1 Identify kinetic term (lattice)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in the moiré lattice system in the real space in the second-quantized form. The degrees of freedom of the system are: spin $s =\uparrow$ and $\downarrow$ coupled with the $+K$ and $-K$ valleys The 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 spin $s =\uparrow$ and $\downarrow$ coupled with the $+K$ and $-K$ valleys and all real space positions. Return the Kinetic Hamiltonian H.
Use the following conventions for the symbols: $t_s(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is the hopping between the moir'e lattice site i and j, fitted from the first moir'e valence band of twisted WSe$_2$ at $\pm K$ valleys in the noninteracting picture. $s =\uparrow$ and $\downarrow$ are coupled with the $+K$ and $-K$ valleys. $c_{i,s}^\dagger$ is the creation operator at site i with spin s. $c_{i,s}$ is the annihilation operator at site i with spin s.
Completion: The kinetic term of the Hamiltonian in the moiré lattice system in the real space in the second-quantized form can be written as:

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

Here, the first summation is over all pairs of sites i and j in the moiré lattice, and the second summation is over all spins $s =\uparrow$ and $\downarrow$ coupled with the $+K$ and $-K$ valleys. The term $t_s(\boldsymbol{R}_i - \boldsymbol{R}_j)$ represents the hopping amplitude between site i and site j for a particle with spin s. The operators $c_{i,s}^\dagger$ and $c_{i,s}$ are the creation and annihilation operators at site i with spin s, respectively. The minus sign in front of the summation indicates that the energy decreases as the hopping process occurs.

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 s, s' and all real space positions. Return the interaction term H_{int} 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): $t_s(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is the hopping between the moir'e lattice site i and j, $s =\uparrow$ and $\downarrow$ are coupled with the $+K$ and $-K$ valleys, $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$ describes the Coulomb repulsion between site i and j.
Completion: The interaction part of the Hamiltonian, H_{int}, in real space in the second-quantized form can be written as:

$$H_{int} = \frac{1}{2} \sum_{i,j} \sum_{s,s'} U(\boldsymbol{R}_i - \boldsymbol{R}_j) n_{i,s} n_{j,s'}$$

Here, the first summation is over all pairs of sites i and j in the moiré lattice, and the second summation is over all spins $s, s' =\uparrow, \downarrow$ coupled with the $+K$ and $-K$ valleys. The term $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$ represents the interaction strength between site i and site j. The operators $n_{i,s} = c_{i,s}^\dagger c_{i,s}$ and $n_{j,s'} = c_{j,s'}^\dagger c_{j,s'}$ are the number operators at site i with spin s and at site j with spin s', respectively. The factor of 1/2 is to avoid double counting of interactions.

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 $c_{\boldsymbol{k},s}^\dagger$ 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 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 $H = \sum_s \sum_{i,j} t_s(\boldsymbol{R}_i - \boldsymbol{R}_j) c_{i,s}^\dagger c_{j,s}$ Express the total noninteracting Hamiltonian H 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): H is the noninteracting Hamiltonian, $t_s(\boldsymbol{R}_i - \boldsymbol{R}_j)$

is the hopping between the moir'e lattice site i and j, $s = \uparrow$ and $\downarrow$ are coupled with the $+K$ and $-K$ valleys, and $c^\dagger_{i,s}$ is the creation operator in real 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 Hamiltonian H. The Fourier transformation is defined as $c^\dagger_{k,s} = \frac{1}{\sqrt{N}} \sum_i c^\dagger_{R_i,s}e^{ik\cdot R_i}$ and its inverse is $c^\dagger_{R_i,s} = \frac{1}{\sqrt{N}} \sum_k c^\dagger_{k,s}e^{-ik\cdot R_i}$.
Substituting these into the Hamiltonian, we get:

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

Simplifying, we get:

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

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

$$H = -\frac{1}{N} \sum_s \sum_{i,n} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} t_s(\boldsymbol{n})c^\dagger_{\boldsymbol{k}_1,s}c_{\boldsymbol{k}_2,s}e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot R_i}e^{-i\boldsymbol{k}_2\cdot\boldsymbol{n}}$$

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

$$H = -\sum_s \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_n t_s(\boldsymbol{n})e^{-i\boldsymbol{k}_2\cdot\boldsymbol{n}}c^\dagger_{\boldsymbol{k}_1,s}c_{\boldsymbol{k}_2,s}\delta(\boldsymbol{k}_1,\boldsymbol{k}_2)$$

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

$$H = -\sum_s \sum_{\boldsymbol{k}_1} \sum_n t_s(\boldsymbol{n})e^{-i\boldsymbol{k}_1\cdot\boldsymbol{n}}c^\dagger_{\boldsymbol{k}_1,s}c_{\boldsymbol{k}_1,s}$$

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

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

If we define the energy dispersion $E_s(\boldsymbol{k}) = \sum_{\boldsymbol{n}} t_s(\boldsymbol{n}) e^{-i\boldsymbol{k}\cdot\boldsymbol{n}}$, where $\boldsymbol{n}$ is the summation of all hopping pairs, the Hamiltonian in the momentum space is:

$$H = -\sum_s \sum_{\boldsymbol{k}} E_s(\boldsymbol{k}) c_{\boldsymbol{k},s}^\dagger c_{\boldsymbol{k},s}$$

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 $c_{k,s}^\dagger = \frac{1}{\sqrt{N}} \sum_i c_{R_i,s}^\dagger e^{ik\cdot R_i}$, where $\boldsymbol{R}_i$ 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 $H_{int} = \frac{1}{2} \sum_{i,j} \sum_{s,s'} U(\boldsymbol{R}_i - \boldsymbol{R}_j) n_{i,s} n_{j,s'}$. 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: To convert the interacting Hamiltonian H_{int} from real space to momentum space, we first express the number operators $n_{i,s}$ and $n_{j,s'}$ in terms of the creation and annihilation operators in momentum space using the Fourier transformation.
The Fourier transformation is defined as $c_{\boldsymbol{k},s}^\dagger = \frac{1}{\sqrt{N}} \sum_i c_{R_i,s}^\dagger e^{i\boldsymbol{k}\cdot R_i}$ and its inverse is $c_{R_i,s}^\dagger = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} c_{\boldsymbol{k},s}^\dagger e^{-i\boldsymbol{k}\cdot R_i}$.
Substituting these into the number operators, we get

$$n_{i,s} = c_{i,s}^\dagger c_{i,s}$$
$$= \frac{1}{N} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} c_{\boldsymbol{k}_1,s}^\dagger c_{\boldsymbol{k}_2,s} e^{-i\boldsymbol{k}_1\cdot R_i} e^{i\boldsymbol{k}_2\cdot R_i}$$

and similarly for $n_{j,s'}$.

Substituting these into the Hamiltonian H_{int}, we get

$H_{int} = \frac{1}{2}\sum_{i,j}\sum_{s,s'}U(\boldsymbol{R}_i - \boldsymbol{R}_j)n_{i,s}n_{j,s'} = \frac{1}{2N^2}\sum_{i,j}\sum_{s,s'}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}U(\boldsymbol{R}_i - \boldsymbol{R}_j)c^\dagger_{\boldsymbol{k}_1,s}c_{\boldsymbol{k}_2,s}e^{-i\boldsymbol{k}_1\cdot R_i}e^{i\boldsymbol{k}_2\cdot R_i}c^\dagger_{\boldsymbol{k}_3,s'}c_{\boldsymbol{k}_4,s'}e^{-i\boldsymbol{k}_3\cdot R_j}e^{i\boldsymbol{k}_4\cdot R_j}$.

Now, we make a replacement by defining $\boldsymbol{n} = \boldsymbol{R}_i - \boldsymbol{R}_j$ and $\boldsymbol{R}_j = \boldsymbol{r}$, we get

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

Using the property of the Kronecker delta function, we get

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

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

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

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 †, 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 $H_{int} = \frac{1}{2N}\sum_{s,s'}\sum_{k,k',q,q'}U(k-q)c^\dagger_{k,s}c_{q,s}c^\dagger_{k',s'}c_{q',s'}\sum_{G}\delta(k-q+k'-q',G)$.Return the expanded interaction term after Hartree-Fock approximation as $H_{int,MF}$.

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):$t_s(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is the hopping between the moir'e lattice site i and j, fitted from the first moir'e valence band of twisted WSe$_2$ at $\pm K$ valleys in the noninteracting picture, and $s =\uparrow$ and $\downarrow$ are coupled with the $+K$ and $-K$ valleys. $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$ describes the Coulomb repulsion between site i and j.

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: Using Wick's theorem, we can expand the four-fermion term in H_{int} into quadratic terms. Following the convention in EXAMPLE 1, we have:

$c^\dagger_{k,s}c_{q,s}c^\dagger_{k',s'}c_{q',s'} = \langle c^\dagger_{k,s}c_{q',s'}\rangle c_{q,s}c_{k',s'} + \langle c_{q,s}c_{k',s'}\rangle c^\dagger_{k,s}c_{q',s'} - \langle c^\dagger_{k,s}c_{q',s'}\rangle\langle c_{q,s}c_{k',s'}\rangle - \langle c^\dagger_{k,s}c_{k',s'}\rangle c_{q,s}c_{q',s'} - \langle c_{q,s}c_{q',s'}\rangle c^\dagger_{k,s}c_{k',s'} + \langle c^\dagger_{k,s}c_{k',s'}\rangle\langle c_{q,s}c_{q',s'}\rangle$.

Substituting this expansion back into H_{int}, we get:

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

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 $H_{int,MF}$.The quadratic terms mean terms that are proportional to $c^\dagger c$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in $H_{int,MF}$, denoted as $H_{quadratic}$.You should recall that $H_{int,MF}$ is

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

Return $H_{quadratic}$.

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):$t_s(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is the hopping between the moir'e lattice site i and j, fitted from the first moir'e valence band of twisted WSe$_2$ at $\pm K$ valleys in the noninteracting picture, and $s = \uparrow$ and $\downarrow$ are coupled with the $+K$ and $-K$ valleys. $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$ describes the Coulomb repulsion between site i and j.

Completion: The quadratic terms in the Hartree-Fock approximation of the interaction Hamiltonian, $H_{\text{int,MF}}$, are those proportional to $c^\dagger c$. These terms do not include expectations or products of expectations.

From the given $H_{\text{int,MF}}$, the quadratic terms are:

$\langle c^\dagger_{k,s} c_{q,s} \rangle c^\dagger_{k',s'} c_{q',s'}$ and $\langle c^\dagger_{k',s'} c_{q',s'} \rangle c^\dagger_{k,s} c_{q,s}$.

Therefore, the quadratic terms in $H_{\text{int,MF}}$, denoted as $H_{\text{quadratic}}$, are:

$H_{\text{quadratic}} = \frac{1}{2N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q) \left[\langle c^\dagger_{k,s} c_{q,s} \rangle c^\dagger_{k',s'} c_{q',s'} + \langle c^\dagger_{k',s'} c_{q',s'} \rangle c^\dagger_{k,s} c_{q,s} \right] \sum_G \delta(k-q+k'-q', G)$.

7 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $H_{\text{quadratic}}$. If you find the $V(q)$ in $H_{\text{quadratic}}$ 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 $H_{\text{quadratic}}$ is $H_{\text{quadratic}} = \frac{1}{2N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q) \left[\langle c^\dagger_{k,s} c_{q,s} \rangle c^\dagger_{k',s'} c_{q',s'} + \langle c^\dagger_{k',s'} c_{q',s'} \rangle c^\dagger_{k,s} c_{q,s} - \langle c^\dagger_{k,s} c_{q',s'} \rangle c^\dagger_{k',s'} c_{q,s} - \langle c^\dagger_{k',s'} c_{q,s} \rangle c^\dagger_{k,s} c_{q',s'} \right] \sum_G \delta(k-q+k'-q', G)$. Return $H_{\text{quadratic}}$ with expanded interaction.

Completion: The interaction term $U(k-q)$ in $H_{\text{quadratic}}$ contains the momentum q which is not in the summation sign. Therefore, we need to expand $U(k-q)$ by replacing q with the momentum $\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta$. After expanding the interaction term, the $H_{\text{quadratic}}$ becomes:

$$H_{\text{quadratic}} = \frac{1}{2N} \sum_{s,s'} \sum_{k,k',q,q'} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \left[\langle c^\dagger_{k,s} c_{q,s} \rangle c^\dagger_{k',s'} c_{q',s'} + \langle c^\dagger_{k',s'} c_{q',s'} \rangle c^\dagger_{k,s} c_{q,s} - \langle c^\dagger_{k,s} c_{q',s'} \rangle c^\dagger_{k',s'} c_{q,s} \right.$$
$$\left. - \langle c^\dagger_{k',s'} c_{q,s} \rangle c^\dagger_{k,s} c_{q',s'} \right] \sum_G \delta(k-q+k'-q', G).$$

8 Relabel the index

Prompt: You will be instructed to simplify the quadratic term H_{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 $\boldsymbol{k}_\gamma \leftrightarrow \boldsymbol{k}_\delta$ is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes nothing here.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} is $H_{\text{quadratic}} = \frac{1}{2N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q) \left[\langle c^\dagger_{k,s} c_{q,s} \rangle c^\dagger_{k',s'} c_{q',s'} + \langle c^\dagger_{k',s'} c_{q',s'} \rangle c^\dagger_{k,s} c_{q,s} - \langle c^\dagger_{k,s} c_{q',s'} \rangle c^\dagger_{k',s'} c_{q,s} - \langle c^\dagger_{k',s'} c_{q,s} \rangle c^\dagger_{k,s} c_{q',s'} \right] \sum_G \delta(k-q+k'-q', G)$ Return the simplified H_{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_{int} by relabeling the index. Specifically, we swap the indices in the expected value and the quadratic operators in the second Hartree or Fock term.

For the second Hartree term, we swap $k \leftrightarrow k'$ and $q \leftrightarrow q'$. After the replacement, the second Hartree term becomes $\langle c_{k',s'}^\dagger c_{q',s'} \rangle c_{k,s}^\dagger c_{q,s}$.

For the second Fock term, we swap $k \leftrightarrow k'$ and $q \leftrightarrow q'$. After the replacement, the second Fock term becomes $-\langle c_{k',s'}^\dagger c_{q,s} \rangle c_{k,s}^\dagger c_{q',s'}$.

Therefore, the simplified H_{int} is:

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

This simplification is valid as long as $U(q) = U(-q)$, which is naturally satisfied in Coulomb interaction.

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 $\langle c_{k,s}^\dagger c_{q,s} \rangle$.The expected value $\langle c_{k,s}^\dagger c_{q,s} \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c_{k,s}^\dagger c_{q,s} \rangle = \langle c_{k,s}^\dagger c_{q,s} \rangle \delta_{k,q}$.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 Hartree term, and another momentum in the quadratic term.You should recall that H_{Hartree} is $H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q) \langle c_{k,s}^\dagger c_{q,s} \rangle c_{k',s'}^\dagger c_{q',s'} \sum_G \delta(k - q + k' - q', G)$..Return the final simplified Hartree term H_{Hartree}.

EXAMPLE:Given a Hamiltonian where the Hartree term

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

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: The Hartree term H_{Hartree} is given by:

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q) \langle c_{k,s}^\dagger c_{q,s} \rangle c_{k',s'}^\dagger c_{q',s'} \sum_G \delta(k - q + k' - q', G)$$

The expected value $\langle c_{k,s}^\dagger c_{q,s} \rangle$ is nonzero only when $k = q$, i.e., $\langle c_{k,s}^\dagger c_{q,s} \rangle = \langle c_{k,s}^\dagger c_{q,s} \rangle \delta_{k,q}$.

Substituting this into the Hartree term, we get:

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q) \langle c_{k,s}^\dagger c_{q,s} \rangle \delta_{k,q} c_{k',s'}^\dagger c_{q',s'} \sum_G \delta(k - q + k' - q', G)$$

Using the property of the Kronecker delta function $\delta_{k,q}$ to sum over q, we get:

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k',q'} U(0) \langle c_{k,s}^\dagger c_{k,s} \rangle c_{k',s'}^\dagger c_{q',s'} \sum_G \delta(k + k' - q', G)$$

The total momentum conservation $\delta(k + k' - q', G)$ is nonzero only when $k' + q' = k + G$, i.e., $\delta(k + k' - q', G) = \delta_{k',q'} \delta_{k,G}$.

Substituting this into the Hartree term, we get:

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k',q'} U(0)\langle c_{k,s}^\dagger c_{k,s}\rangle \delta_{k',q'} c_{k',s'}^\dagger c_{q',s'} \sum_G \delta_{k,G}$$

Using the property of the Kronecker delta function $\delta_{k',q'}$ to sum over q', we get:

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k'} U(0)\langle c_{k,s}^\dagger c_{k,s}\rangle c_{k',s'}^\dagger c_{k',s'} \sum_G \delta_{k,G}$$

Finally, we can simplify the Hartree term by summing over G:

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k'} U(0)\langle c_{k,s}^\dagger c_{k,s}\rangle c_{k',s'}^\dagger c_{k',s'}$$

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

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k'} U(0)\langle c_{k,s}^\dagger c_{k,s}\rangle c_{k',s'}^\dagger c_{k',s'}$$

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 $\langle c_{k,s}^\dagger c_{q',s'}\rangle$.The expected value $\langle c_{k,s}^\dagger c_{q',s'}\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c_{k,s}^\dagger c_{q',s'}\rangle = \langle c_{k,s}^\dagger c_{q',s'}\rangle \delta_{k,q'}$.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 $H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q)\langle c_{k,s}^\dagger c_{q',s'}\rangle c_{k',s'}^\dagger c_{q,s} \sum_G \delta(k-q+k'-q',G)$.Return the final simplified Fock term H_{Fock}.
EXAMPLE:Given a Hamiltonian where the Fock term $\hat{H}^{Fock} = -\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, 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

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

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

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: Given the Fock term $H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q)\langle c_{k,s}^\dagger c_{q',s'}\rangle c_{k',s'}^\dagger c_{q,s} \sum_G \delta(k-q+k'-q',G)$, we can simplify it by reducing the momentum inside the expected value $\langle c_{k,s}^\dagger c_{q',s'}\rangle$.
We know that $\langle c_{k,s}^\dagger c_{q',s'}\rangle$ is nonzero only when $k=q'$, i.e., $\langle c_{k,s}^\dagger c_{q',s'}\rangle = \langle c_{k,s}^\dagger c_{q',s'}\rangle \delta_{k,q'}$.
Substituting this into the Fock term, we get:
$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,k',q,q'} U(k-q)\langle c_{k,s}^\dagger c_{q',s'}\rangle \delta_{k,q'} c_{k',s'}^\dagger c_{q,s} \sum_G \delta(k-q+k'-q',G)$.
Using the property of the Kronecker delta function $\delta_{k,q'}$ to sum over q', we obtain:

$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,k',q} U(k-q) \langle c^\dagger_{k,s} c_{k,s'} \rangle c^\dagger_{k',s'} c_{q,s} \sum_G \delta(k - q + k' - q, G).$

Next, we notice that the total momentum conservation will reduce another momentum in the quadratic term. The Kronecker delta function $\delta(k - q + k' - q, G)$ is nonzero only when $k' - q = k$, i.e., $\delta(k - q + k' - q, G) = \delta_{k,k'} \delta_{G,0}$.

Substituting this into the Fock term, we get:

$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,k',q} U(k-q) \langle c^\dagger_{k,s} c_{k,s'} \rangle c^\dagger_{k',s'} c_{q,s} \delta_{k,k'} \delta_{G,0}.$

Using the property of the Kronecker delta function $\delta_{k,k'}$ to sum over k', we obtain:

$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,q} U(k-q) \langle c^\dagger_{k,s} c_{k,s'} \rangle c^\dagger_{k,s'} c_{q,s} \delta_{G,0}.$

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

$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,q} U(k-q) \langle c^\dagger_{k,s} c_{k,s'} \rangle c^\dagger_{k,s'} c_{q,s} \delta_{G,0}.$

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 $H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k'} U(0) \langle c^\dagger_{k,s} c_{k,s} \rangle c^\dagger_{k',s'} c_{k',s'}$, and the Fock term $H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,q} U(k-q) \langle c^\dagger_{k,s} c_{k,s'} \rangle c^\dagger_{q,s'} c_{q,s}$. 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 : Not needed. 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} can be combined as follows:

First, we relabel the indices in the Fock term. Since the instruction specifies that no swap is needed, the Fock term remains the same:

$$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k,q} U(k-q) \langle c^\dagger_{k,s} c_{k,s'} \rangle c^\dagger_{q,s'} c_{q,s}$$

Next, we add the Hartree term and the Fock term:

$$H_{\text{HF}} = H_{\text{Hartree}} + H_{\text{Fock}}$$

Substituting the expressions for the Hartree and Fock terms, we get:

$$H_{\text{HF}} = \frac{1}{N} \sum_{s,s'} \sum_{k,k'} U(0) \langle c^\dagger_{k,s} c_{k,s} \rangle c^\dagger_{k',s'} c_{k',s'} - \frac{1}{N} \sum_{s,s'} \sum_{k,q} U(k-q) \langle c^\dagger_{k,s} c_{k,s'} \rangle c^\dagger_{q,s'} c_{q,s}$$

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