k_3) e^{ik_3\cdot R_j} \frac{1}{\sqrt{N}} \sum_{k_4} c_s(k_4) e^{ik_4\cdot R_i}$$

$$= \sum_{s,s'} \sum_{i,j} \frac{1}{N^2} \sum_{k_1,k_2,k_3,k_4} U(R_i - R_j) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) e^{-i(k_1-k_4)\cdot R_i} e^{-i(k_2-k_3)\cdot R_j}$$

Now make a replacement by defining $n = R_i - R_j$The Hamiltonian become

$$\hat{H}^{int} = \frac{1}{N^2} \sum_{j,n} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(n) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) e^{-i(k_1-k_4)\cdot n} e^{-i(k_1-k_4+k_2-k_3)\cdot r_j}$$

Because $\frac{1}{N} \sum_i e^{-i(k_1-k_4+k_2-k_3)\cdot R_i} = \sum \delta(k_1 - k_4 + k_2 - k_3, G)$, where $\delta(..,..)$ is the Kronecker delta function, and G is the all reciprocal lattices in the momentum space.Therefore,

$$\hat{H}^{int} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} \sum_n U(n) e^{-i(k_1-k_4)\cdot n} c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(k_1 - k_4 + k_2 - k_3, G)$$

If we define interaction in the momentum space $U(k) = \sum_n U(n) e^{-ik\cdot n}$, where n is the summation of all hopping pairs, the interacting Hamiltonian in the momentum space is

$$\hat{H}^{int} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1 - k_4) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(k_1 - k_4 + k_2 - k_3, G)$$

Completion: Following the example, we first apply the Fourier transformation to the creation and annihilation operators in the interacting Hamiltonian H_{Coulomb}. Substituting these into the Hamiltonian H_{Coulomb}, we get

$$H_{\text{Coulomb}} = \frac{1}{2N^2} \sum_{s,s'} \sum_{i,j} \sum_{\bm{k}_1,\bm{k}_2,\bm{k}_3,\bm{k}_4} U(\bm{R}_i - \bm{R}_j) c_{\bm{k}_1,s}^\dagger c_{\bm{k}_2,s'}^\dagger c_{\bm{k}_3,s'} c_{\bm{k}_4,s} e^{-i(\bm{k}_1-\bm{k}_4)\cdot\bm{R}_i} e^{-i(\bm{k}_2-\bm{k}_3)\cdot\bm{R}_j}.$$

Next, we make a replacement by defining $\bm{n} = \bm{R}_i - \bm{R}_j$, and the Hamiltonian becomes

$$H_{\text{Coulomb}} = \frac{1}{2N^2} \sum_{s,s'} \sum_{\bm{n},j} \sum_{\bm{k}_1,\bm{k}_2,\bm{k}_3,\bm{k}_4} U(\bm{n}) c_{\bm{k}_1,s}^\dagger c_{\bm{k}_2,s'}^\dagger c_{\bm{k}_3,s'} c_{\bm{k}_4,s} e^{-i(\bm{k}_1-\bm{k}_4)\cdot\bm{n}} e^{-i(\bm{k}_1-\bm{k}_4+\bm{k}_2-\bm{k}_3)\cdot\bm{R}_j}.$$

Using the property of the Kronecker delta function and summing over $\boldsymbol{R}_j$, we obtain

$$H_{\text{Coulomb}} = \frac{1}{2N} \sum_{s,s'} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \sum_{\boldsymbol{n}} U(\boldsymbol{n}) e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_4)\cdot\boldsymbol{n}} c^\dagger_{\boldsymbol{k}_1,s} c^\dagger_{\boldsymbol{k}_2,s'} c_{\boldsymbol{k}_3,s'} c_{\boldsymbol{k}_4,s} \sum_{\boldsymbol{G}} \delta(\boldsymbol{k}_1 - \boldsymbol{k}_4 + \boldsymbol{k}_2 - \boldsymbol{k}_3, \boldsymbol{G}).$$

If we define the interaction in the momentum space $U(\boldsymbol{k}) = \sum_{\boldsymbol{n}} U(\boldsymbol{n}) e^{-i\boldsymbol{k}\cdot\boldsymbol{n}}$, where $\boldsymbol{n}$ is the summation of all hopping pairs, the interacting Hamiltonian H_{Coulomb} in the momentum space is

$$H_{\text{Coulomb}} = \frac{1}{2N} \sum_{s,s'} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} U(\boldsymbol{k}_1 - \boldsymbol{k}_4) c^\dagger_{\boldsymbol{k}_1,s} c^\dagger_{\boldsymbol{k}_2,s'} c_{\boldsymbol{k}_3,s'} c_{\boldsymbol{k}_4,s} \sum_{\boldsymbol{G}} \delta(\boldsymbol{k}_1 - \boldsymbol{k}_4 + \boldsymbol{k}_2 - \boldsymbol{k}_3, \boldsymbol{G}).$$

5 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, H_{Coulomb}.You should use Wick's theorem to expand the four-fermion term in H_{Coulomb} 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 $\dagger$, 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_{Coulomb} is $H_{\text{Coulomb}} = \frac{1}{2N} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} c^\dagger_{\boldsymbol{k}_\alpha,s} c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} c_{\boldsymbol{k}_\delta,s}$, where $\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} = \sum_{\boldsymbol{G}} \delta(\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta - \boldsymbol{k}_\gamma - \boldsymbol{k}_\delta, \boldsymbol{G})$ is the Kronecker delta function.Return the expanded interaction term after Hartree-Fock approximation as $H_{\text{int,MF}}$.
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):H_{int} is the interaction term, $\mathcal{N}$ is a normalization constant, s and s' are spin indices, $\boldsymbol{k}$ is the momentum vector, $U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$ is the interaction potential, $\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} = \sum_{\boldsymbol{G}} \delta(\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta - \boldsymbol{k}_\gamma - \boldsymbol{k}_\delta, \boldsymbol{G})$ is the Kronecker delta function, $c^\dagger_{\boldsymbol{k}_\alpha,s}$ and $c_{\boldsymbol{k}_\delta,s}$ are creation and annihilation operators respectively, and $\langle ... \rangle$ denotes expectation values.
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_{Coulomb} into quadratic terms. The order of the four-term product in H_{Coulomb} matches with the order in EXAMPLE 1. Therefore, we use EXAMPLE 1 as a guide to expand the four-fermion term in H_{Coulomb}.
The expanded interaction term after Hartree-Fock approximation is:
$H_{\text{int,MF}} \quad = \quad \frac{1}{2N} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} [\langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\delta,s} \rangle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} + \langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} \rangle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\delta,s} \rangle \langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} \rangle - \langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\gamma,s'} \rangle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s} \rangle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\gamma,s'} + \langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\gamma,s'} \rangle \langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s} \rangle]$
This is the expanded interaction term after Hartree-Fock approximation.

6 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the $H_{\text{int,MF}}$.The quadratic terms mean terms that are proportional to $c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'}$ and $c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s}$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in $H_{\text{int,MF}}$, denoted as $H^{(2)}_{\text{int}}$.You should recall that $H_{\text{int,MF}}$ is

$$H_{\text{Coulomb}} = \frac{1}{2\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \left[\langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\delta,s} \rangle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} + \langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} \rangle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\delta,s} \right.$$

$$\left. - \langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\delta,s} \rangle \langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} \rangle - \langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\gamma,s'} \rangle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s} \rangle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\gamma,s'} + \langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\gamma,s'} \rangle \langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s} \rangle \right],$$

where $\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} = \sum_{\boldsymbol{G}} \delta(\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta - \boldsymbol{k}_\gamma - \boldsymbol{k}_\delta, \boldsymbol{G})$ .Return $H^{(2)}_{\text{int}}$.
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):H_{int} is the interaction Hamiltonian, $\mathcal{N}$ is a normalization factor, s and s' are spin indices, $\boldsymbol{k}$ is the momentum vector, $U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$ is the interaction

potential, $\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta}$ is the Kronecker delta function, $c^\dagger_{\boldsymbol{k}_\alpha,s}$ and $c_{\boldsymbol{k}_\delta,s}$ are creation and annihilation operators, and $\langle...\rangle$ denotes expectation values.

Completion: The quadratic terms in $H_{\text{int,MF}}$ that are proportional to $c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'}$ and $c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s}$, excluding terms that are solely expectations or products of expectations, are given by:

$$H^{(2)}_{\text{int}} = \frac{1}{2\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \left[\langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s}\rangle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'} + \langle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'}\rangle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'}\rangle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s} \right.$$
$$\left. - \langle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s}\rangle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'} \right]$$

This is the desired $H^{(2)}_{\text{int}}$.

7 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $H^{(2)}_{\text{int}}$. If you find the $V(q)$ in $H^{(2)}_{\text{int}}$ 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 $\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta$. You should recall that $H^{(2)}_{\text{int}} = \frac{1}{2\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \left[\langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s}\rangle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'} + \langle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'}\rangle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'}\rangle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s}\rangle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'} \right]$, where $\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} = \sum_{\boldsymbol{G}} \delta(\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta - \boldsymbol{k}_\gamma - \boldsymbol{k}_\delta, \boldsymbol{G})$. Return $H^{(2)}_{\text{int}}$ with expanded interaction.

Completion: The interaction term $U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$ in $H^{(2)}_{\text{int}}$ does not contain any momentum that is not in the summation sign. Therefore, the interaction term is already expanded and no further action is required. The expanded interaction term remains as $U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$.

So, the $H^{(2)}_{\text{int}}$ with expanded interaction is:

$$H^{(2)}_{\text{int}} = \frac{1}{2\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \left[\langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s}\rangle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'} + \langle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'}\rangle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'}\rangle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s} \right.$$
$$\left. - \langle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s}\rangle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'} \right].$$

8 Relabel the index

Prompt: You will be instructed to simplify the quadratic term $H^{(2)}_{\text{int}}$ through relabeling the index.The logic is that the expected value ($\langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s}\rangle$ and $\langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'}\rangle$) in the first Hartree term ($c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'}$) has the same form as the quadratic operators in the second Hartree term ($c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s}$), and vice versa. The same applies to the Fock term.Namely, a replacement of $\boldsymbol{k}_\alpha, \leftrightarrow \boldsymbol{k}_\beta$ and $\boldsymbol{k}_\gamma \leftrightarrow \boldsymbol{k}_\delta$ is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes nothings in this case.This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree or Fock term, you can make the second Hartree or Fock term look identical to the first Hartree or Fock 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 recall that $H^{(2)}_{\text{int}}$ is $H^{(2)}_{\text{int}} = \frac{1}{2\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \left[\langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s}\rangle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'} + \langle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\gamma,s'}\rangle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'}\rangle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s} - \langle c^\dagger_{\boldsymbol{k}_\beta,s'}c_{\boldsymbol{k}_\delta,s}\rangle c^\dagger_{\boldsymbol{k}_\alpha,s}c_{\boldsymbol{k}_\gamma,s'} \right]$, where $\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} = \sum_{\boldsymbol{G}} \delta(\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta - \boldsymbol{k}_\gamma - \boldsymbol{k}_\delta, \boldsymbol{G})$ Return the simplified $H^{(2)}_{\text{int}}$.

EXAMPLE:Given a Hamiltonian $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)(\langle c^\dagger_{d,\sigma_1}(k_1)c_{d,\sigma_4}(k_4)\rangle c^\dagger_{p,\sigma_2}(k_2)c_{p,\sigma_3}(k_3) + \langle c^\dagger_{p,\sigma_2}(k_2)c_{d,\sigma_3}(k_3)\rangle c^\dagger_{d,\sigma_1}(k_1)c_{\sigma_4}(k_4))\delta_{k_1+k_2,k_3+k_4}$, 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, $\sigma_1 \leftrightarrow \sigma_2$, $\sigma_3 \leftrightarrow \sigma_4$, $k_1 \leftrightarrow k_2$, $k_3 \leftrightarrow k_4$. Important: d and p cannot be swapped because they are not indices in the summation.After the replacement, the second term becomes $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_2 - k_3)\langle c^\dagger_{p,\sigma_1}(k_1)c_{p,\sigma_4}(k_4)\rangle c^\dagger_{d,\sigma_2}(k_2)c_{d,\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$.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 $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_4 - k_1)\langle c^\dagger_{p,\sigma_1}(k_1)c_{p,\sigma_4}(k_4)\rangle c^\dagger_{d,\sigma_2}(k_2)c_{d,\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Because $V(q) = V(-q)$, meaning $V(k_4 - k_1) = V(k_1 - k_4)$, the second term further simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)\langle c^\dagger_{p,\sigma_1}(k_1)c_{p,\sigma_4}(k_4)\rangle c^\dagger_{d,\sigma_2}(k_2)c_{d,\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$.Finally, we have the simplified Hamiltonian as $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)(\langle c^\dagger_{d,\sigma_1}(k_1)c_{d,\sigma_4}(k_4)\rangle c^\dagger_{p,\sigma_2}(k_2)c_{p,\sigma_3}(k_3) + \langle c^\dagger_{p,\sigma_1}(k_1)c_{p,\sigma_4}(k_4)\rangle c^\dagger_{d,\sigma_2}(k_2)c_{d,\sigma_3}(k_3))\delta_{k_4+k_3,k_2+k_1}$.

Completion: Following the logic and example provided, we can simplify the quadratic term $H^{(2)}_{\text{int}}$ by relabeling the index. We swap the indices in the expected value and the quadratic operators in the

second Hartree and Fock terms. Specifically, we replace $\boldsymbol{k}_\alpha \leftrightarrow \boldsymbol{k}_\beta$ and $\boldsymbol{k}_\gamma \leftrightarrow \boldsymbol{k}_\delta$ in the second Hartree and Fock terms.

After the replacement, the second Hartree term becomes $\langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} \rangle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\delta,s}$ and the second Fock term becomes $\langle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s} \rangle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\gamma,s'}$.

The Kronecker delta function $\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta}$ implies $\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta = \boldsymbol{k}_\gamma + \boldsymbol{k}_\delta$, i.e., $\boldsymbol{k}_\beta - \boldsymbol{k}_\gamma = \boldsymbol{k}_\delta - \boldsymbol{k}_\alpha$. Thus, the interaction potential $U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$ in the second Hartree and Fock terms can be replaced by $U(\boldsymbol{k}_\beta - \boldsymbol{k}_\gamma)$. Because $U(q) = U(-q)$, meaning $U(\boldsymbol{k}_\beta - \boldsymbol{k}_\gamma) = U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$, the simplified $H^{(2)}_{\text{int}}$ is:

$$H^{(2)}_{\text{int}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \left[\langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\delta,s} \rangle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} - \langle c^\dagger_{\boldsymbol{k}_\alpha,s} c_{\boldsymbol{k}_\gamma,s'} \rangle c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\delta,s} \right].$$

9 Identify order parameters in Hartree term (extended BZ)

Prompt: You will be instructed to simplify the Hartree term in H_{Hartree} by reducing the momentum inside the expected value $\langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\delta,\boldsymbol{q}_\delta,s} \rangle$.The expected value $\langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\delta,\boldsymbol{q}_\delta,s} \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\delta,\boldsymbol{q}_\delta,s} \rangle = \langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\delta,\boldsymbol{q}_\delta,s} \rangle \delta_{c_{\boldsymbol{p}_\alpha,\boldsymbol{p}_\delta}}$.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 H_{Hartree} is $H_{\text{Hartree}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{p}_\alpha + \boldsymbol{q}_\alpha - \boldsymbol{p}_\delta - \boldsymbol{q}_\delta) \delta_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha+\boldsymbol{p}_\beta+\boldsymbol{q}_\beta,\boldsymbol{p}_\gamma+\boldsymbol{q}_\gamma+\boldsymbol{p}_\delta+\boldsymbol{q}_\delta} \langle c^\dagger_{\boldsymbol{q}_\alpha,s}(\boldsymbol{p}_\alpha) c_{\boldsymbol{q}_\delta,s}(\boldsymbol{p}_\delta) \rangle c^\dagger_{\boldsymbol{q}_\beta,s'}(\boldsymbol{p}_\beta) c_{\boldsymbol{q}_\gamma,s'}(\boldsymbol{p}_\gamma)$..Return the final simplified Hartree term H_{Hartree}.

EXAMPLE:Given a Hamiltonian where the Hartree term $\hat{H}^{Hartree} = \sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, where k_i is the momentum inside first Brilloun zone and b_i is the reciprocal lattice.Inside the expected value, we realize $\langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle$ is nonzero only when $k_1 = k_4$, i.e., $\langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle = \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle \delta_{k_1,k_4}$.Thus, the Hartree term becomes $\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle \delta_{k_1,k_4} c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.Use the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have

$$\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(k_1 - k_1 + b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_1) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{k_1+k_2+b_1+b_2,k_3+k_1+b_3+b_4}$$
$$= \sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_1) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{k_2+b_1+b_2,k_3+b_3+b_4}.$$

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 $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_1) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{b_1+b_2,b_3+b_4} \delta_{k_2,k_3} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_1) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_2) \delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Hartree term after reducing two momenta is $\hat{H}^{Hartree} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_1) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_2) \delta_{b_1+b_2,b_3+b_4}$

Completion: The Hartree term H_{Hartree} can be simplified by reducing the momentum inside the expected value $\langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\delta,\boldsymbol{q}_\delta,s} \rangle$. This expected value is nonzero only when $\boldsymbol{p}_\alpha = \boldsymbol{p}_\delta$, i.e., $\langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\delta,\boldsymbol{q}_\delta,s} \rangle = \langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\delta,\boldsymbol{q}_\delta,s} \rangle \delta_{\boldsymbol{p}_\alpha,\boldsymbol{p}_\delta}$.

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

$H_{\text{Hartree}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{p}_\alpha + \boldsymbol{q}_\alpha - \boldsymbol{p}_\alpha - \boldsymbol{q}_\delta) \delta_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha+\boldsymbol{p}_\beta+\boldsymbol{q}_\beta,\boldsymbol{p}_\alpha+\boldsymbol{q}_\gamma+\boldsymbol{p}_\alpha+\boldsymbol{q}_\delta} \langle c^\dagger_{\boldsymbol{q}_\alpha,s}(\boldsymbol{p}_\alpha) c_{\boldsymbol{q}_\delta,s}(\boldsymbol{p}_\alpha) \rangle c^\dagger_{\boldsymbol{q}_\beta,s'}(\boldsymbol{p}_\beta) c_{\boldsymbol{q}_\gamma,s'}(\boldsymbol{p}_\gamma)$.

This simplifies to:

$H_{\text{Hartree}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{q}_\alpha - \boldsymbol{q}_\delta) \delta_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha+\boldsymbol{p}_\beta+\boldsymbol{q}_\beta,\boldsymbol{p}_\alpha+\boldsymbol{q}_\gamma+\boldsymbol{p}_\alpha+\boldsymbol{q}_\delta} \langle c^\dagger_{\boldsymbol{q}_\alpha,s}(\boldsymbol{p}_\alpha) c_{\boldsymbol{q}_\delta,s}(\boldsymbol{p}_\alpha) \rangle c^\dagger_{\boldsymbol{q}_\beta,s'}(\boldsymbol{p}_\beta) c_{\boldsymbol{q}_\gamma,s'}(\boldsymbol{p}_\gamma)$.

The total momentum conservation will reduce another momentum in the quadratic term. The Kronecker delta function $\delta_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha+\boldsymbol{p}_\beta+\boldsymbol{q}_\beta,\boldsymbol{p}_\alpha+\boldsymbol{q}_\gamma+\boldsymbol{p}_\alpha+\boldsymbol{q}_\delta}$ implies $\boldsymbol{p}_\beta + \boldsymbol{q}_\beta = \boldsymbol{p}_\gamma + \boldsymbol{q}_\gamma$, i.e., $\boldsymbol{p}_\beta = \boldsymbol{p}_\gamma$ and $\boldsymbol{q}_\beta = \boldsymbol{q}_\gamma$. Therefore, the final simplified Hartree term H_{Hartree} is:

$H_{\text{Hartree}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{q}_\alpha - \boldsymbol{q}_\delta) \delta_{\boldsymbol{q}_\alpha+\boldsymbol{q}_\beta,\boldsymbol{q}_\gamma+\boldsymbol{q}_\delta} \langle c^\dagger_{\boldsymbol{q}_\alpha,s}(\boldsymbol{p}_\alpha) c_{\boldsymbol{q}_\delta,s}(\boldsymbol{p}_\alpha) \rangle c^\dagger_{\boldsymbol{q}_\beta,s'}(\boldsymbol{p}_\alpha) c_{\boldsymbol{q}_\beta,s'}(\boldsymbol{p}_\alpha)$.

10 Identify order parameters in Fock term (extended BZ)

Prompt: You will be instructed to simplify the Fock term in H_{Fock} by reducing the momentum inside the expected value $\langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\gamma,\boldsymbol{q}_\gamma,s'} \rangle$.The expected value $\langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\gamma,\boldsymbol{q}_\gamma,s'} \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\gamma,\boldsymbol{q}_\gamma,s'} \rangle = \langle c^\dagger_{\boldsymbol{p}_\alpha,\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\gamma,\boldsymbol{q}_\gamma,s'} \rangle \delta_{c_{\boldsymbol{p}_\alpha,\boldsymbol{p}_\gamma}}$.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 $\langle \ldots \rangle$. 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 H_{Fock} is $H_{\text{Fock}} = -\frac{1}{N}\sum_{s,s'}\sum_{p,q} U(p_\alpha + q_\alpha - p_\delta - q_\delta)\delta_{p_\alpha+q_\alpha+p_\beta+q_\beta,p_\gamma+q_\gamma+p_\delta+q_\delta}\langle c_{q_\alpha,s}^\dagger(p_\alpha)c_{q_\gamma,s'}(p_\gamma)\rangle c_{q_\beta,s'}^\dagger(p_\beta)c_{q_\delta,s}(p_\delta)$..Return the final simplified Fock term H_{Fock}.

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

$$- \sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle\delta_{k_1,k_3} c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4} \cdot$$

Use the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we have

$$- \sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_1+k_4+b_3+b_4}$$

$$= - \sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_2+b_1+b_2,k_4+b_3+b_4} \cdot$$

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 provided, we can simplify the Fock term in H_{Fock} by reducing the momentum inside the expected value $\langle c_{p_\alpha,q_\alpha,s}^\dagger c_{p_\gamma,q_\gamma,s'}\rangle$.

We realize that $\langle c_{p_\alpha,q_\alpha,s}^\dagger c_{p_\gamma,q_\gamma,s'}\rangle$ is nonzero only when $p_\alpha = p_\gamma$, i.e., $\langle c_{p_\alpha,q_\alpha,s}^\dagger c_{p_\gamma,q_\gamma,s'}\rangle = \langle c_{p_\alpha,q_\alpha,s}^\dagger c_{p_\gamma,q_\gamma,s'}\rangle\delta_{p_\alpha,p_\gamma}$.

Thus, the Fock term becomes

$$-\frac{1}{N}\sum_{s,s'}\sum_{p,q} U(p_\alpha + q_\alpha - p_\delta - q_\delta)\delta_{p_\alpha+q_\alpha+p_\beta+q_\beta,p_\gamma+q_\gamma+p_\delta+q_\delta}\langle c_{q_\alpha,s}^\dagger(p_\alpha)c_{q_\gamma,s'}(p_\gamma)\rangle\delta_{p_\alpha,p_\gamma} c_{q_\beta,s'}^\dagger(p_\beta)c_{q_\delta,s}(p_\delta) \cdot$$

Using the property of the Kronecker delta function $\delta_{p_\alpha,p_\gamma}$ to sum over p_γ, we have $-\frac{1}{N}\sum_{s,s'}\sum_{p,q} U(p_\alpha + q_\alpha - p_\delta - q_\delta)\delta_{p_\alpha+q_\alpha+p_\beta+q_\beta,p_\alpha+q_\gamma+p_\delta+q_\delta}\langle c_{q_\alpha,s}^\dagger(p_\alpha)c_{q_\gamma,s'}(p_\alpha)\rangle c_{q_\beta,s'}^\dagger(p_\beta)c_{q_\delta,s}(p_\delta)$.

Because p_α is the momentum inside the first Brillouin zone while q_α is the reciprocal lattice, it is only when $p_\beta = p_\delta$ that $\delta_{p_\alpha+q_\alpha+p_\beta+q_\beta,p_\alpha+q_\gamma+p_\delta+q_\delta}$ is nonzero, i.e., $\delta_{p_\alpha+q_\alpha+p_\beta+q_\beta,p_\alpha+q_\gamma+p_\delta+q_\delta} = \delta_{q_\alpha+q_\beta,q_\gamma+q_\delta}\delta_{p_\beta,p_\delta}$.

Therefore, the Fock term simplifies to $-\frac{1}{N}\sum_{s,s'}\sum_{p,q} U(p_\alpha + q_\alpha - p_\beta - q_\delta)\delta_{q_\alpha+q_\beta,q_\gamma+q_\delta}\langle c_{q_\alpha,s}^\dagger(p_\alpha)c_{q_\gamma,s'}(p_\alpha)\rangle c_{q_\beta,s'}^\dagger(p_\beta)c_{q_\delta,s}(p_\beta)$.

Therefore, the final simplified Fock term after reducing two momenta is

$$H_{\text{Fock}} = -\frac{1}{N}\sum_{s,s'}\sum_{p,q} U(p_\alpha + q_\alpha - p_\beta - q_\delta)\delta_{q_\alpha+q_\beta,q_\gamma+q_\delta}\langle c_{q_\alpha,s}^\dagger(p_\alpha)c_{q_\gamma,s'}(p_\alpha)\rangle c_{q_\beta,s'}^\dagger(p_\beta)c_{q_\delta,s}(p_\beta) \cdot$$

11 Final form of iteration in quadratic terms

Prompt: You will now be instructed to combine the Hartree term H_{Hartree} and the Fock term H_{Fock}.You should recall that the Hartree term $H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{p,q} U(q_\alpha - q_\delta)\delta_{q_\alpha+q_\beta,q_\gamma+q_\delta}\langle c_{q_\alpha,s}^\dagger(p_\alpha)c_{q_\delta,s}(p_\alpha)\rangle c_{q_\beta,s'}^\dagger(p_\beta)c_{q_\gamma,s'}(p_\beta)$,and the Fock term $H_{\text{Fock}} = -\frac{1}{N}\sum_{s,s'}\sum_{p,q} U(p_\alpha + q_\alpha - p_\beta - q_\delta)\delta_{q_\alpha+q_\beta,q_\gamma+q_\delta}\langle c_{q_\alpha,s}^\dagger(p_\alpha)c_{q_\gamma,s'}(p_\alpha)\rangle c_{q_\beta,s'}^\dagger(p_\beta)c_{q_\delta,s}(p_\beta)$.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 H_{Hartree} and the Fock term H_{Fock}, we first 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.

In the Fock term, we apply the replacement $\boldsymbol{q}_\alpha \leftrightarrow \boldsymbol{q}_\beta$ and $\boldsymbol{q}_\gamma \leftrightarrow \boldsymbol{q}_\delta$. After the replacement, the Fock term becomes $-\frac{1}{N} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{p}_\beta + \boldsymbol{q}_\beta - \boldsymbol{p}_\beta - \boldsymbol{q}_\delta) \delta_{\boldsymbol{q}_\beta + \boldsymbol{q}_\beta, \boldsymbol{q}_\delta + \boldsymbol{q}_\delta} \langle c^\dagger_{\boldsymbol{q}_\beta, s}(\boldsymbol{p}_\beta) c_{\boldsymbol{q}_\delta, s'}(\boldsymbol{p}_\beta) \rangle c^\dagger_{\boldsymbol{q}_\alpha, s'}(\boldsymbol{p}_\alpha) c_{\boldsymbol{q}_\gamma, s}(\boldsymbol{p}_\alpha)$.

Now, the quadratic operators in the Fock term are the same as those in the Hartree term. We can add them together to get the final sum of Hartree and Fock term:

$H_{\mathrm{HF}} \;=\; H_{\mathrm{Hartree}} \;+\; H_{\mathrm{Fock}} \;=\; \frac{1}{N} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{q}_\alpha - \boldsymbol{q}_\delta) \delta_{\boldsymbol{q}_\alpha + \boldsymbol{q}_\beta, \boldsymbol{q}_\gamma + \boldsymbol{q}_\delta} \langle c^\dagger_{\boldsymbol{q}_\alpha, s}(\boldsymbol{p}_\alpha) c_{\boldsymbol{q}_\delta, s}(\boldsymbol{p}_\alpha) \rangle c^\dagger_{\boldsymbol{q}_\beta, s'}(\boldsymbol{p}_\beta) c_{\boldsymbol{q}_\gamma, s'}(\boldsymbol{p}_\beta) \;-$

$\frac{1}{N} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{p}_\beta + \boldsymbol{q}_\beta - \boldsymbol{p}_\beta - \boldsymbol{q}_\delta) \delta_{\boldsymbol{q}_\beta + \boldsymbol{q}_\beta, \boldsymbol{q}_\delta + \boldsymbol{q}_\delta} \langle c^\dagger_{\boldsymbol{q}_\beta, s}(\boldsymbol{p}_\beta) c_{\boldsymbol{q}_\delta, s'}(\boldsymbol{p}_\beta) \rangle c^\dagger_{\boldsymbol{q}_\alpha, s'}(\boldsymbol{p}_\alpha) c_{\boldsymbol{q}_\gamma, s}(\boldsymbol{p}_\alpha)$.

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