1 Identify kinetic term (lattice)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in the TTMD 2D moiré materials in the real space in the second-quantized form.The degrees of freedom of the system are: valley index s, spin-up or down, coupled with $+K$ or $-K$ valley, respectively, in the Brillouin zoneThe kinetic term is a tight-binding model composed of the following hopping process: between site i and site j with the amplitude hopping t_s.
The summation should be taken over all valley index s, spin-up or down, coupled with $+K$ or $-K$ valley, respectively, in the Brillouin zone and all real space positions.Return the Kinetic Hamiltonian H.
Use the following conventions for the symbols:t_s represents band structures (depending on θ), and effective interparticle Coulomb interactions U represent the correlation effect (depending on ϵ). Both t and U involve distant nearest neighbors (i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term U up to 1993 distant sites).
Completion: The kinetic term of the Hamiltonian in the second-quantized form for the TTMD 2D moiré materials in real space can be written as:

$$H = -\sum_{i,j,s} t_s c_{i,s}^\dagger c_{j,s}$$

where $c_{i,s}^\dagger$ and $c_{j,s}$ are the creation and annihilation operators at sites i and j with valley index s, respectively. The sum is taken over all valley indices s and all real space positions. The hopping amplitude t_s depends on the band structures and the angle θ.

2 Identify interacting term (real space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian, H^{int} 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 valley indices s and s' and all real space positions.Return the interaction term H^{int} in terms of $c_{i,s}^\dagger c_{i,s}$.
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): t_s represents band structures, U represents the correlation effect, $c_{i,s}^\dagger$ and $c_{j,s'}$ are creation and annihilation operators, respectively, and $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$ are real space positions.
Completion: The interaction part of the Hamiltonian, H^{int}, in real space in the second-quantized form can be constructed as follows:
$H^{int} = \frac{1}{2} \sum_{i,j,s,s'} U(\boldsymbol{R}_i - \boldsymbol{R}_j) c_{i,s}^\dagger c_{i,s} c_{j,s'}^\dagger c_{j,s'}$
Here, the sum is taken over all valley indices s and s' and all real space positions. The factor of 1/2 is included to avoid double counting of interactions. The operators $c_{i,s}^\dagger$ and $c_{j,s'}$ are creation and annihilation operators, respectively. The interaction strength $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$ represents the density-density interaction between site i and site j.

3 Fourier transform noninteracting term to momentum space (lattice)

Prompt: You will be instructed to convert the noninteracting Hamiltonian H 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 $c_{i,s}^\dagger$ in the real space to the $c_{k,s}^\dagger$ in the momentum space, which is defined as $c_{k,s}^\dagger = \frac{1}{\sqrt{N}} \sum_i c_{i,s}^\dagger e^{ik \cdot R_i}$, where 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 is $\sum_s \sum_{i,j} t_s (\boldsymbol{R}_i - \boldsymbol{R}_j) c_{i,s}^\dagger c_{j,s}$ Express the total noninteracting Hamiltonian H in terms of $c_{k,s}^\dagger$. 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): The hopping terms t_s represent band structures (depending on θ), and effective interparticle Coulomb interactions U represent the correlation effect (depending on ε). Valley index s, spin-up or down, is coupled with +K or -K valley, respectively,

in the Brillouin zone. Both t and U involve distant nearest neighbors (i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term U up to 1993 distant sites).

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 Hamiltonian H. The Fourier transformation is defined as $c^\dagger_{k,s} = \frac{1}{\sqrt{N}}\sum_i c^\dagger_{i,s}e^{ik \cdot R_i}$ and its inverse is $c^\dagger_{i,s} = \frac{1}{\sqrt{N}}\sum_k c^\dagger_{k,s}e^{-ik \cdot R_i}$.

Substituting these into the Hamiltonian H, we get:
$H = -\sum_s \sum_{i,j} t_s(\boldsymbol{R}_i - \boldsymbol{R}_j) \frac{1}{\sqrt{N}} \sum_{k_1} c^\dagger_{k_1,s} e^{-ik_1 \cdot R_i} \frac{1}{\sqrt{N}} \sum_{k_2} c_{k_2,s} e^{ik_2 \cdot R_j}$
Simplifying, we get:
$H = -\frac{1}{N}\sum_s \sum_{i,j} \sum_{k_1,k_2} t_s(\boldsymbol{R}_i - \boldsymbol{R}_j) c^\dagger_{k_1,s} c_{k_2,s} e^{-i(k_1 \cdot R_i - k_2 \cdot R_j)}$
Now, we make a replacement by defining $n = \boldsymbol{R}_i - \boldsymbol{R}_j$, and the Hamiltonian becomes:
$H = -\frac{1}{N}\sum_s \sum_{i,n} \sum_{k_1,k_2} t_s(n) c^\dagger_{k_1,s} c_{k_2,s} e^{-i(k_1-k_2) \cdot R_i} e^{-ik_2 \cdot n}$
Using the property of the Kronecker delta function, $\frac{1}{N}\sum_i e^{-i(k_1-k_2) \cdot R_i} = \delta(k_1,k_2)$, we get:
$H = -\sum_s \sum_{k_1,k_2} \sum_n t_s(n) c^\dagger_{k_1,s} c_{k_2,s} e^{-ik_2 \cdot n} \delta(k_1,k_2)$
Using the property of the Kronecker delta function and summing over k_2, we obtain:
$H = -\sum_s \sum_{k_1} \sum_n t_s(n) e^{-ik_1 \cdot n} c^\dagger_{k_1,s} c_{k_1,s}$
For simplicity, we replace k_1 with k, and we obtain:
$H = -\sum_s \sum_k \sum_n t_s(n) e^{-ik \cdot n} c^\dagger_{k,s} c_{k,s}$
If we define the energy dispersion $E_s(k) = \sum_n t_s(n)e^{-ik \cdot n}$, where n is the summation of all hopping pairs, the Hamiltonian in the momentum space is:
$H = -\sum_s \sum_k E_s(k) c^\dagger_{k,s} c_{k,s}$

4 Fourier transform interacting term to momentum space (lattice)

Prompt: You will be instructed to convert the interacting Hamiltonian, H_{int}, 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 $c_{i,s}^\dagger$ in the real space to the $c_{k,s}^\dagger$ in the momentum space, which is defined as $c_{k,s}^\dagger = \frac{1}{\sqrt{N}} \sum_i c_{i,s}^\dagger e^{ik \cdot R_i}$, where i is integrated over all sites in the entire real space, and k is defined within the first Brillouin zone. You should follow the EXAMPLE below to apply the Fourier transformation.You should recall that H_{int} is $H_{int} = \frac{1}{2} \sum_{i,j,s,s'} U(\boldsymbol{R}_i - \boldsymbol{R}_j) c_{i,s}^\dagger c_{i,s} c_{j,s'}^\dagger c_{j,s'}$. Express H_{int} in terms of $c_{k,s}^\dagger$. 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 interaction Hamiltonian H_{int}. The Fourier transformation is defined as $c_{k,s}^\dagger = \frac{1}{\sqrt{N}} \sum_i c_{i,s}^\dagger e^{ik \cdot R_i}$ and its inverse is $c_{i,s}^\dagger = \frac{1}{\sqrt{N}} \sum_k c_{k,s}^\dagger e^{-ik \cdot R_i}$. Substituting these into the Hamiltonian H_{int}, we get:

$H_{int} = \frac{1}{2N^2} \sum_{i,j,s,s'} \sum_{k_1,k_2,k_3,k_4} U(\boldsymbol{R}_i - \boldsymbol{R}_j) c_{k_1,s}^\dagger e^{-ik_1 \cdot R_i} c_{k_2,s} e^{ik_2 \cdot R_i} c_{k_3,s'}^\dagger e^{-ik_3 \cdot R_j} c_{k_4,s'} e^{ik_4 \cdot R_j}$

Now, we make a replacement by defining $n = \boldsymbol{R}_i - \boldsymbol{R}_j$. The Hamiltonian becomes:

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

Using the property of the Kronecker delta function, $\frac{1}{N} \sum_j e^{-i(k_1-k_2+k_3-k_4) \cdot R_j} = \delta(k_1 - k_2 + k_3 - k_4, G)$, where G is the all reciprocal lattices in the momentum space, we get:

$H_{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1 - k_2) c_{k_1,s}^\dagger c_{k_2,s} c_{k_3,s'}^\dagger c_{k_4,s'} \delta(k_1 - k_2 + k_3 - k_4, G)$

If we define the 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:

$H_{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1 - k_2) c_{k_1,s}^\dagger c_{k_2,s} c_{k_3,s'}^\dagger c_{k_4,s'} \delta(k_1 - k_2 + k_3 - k_4, G)$

5 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, H_{int}.You should use Wick's theorem to expand the four-fermion term in H_{int} 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_{int} is

$$H_{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1-k_2) c^\dagger_{k_1,s} c_{k_2,s} c^\dagger_{k_3,s'} c_{k_4,s'} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)..$$

Return the expanded interaction term after Hartree-Fock approximation as H^{HF}_{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):The hopping terms t_s represent band structures (depending on θ), and effective interparticle Coulomb interactions U represent the correlation effect (depending on ϵ). Valley index s , spin-up or down, is coupled with $+K$ or $-K$ valley, respectively, in the Brillouin zone. Both t and U involve distant nearest neighbors.
EXAMPLE 1:For a four-fermion term $a^\dagger_1 a^\dagger_2 a_3 a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a^\dagger_1 a^\dagger_2 a_3 a_4 = \langle a^\dagger_1 a_4 \rangle a^\dagger_2 a_3 + \langle a^\dagger_2 a_3 \rangle a^\dagger_1 a_4 - \langle a^\dagger_1 a_4 \rangle \langle a^\dagger_2 a_3 \rangle - \langle a^\dagger_1 a_3 \rangle a^\dagger_2 a_4 - \langle a^\dagger_2 a_4 \rangle a^\dagger_1 a_3 + \langle a^\dagger_1 a_3 \rangle \langle a^\dagger_2 a_4 \rangle$Be cautious about the order of the index and sign before each term here.
EXAMPLE 2:For a four-fermion term $a^\dagger_1 a_2 a^\dagger_3 a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a^\dagger_1 a_2 a^\dagger_3 a_4 = \langle a^\dagger_1 a_2 \rangle a^\dagger_3 a_4 + \langle a^\dagger_3 a_4 \rangle a^\dagger_1 a_2 - \langle a^\dagger_1 a_2 \rangle \langle a^\dagger_3 a_4 \rangle - \langle a^\dagger_1 a_4 \rangle a^\dagger_3 a_2 - \langle a^\dagger_3 a_2 \rangle a^\dagger_1 a_4 + \langle a^\dagger_1 a_4 \rangle \langle a^\dagger_3 a_2 \rangle$Be cautious about the order of the index and sign before each term here.
Completion: Following the examples provided, we can apply Wick's theorem to the interaction term H_{int} and expand it into quadratic terms. The four-fermion term in H_{int} is $c^\dagger_{k_1,s} c_{k_2,s} c^\dagger_{k_3,s'} c_{k_4,s'}$.
Following the pattern in Example 2, we can expand this term as:
$c^\dagger_{k_1,s} c_{k_2,s} c^\dagger_{k_3,s'} c_{k_4,s'} = \langle c^\dagger_{k_1,s} c_{k_2,s} \rangle c^\dagger_{k_3,s'} c_{k_4,s'} + \langle c^\dagger_{k_3,s'} c_{k_4,s'} \rangle c^\dagger_{k_1,s} c_{k_2,s} - \langle c^\dagger_{k_1,s} c_{k_2,s} \rangle \langle c^\dagger_{k_3,s'} c_{k_4,s'} \rangle - \langle c^\dagger_{k_1,s} c_{k_4,s'} \rangle c^\dagger_{k_3,s'} c_{k_2,s} - \langle c^\dagger_{k_3,s'} c_{k_2,s} \rangle c^\dagger_{k_1,s} c_{k_4,s'} + \langle c^\dagger_{k_1,s} c_{k_4,s'} \rangle \langle c^\dagger_{k_3,s'} c_{k_2,s} \rangle$
Substituting this expansion back into H_{int}, we get:

$$H^{HF}_{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1-k_2) \left[\langle c^\dagger_{k_1,s} c_{k_2,s} \rangle c^\dagger_{k_3,s'} c_{k_4,s'} + \langle c^\dagger_{k_3,s'} c_{k_4,s'} \rangle c^\dagger_{k_1,s} c_{k_2,s} - \langle c^\dagger_{k_1,s} c_{k_2,s} \rangle \langle c^\dagger_{k_3,s'} c_{k_4,s'} \rangle \right.$$
$$\left. - \langle c^\dagger_{k_1,s} c_{k_4,s'} \rangle c^\dagger_{k_3,s'} c_{k_2,s} - \langle c^\dagger_{k_3,s'} c_{k_2,s} \rangle c^\dagger_{k_1,s} c_{k_4,s'} + \langle c^\dagger_{k_1,s} c_{k_4,s'} \rangle \langle c^\dagger_{k_3,s'} c_{k_2,s} \rangle \right] \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)$$

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^{HF}_{int}.The quadratic terms mean terms that are proportional to $c^\dagger_{i,s} c_{j,s}$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in H^{HF}_{int}, denoted as $H^{HF,2}_{int}$.You should recall that H^{HF}_{int} is

$$H_{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1-k_2) \left[\langle c^\dagger_{k_1,s} c_{k_2,s} \rangle c^\dagger_{k_3,s'} c_{k_4,s'} + \langle c^\dagger_{k_3,s'} c_{k_4,s'} \rangle c^\dagger_{k_1,s} c_{k_2,s} - \langle c^\dagger_{k_1,s} c_{k_2,s} \rangle \langle c^\dagger_{k_3,s'} c_{k_4,s'} \rangle \right.$$
$$\left. - \langle c^\dagger_{k_1,s} c_{k_4,s'} \rangle c^\dagger_{k_3,s'} c_{k_2,s} - \langle c^\dagger_{k_3,s'} c_{k_2,s} \rangle c^\dagger_{k_1,s} c_{k_4,s'} + \langle c^\dagger_{k_1,s} c_{k_4,s'} \rangle \langle c^\dagger_{k_3,s'} c_{k_2,s} \rangle \right] \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)..$$

Return $H^{HF,2}_{int}$.
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):t_s represents the hopping terms which are band structures (depending on θ), and effective interparticle Coulomb interactions U represent the correlation effect (depending on ϵ). Valley index s , spin-up or down, is coupled with $+K$ or $-K$ valley, respectively, in the Brillouin zone. Both t and U involve distant nearest neighbors.
Completion: The quadratic terms in the Hartree-Fock approximation of the interaction Hamiltonian, $H^{HF,2}_{int}$, are those terms that are proportional to $c^\dagger_{i,s} c_{j,s}$, excluding terms that are solely expectations or products of expectations.
From the given H^{HF}_{int}, we can identify the quadratic terms as:

$$H^{HF,2}_{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1-k_2) \left[\langle c^\dagger_{k_1,s} c_{k_2,s} \rangle c^\dagger_{k_3,s'} c_{k_4,s'} + \langle c^\dagger_{k_3,s'} c_{k_4,s'} \rangle c^\dagger_{k_1,s} c_{k_2,s} - \langle c^\dagger_{k_1,s} c_{k_4,s'} \rangle c^\dagger_{k_3,s'} c_{k_2,s} \right.$$
$$\left. - \langle c^\dagger_{k_3,s'} c_{k_2,s} \rangle c^\dagger_{k_1,s} c_{k_4,s'} \right] \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) .$$

This is the result after removing the terms that are products of expectations, which are not quadratic terms.

7 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term H{int}^{HF,2}. If you find the $V(q)$ in H{int}^{HF,2} 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 $k_\alpha - k_\delta$. You should recall that $H_{int}^{HF,2}$ is

$$H_{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1 - k_2) \left[\langle c_{k_1,s}^\dagger c_{k_2,s} \rangle c_{k_3,s'}^\dagger c_{k_4,s'} + \langle c_{k_3,s'}^\dagger c_{k_4,s'} \rangle c_{k_1,s}^\dagger c_{k_2,s} - \langle c_{k_1,s}^\dagger c_{k_4,s'} \rangle c_{k_3,s'}^\dagger c_{k_2,s} \right.$$
$$\left. - \langle c_{k_3,s'}^\dagger c_{k_2,s} \rangle c_{k_1,s}^\dagger c_{k_4,s'} \right] \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)..$$

Return $H_{int}^{HF,2}$ with expanded interaction.
Completion: The interaction term $V(q)$ in $H_{int}^{HF,2}$ is already expanded as $U(k_1 - k_2)$. However, if we were to replace q with the momentum $k_\alpha - k_\delta$, the expanded interaction term would be $U(k_\alpha - k_\delta)$. Therefore, the expanded $H_{int}^{HF,2}$ would be:

$$H_{int}^{HF,2} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_\alpha - k_\delta) \left[\langle c_{k_1,s}^\dagger c_{k_2,s} \rangle c_{k_3,s'}^\dagger c_{k_4,s'} + \langle c_{k_3,s'}^\dagger c_{k_4,s'} \rangle c_{k_1,s}^\dagger c_{k_2,s} - \langle c_{k_1,s}^\dagger c_{k_4,s'} \rangle c_{k_3,s'}^\dagger c_{k_2,s} \right.$$
$$\left. - \langle c_{k_3,s'}^\dagger c_{k_2,s} \rangle c_{k_1,s}^\dagger c_{k_4,s'} \right] \sum_G \delta(k_1 - k_2 + k_3 - k_4, G).$$

8 Relabel the index

Prompt: You will be instructed to simplify the quadratic term H_{int}^{HF,2} through relabeling the index.The logic is that the expected value ($\langle c_{k_\alpha,s}^\dagger c_{k_\delta,s} \rangle$ and $\langle c_{k_\alpha,s}^\dagger c_{k_\gamma,s'} \rangle$) in the first Hartree term ($c_{k_\beta,s'}^\dagger c_{k_\gamma,s'}$) has the same form as the quadratic operators in the second Hartree term ($c_{k_\beta,s'}^\dagger c_{k_\delta,s}$), and vice versa. The same applies to the Fock term.Namely, a replacement of $k_1 \leftrightarrow k_3$, $k_2 \leftrightarrow k_4$, and s and s' is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes nothing.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 $H_{int}^{HF,2}$ is $H_{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1 - k_2) \left[\langle c_{k_1,s}^\dagger c_{k_2,s} \rangle c_{k_3,s'}^\dagger c_{k_4,s'} + \langle c_{k_3,s'}^\dagger c_{k_4,s'} \rangle c_{k_1,s}^\dagger c_{k_2,s} - \langle c_{k_1,s}^\dagger c_{k_4,s'} \rangle c_{k_3,s'}^\dagger c_{k_2,s} - \langle c_{k_3,s'}^\dagger c_{k_2,s} \rangle c_{k_1,s}^\dagger c_{k_4,s'} \right] \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)$. Return the simplified $H_{int}^{HF,2}$.
EXAMPLE:Given a Hamiltonian $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)(\langle c_{d,\sigma_1}^\dagger(k_1) c_{d,\sigma_4}(k_4) \rangle c_{p,\sigma_2}^\dagger(k_2) c_{p,\sigma_3}(k_3) + \langle c_{p,\sigma_2}^\dagger(k_2) c_{d,\sigma_3}(k_3) \rangle c_{d,\sigma_1}^\dagger(k_1) c_{d,\sigma_4}(k_4)) \delta_{k_1+k_2,k_3+k_4}$, 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 $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_2 - k_3) \langle c_{p,\sigma_1}^\dagger(k_1) c_{p,\sigma_4}(k_4) \rangle c_{d,\sigma_2}^\dagger(k_2) c_{d,\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$.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 $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_4 - k_1) \langle c_{p,\sigma_1}^\dagger(k_1) c_{p,\sigma_4}(k_4) \rangle c_{d,\sigma_2}^\dagger(k_2) c_{d,\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$. Because $V(q) = V(-q)$, meaning $V(k_4 - k_1) = V(k_1 - k_4)$, the second term further simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4) \langle c_{p,\sigma_1}^\dagger(k_1) c_{p,\sigma_4}(k_4) \rangle c_{d,\sigma_2}^\dagger(k_2) c_{d,\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$.Finally, we have the simplified Hamiltonian as

$$\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)(\langle c_{d,\sigma_1}^\dagger(k_1) c_{d,\sigma_4}(k_4) \rangle c_{p,\sigma_2}^\dagger(k_2) c_{p,\sigma_3}(k_3)$$
$$+ \langle c_{p,\sigma_1}^\dagger(k_1) c_{p,\sigma_4}(k_4) \rangle c_{d,\sigma_2}^\dagger(k_2) c_{d,\sigma_3}(k_3)) \delta_{k_4+k_3,k_2+k_1}.$$

Completion: Following the example, we can simplify the quadratic term $H_{int}^{HF,2}$ by relabeling the index. We apply the replacement $k_1 \leftrightarrow k_3$, $k_2 \leftrightarrow k_4$, and $s \leftrightarrow s'$ to ONLY the second Hartree or Fock term.

After the replacement, the second Hartree term becomes $\langle c_{k_3,s'}^\dagger c_{k_4,s'}\rangle c_{k_1,s}^\dagger c_{k_2,s}$ and the second Fock term becomes $-\langle c_{k_3,s'}^\dagger c_{k_2,s}\rangle c_{k_1,s}^\dagger c_{k_4,s'}$.

The Kronecker delta function $\delta(k_1 - k_2 + k_3 - k_4, G)$ implies $k_1 - k_2 = k_4 - k_3$, i.e., $k_\alpha - k_\delta = k_4 - k_3$. Thus, the interaction term $U(k_\alpha - k_\delta)$ simplifies to $U(k_4 - k_3)$.

Because $U(q) = U(-q)$, meaning $U(k_4 - k_3) = U(k_3 - k_4)$, the interaction term further simplifies to $U(k_3 - k_4)$.

Finally, we have the simplified $H_{int}^{HF,2}$ as:

$$H_{int}^{HF,2} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_3 - k_4) \left[\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle c_{k_3,s'}^\dagger c_{k_4,s'} + \langle c_{k_3,s'}^\dagger c_{k_4,s'}\rangle c_{k_1,s}^\dagger c_{k_2,s} - \langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle c_{k_3,s'}^\dagger c_{k_2,s} \right.$$
$$\left. - \langle c_{k_3,s'}^\dagger c_{k_2,s}\rangle c_{k_1,s}^\dagger c_{k_4,s'} \right] \sum_G \delta(k_1 - k_2 + k_3 - k_4, G).$$

9 Identify order parameters in Hartree term

Prompt: You will be instructed to simplify the Hartree term, H_{Hartree}, by reducing the momentum inside the expected value $\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle$.The expected value $\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle = \delta_{k_1,k_2}\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle$.You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_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 Hartree term, and another momentum in the quadratic term.You should recall that H_{Hartree} is $H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_3 - k_4)\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle c_{k_3,s'}^\dagger c_{k_4,s'} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)$..Return the final simplified Hartree term H_{Hartree}.

EXAMPLE:Given a Hamiltonian where the Hartree term $\hat{H}^{Hartree} = \sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \sum_G \delta_{k_1+k_2-k_3-k_4,G}$, where k_i is the momentum inside first Brilloun zone, G is the reciprocal lattice vectors, and s_i is a certain index for the degree of freedom other than momentum.Inside the expected value, we realize $\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4)\rangle$ is nonzero only when $k_1 = k_4$, i.e., $\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4)\rangle = \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4)\rangle\delta_{k_1,k_4}$.Thus, the Hartree term becomes $\sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4)\rangle\delta_{k_1,k_4} c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \sum_G \delta_{k_1+k_2-k_3-k_4,G}$.Use the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have $\sum_{k_1,k_2,k_3,s_1,s_2} V(k_1 - k_1)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \sum_G \delta_{k_1+k_2-k_3-k_1,G} = \sum_{k_1,k_2,k_3,s_1,s_2} V(0)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \sum_G \delta_{k_2-k_3,G}$.We can further simplify $\sum_G \delta_{k_2-k_3,G}$. Because k_i is momentum inside first Brilloun zone, and the difference between k_2 and k_3 cannot exceed the first shell of reciprocal lattice vector, which means G can only take the value of the origin point in the reciprocal lattice, therefore, $\sum_G \delta_{k_2-k_3,G} = \delta_{k_2-k_3,0}$.Thus, the Hartree term simplifies to $\sum_{k_1,k_2,k_3,s_1,s_2} V(0)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3)\delta_{k_2-k_3,0} = \sum_{k_1,k_2,s_1,s_2} V(0)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_2)$.Therefore, the final simplified Hartree term after reducing one momentum is $\hat{H}^{Hartree} = \sum_{k_1,k_2,s_1,s_2} V(0)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_2)$

Completion: The Hartree term H_{Hartree} is given by:
$H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_3 - k_4)\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle c_{k_3,s'}^\dagger c_{k_4,s'} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)$.

The expected value $\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle$ is nonzero only when $k_1 = k_2$, so we can write $\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle = \delta_{k_1,k_2}\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle$.

Substituting this into the Hartree term, we get:
$H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_3 - k_4)\delta_{k_1,k_2}\langle c_{k_1,s}^\dagger c_{k_2,s}\rangle c_{k_3,s'}^\dagger c_{k_4,s'} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)$.

Using the property of the Kronecker delta function δ_{k_1,k_2} to sum over k_2, we get:
$H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_3,k_4} U(k_3 - k_4)\langle c_{k_1,s}^\dagger c_{k_1,s}\rangle c_{k_3,s'}^\dagger c_{k_4,s'} \sum_G \delta(2k_1 + k_3 - k_4, G)$.

The total momentum conservation $\delta(2k_1 + k_3 - k_4, G)$ will reduce another momentum in the quadratic term. Since G can only take the value of the origin point in the reciprocal lattice, we have $\delta(2k_1 + k_3 - k_4, 0)$, which simplifies to $\delta(k_3 - k_4, 2k_1)$.

Substituting this into the Hartree term, we get:
$H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_3} U(k_3 - k_3)\langle c_{k_1,s}^\dagger c_{k_1,s}\rangle c_{k_3,s'}^\dagger c_{k_3,s'}$.

Therefore, the final simplified Hartree term after reducing one momentum is:
$H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_3} U(0)\langle c_{k_1,s}^\dagger c_{k_1,s}\rangle c_{k_3,s'}^\dagger c_{k_3,s'}$.

10 Identify order parameters in Fock term

Prompt: You will be instructed to simplify the Fock term in H_{Fock} by reducing the momentum inside the expected value $\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle$.The expected value $\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle$ is only nonzero when the two momenta

k_i, k_j are the same, namely, $\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle = \delta_{k_1,k_4}\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle$. You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_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 H_{Fock} is $H_{Fock} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_3 - k_4)\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle c_{k_3,s'}^\dagger c_{k_2,s}\sum_G \delta(k_1 - k_2 + k_3 - k_4, G)$. Return the final simplified Fock term H_{Fock}.

EXAMPLE: Given a Hamiltonian where the Fock term $\hat{H}^{Fock} = -\sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4)\langle c_{s_1}^\dagger(k_1)c_{s_2}(k_3)\rangle c_{s_2}^\dagger(k_2)c_{s_1}(k_4)\sum_G \delta_{k_1+k_2-k_3-k_4,G}$, where k_i is the momentum inside first Brilloun zone, G is the reciprocal lattice vectors, and s_i is a certain index for the degree of freedom other than momentum. Inside the expected value, we realize $\langle c_{s_1}^\dagger(k_1)c_{s_2}(k_3)\rangle$ is nonzero only when $k_1 = k_3$, i.e., $\langle c_{s_1}^\dagger(k_1)c_{s_2}(k_3)\rangle = \langle c_{s_1}^\dagger(k_1)c_{s_2}(k_3)\rangle\delta_{k_1,k_3}$. Thus, the Fock term becomes $-\sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4)\langle c_{s_1}^\dagger(k_1)c_{s_2}(k_3)\rangle\delta_{k_1,k_3} c_{s_2}^\dagger(k_2)c_{s_1}(k_4)\sum_G \delta_{k_1+k_2-k_3-k_4,G}$. Use the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we have $-\sum_{k_1,k_2,k_4,s_1,s_2} V(k_1 - k_4)\langle c_{s_1}^\dagger(k_1)c_{s_2}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_1}(k_4)\sum_G \delta_{k_2-k_4,G}$. We can further simplify $\sum_G \delta_{k_2-k_4,G}$. Because k_i is momentum inside first Brilloun zone, and the difference between k_2 and k_4 cannot exceed the first shell of reciprocal lattice vector, which means G can only take the value of the origin point in the reciprocal lattice, therefore, $\sum_G \delta_{k_2-k_4,G} = \delta_{k_2-k_4,0}$. Thus, the Fock term simplifies to $-\sum_{k_1,k_2,k_4,s_1,s_2} V(k_1 - k_4)\langle c_{s_1}^\dagger(k_1)c_{s_2}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_1}(k_4)\delta_{k_2-k_4,0} = -\sum_{k_1,k_2,s_1,s_2} V(k_1 - k_2)\langle c_{s_1}^\dagger(k_1)c_{s_2}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_1}(k_2)$. Therefore, the final simplified Fock term after reducing one momentum is $\hat{H}^{Fock} = -\sum_{k_1,k_2,s_1,s_2} V(k_1 - k_2)\langle c_{s_1}^\dagger(k_1)c_{s_2}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_1}(k_2)$

Completion: The Fock term in the Hamiltonian is given by:
$H_{Fock} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_3 - k_4)\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle c_{k_3,s'}^\dagger c_{k_2,s}\sum_G \delta(k_1 - k_2 + k_3 - k_4, G)$.

We know that the expected value $\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle$ is nonzero only when $k_1 = k_4$, i.e., $\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle = \delta_{k_1,k_4}\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle$.

Substituting this into the Fock term, we get:
$H_{Fock} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_3 - k_4)\delta_{k_1,k_4}\langle c_{k_1,s}^\dagger c_{k_4,s'}\rangle c_{k_3,s'}^\dagger c_{k_2,s}\sum_G \delta(k_1 - k_2 + k_3 - k_4, G)$.

Using the property of the Kronecker delta function δ_{k_1,k_4} to sum over k_4, we get:
$H_{Fock} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3} U(k_3 - k_1)\langle c_{k_1,s}^\dagger c_{k_1,s'}\rangle c_{k_3,s'}^\dagger c_{k_2,s}\sum_G \delta(k_1 - k_2 + k_3 - k_1, G)$.

Simplifying the delta function $\delta(k_1 - k_2 + k_3 - k_1, G)$, we get $\delta(k_3 - k_2, G)$.

So, the Fock term becomes:
$H_{Fock} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3} U(k_3 - k_1)\langle c_{k_1,s}^\dagger c_{k_1,s'}\rangle c_{k_3,s'}^\dagger c_{k_2,s}\sum_G \delta(k_3 - k_2, G)$.

Finally, using the property of the Kronecker delta function $\delta(k_3 - k_2, G)$ to sum over k_3, we get:
$H_{Fock} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2} U(k_2 - k_1)\langle c_{k_1,s}^\dagger c_{k_1,s'}\rangle c_{k_2,s'}^\dagger c_{k_2,s}$.

This is the final simplified Fock term after reducing one momentum in the expected value and another momentum in the quadratic term.

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 $H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_3} U(0)\langle c_{k_1,s}^\dagger c_{k_1,s}\rangle c_{k_3,s'}^\dagger c_{k_3,s'}$, and the Fock term $H_{Fock} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2} U(k_2 - k_1)\langle c_{k_1,s}^\dagger c_{k_1,s'}\rangle c_{k_2,s'}^\dagger c_{k_2,s}$. 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: The Hartree term H_{Hartree} and the Fock term H_{Fock} are given by:
$H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_3} U(0)\langle c_{k_1,s}^\dagger c_{k_1,s}\rangle c_{k_3,s'}^\dagger c_{k_3,s'}$,
$H_{\text{Fock}} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2} U(k_2 - k_1)\langle c_{k_1,s}^\dagger c_{k_1,s'}\rangle c_{k_2,s'}^\dagger c_{k_2,s}$.

As per the instructions, we need to relabel the index in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. However, the instruction specifies that no swap is needed. This means that the Fock term remains the same.

Adding the Hartree term and the Fock term, we get:
$H_{\text{Hartree+Fock}} = H_{\text{Hartree}} + H_{\text{Fock}}$
$= \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_3} U(0)\langle c_{k_1,s}^\dagger c_{k_1,s}\rangle c_{k_3,s'}^\dagger c_{k_3,s'} - \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2} U(k_2 - k_1)\langle c_{k_1,s}^\dagger c_{k_1,s'}\rangle c_{k_2,s'}^\dagger c_{k_2,s}$.
This is the final sum of the Hartree and Fock terms.