1 Identify kinetic term (lattice)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in a system with a triangular lattice in the real space in the second-quantized form.The degrees of freedom of the system are: spin states associated with $+K$ and $-K$ valleysThe kinetic term is a tight-binding model composed of the following hopping process: between site i and site j with the amplitude $t_s\left(\boldsymbol{R}_i-\boldsymbol{R}_j\right)$

The summation should be taken over all spin states associated with $+K$ and $-K$ valleys and all real space positions.Return the Kinetic Hamiltonian H_{TB}.

Use the following conventions for the symbols:$s= \uparrow,\downarrow$ represents spin $\uparrow$ and $\downarrow$ states associated respectively with $+K$ and $-K$ valleys, $\boldsymbol{R}_i$ represents a site in the triangular lattice, and $c_{j,s}$ ($c_{j,s}^{\dagger}$) is electron annihilation (creation) operator. $t_s\left(\boldsymbol{R}_i-\boldsymbol{R}_j\right)$ is the hopping parameter.

Completion: The kinetic term of the Hamiltonian in the second-quantized form for a system with a triangular lattice in real space, considering the given degrees of freedom and hopping process, can be written as:

$$H_{\mathrm{TB}}=-\sum_{\boldsymbol{R}_i,\boldsymbol{R}_j,s} t_s\left(\boldsymbol{R}_i-\boldsymbol{R}_j\right) c_{i,s}^{\dagger} c_{j,s} \tag{1}$$

Here, the summation is taken over all spin states associated with $+K$ and $-K$ valleys ($s=\uparrow,\downarrow$) and all real space positions ($\boldsymbol{R}_i$ and $\boldsymbol{R}_j$). The term $c_{i,s}^{\dagger} c_{j,s}$ represents the process of an electron hopping from site j to site i with spin state s. The hopping parameter $t_s\left(\boldsymbol{R}_i-\boldsymbol{R}_j\right)$ determines the amplitude of this process. The negative sign in front of the summation indicates that the energy of the system 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, $\hat{H}^{int}$ in the real space in the second-quantized form.The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian $\hat{H}_{Kinetic}$.The interaction is a density-density interaction composed of the following process: between sites i and 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 $\hat{H}^{int}$ in terms of $n_s^{\dagger}(R_i)$.

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 is the hopping parameter, $c_{i,s}^{\dagger}$ and $c_{j,s}$ are the creation and annihilation operators, respectively, $U(\boldsymbol{R}_i-\boldsymbol{R}_j)$ is the repulsion between sites i and j, and ϵ is the effective background dielectric constant.

Completion: The interaction part of the Hamiltonian, $\hat{H}^{int}$, in the real space in the second-quantized form can be constructed as follows:

$$\hat{H}^{int} = \frac{1}{2} \sum_{s,s'=\uparrow,\downarrow} \sum_{\boldsymbol{R}_i,\boldsymbol{R}_j} U(\boldsymbol{R}_i - \boldsymbol{R}_j) n_s(\boldsymbol{R}_i) n_{s'}(\boldsymbol{R}_j) \tag{2}$$

Here, $n_s(\boldsymbol{R}_i) = c^\dagger_{i,s} c_{i,s}$ is the number operator, representing the electron density at site i with spin s. The factor of 1/2 is to avoid double counting of interactions. The sum is taken over all spin states s and s' and all real space positions $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$. The interaction strength $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$ represents the repulsion between sites i and j.

3 Fourier transform noninteracting term to momentum space (lattice)

Prompt: You will be instructed to convert the noninteracting Hamiltonian $\hat{H}_{Kinetic}$ 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 $c_s^\dagger(R_i)$ in the real space to the $c_s^\dagger(k)$ in the momentum space, which is defined as $c_s^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_s^\dagger(R_i) e^{ik\cdot R_i}$, where i is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. You should recall that

$$\hat{H}_{Kinetic} = \sum_{R_i,R_j} \sum_{s=\uparrow,\downarrow} t_s(R_i - R_j)\, c_s^\dagger(R_i) c_s(R_j) \tag{3}$$

Express the total noninteracting Hamiltonian $\hat{H}_{Kinetic}$ in terms of $c_s^\dagger(k)$. 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): $c_s(k)$: electron annihilation operator at momentum k, spin $sc_s^\dagger(k)$: electron creation operator at momentum k, spin sN : number of the unit cells in the 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

$$\begin{aligned} \hat{H} &= \sum_{i,j} t(R_i - R_j) \frac{1}{\sqrt{N}} \sum_{k_1} c^\dagger(k_1) e^{-ik_1\cdot R_i} \frac{1}{\sqrt{N}} \sum_{k_2} c(k_2) e^{ik_2\cdot R_j} \\ &= \frac{1}{N} \sum_{i,j} \sum_{k_1,k_2} c^\dagger(k_1) c(k_2) e^{-ik_1\cdot R_i} e^{ik_2\cdot R_j} t(R_i - R_j) \end{aligned} \tag{4}$$

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

$$\hat{H} = \frac{1}{N} \sum_{i,n} \sum_{k_1,k_2} c^\dagger(k_1) c(k_2) t(n) e^{-i(k_1-k_2)\cdot R_i} e^{-ik_2\cdot n} \tag{5}$$

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

$$\hat{H} = \sum_{k_1,k_2} \sum_n t(n) e^{-ik_2\cdot n} c^\dagger(k_1) c(k_2) \delta(k_1, k_2) \tag{6}$$

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

$$\hat{H} = \sum_{k_1} \sum_n t(n) e^{-ik_1\cdot n} c^\dagger(k_1) c(k_1) \tag{7}$$

For simplicity, we replace k_1 with k, we obtain

$$\hat{H} = \sum_k \sum_n t(n) e^{-ik\cdot n} c^\dagger(k) c(k) \tag{8}$$

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

$$\hat{H} = \sum_k E(k) c^\dagger(k) c(k) \tag{9}$$

Completion: To convert the noninteracting Hamiltonian $\hat{H}_{Kinetic}$ from the basis in real space to the basis in momentum space, we first apply the Fourier transformation to the creation and annihilation operators.

The Fourier transformations are defined as:

$c_s^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_s^\dagger(R_i) e^{ik\cdot R_i}$

$c_s(k) = \frac{1}{\sqrt{N}} \sum_i c_s(R_i) e^{-ik\cdot R_i}$

Substituting these into the kinetic Hamiltonian, we get:

$\hat{H}_{Kinetic} = \sum_{R_i,R_j} \sum_{s=\uparrow,\downarrow} t_s(R_i - R_j) \frac{1}{N} \sum_{k_1} c_s^\dagger(k_1) e^{-ik_1\cdot R_i} \frac{1}{N} \sum_{k_2} c_s(k_2) e^{ik_2\cdot R_j}$

Simplifying, we get:

$\hat{H}_{Kinetic} = \frac{1}{N} \sum_{R_i,R_j} \sum_{s=\uparrow,\downarrow} \sum_{k_1,k_2} t_s(R_i - R_j)\, c_s^\dagger(k_1) c_s(k_2) e^{-i(k_1\cdot R_i - k_2\cdot R_j)}$

Now, we make a replacement by defining $n = R_i - R_j$, and the Hamiltonian becomes:

$\hat{H}_{Kinetic} = \frac{1}{N} \sum_{R_i,n} \sum_{s=\uparrow,\downarrow} \sum_{k_1,k_2} t_s(n)\, c_s^\dagger(k_1) c_s(k_2) e^{-i(k_1-k_2)\cdot R_i} e^{-ik_2\cdot n}$

Using the property of the Kronecker delta function, $\frac{1}{N} \sum_{R_i} e^{-i(k_1-k_2)\cdot R_i} = \delta(k_1, k_2)$, we get:

$\hat{H}_{Kinetic} = \sum_n \sum_{s=\uparrow,\downarrow} \sum_{k_1,k_2} t_s(n)\, c_s^\dagger(k_1) c_s(k_2) e^{-ik_2\cdot n} \delta(k_1, k_2)$

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

$\hat{H}_{Kinetic} = \sum_n \sum_{s=\uparrow,\downarrow} \sum_k t_s(n)\, c_s^\dagger(k) c_s(k) e^{-ik\cdot n}$

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 kinetic Hamiltonian in the momentum space is:

$\hat{H}_{Kinetic} = \sum_{s=\uparrow,\downarrow} \sum_k E_s(k) c_s^\dagger(k) c_s(k)$

4 Fourier transform interacting term to momentum space (lattice)

Prompt: You will be instructed to convert the interacting Hamiltonian, $\hat{H}^{int}$, 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 $c_s^\dagger(R_i)$ in the real space to the $c_s^\dagger(k)$ in the momentum space, which is defined as c*s^\dagger(k)= \frac{1}{\sqrt{N}} \sum*i c*s^\dagger(R*i) e^{i k \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 $\hat{H}^{int}$ is

$$\hat{H}^{int} = \frac{1}{2} \sum_{R_i, R_j} \sum_{s,s'=\uparrow,\downarrow} U(R_i - R_j)\, n_s(R_i) n_{s'}(R_j)\,. \tag{10}$$

Express $\hat{H}^{int}$ in terms of $c_s^\dagger(k)$. 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

$$\begin{aligned} \hat{H}^{int} &= \sum_{s,s'} \sum_{i,j} U(R_i \\ &- R_j) \frac{1}{\sqrt{N}} \sum_{k_1} c_s^\dagger(k_1) e^{-ik_1\cdot R_i} \frac{1}{\sqrt{N}} \sum_{k_2} c_{s'}^\dagger(k_2) e^{-ik_2\cdot R_j} \frac{1}{\sqrt{N}} \sum_{k_3} c_{s'}(k_3) e^{ik_3\cdot R_j} \frac{1}{\sqrt{N}} \sum_{k_4} c_s(k_4) e^{ik_4\cdot R_i} \\ &= \sum_{s,s'} \sum_{i,j} \frac{1}{N^2} \sum_{k_1,k_2,k_3,k_4} U(R_i \\ &\qquad - R_j) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) e^{-i(k_1-k_4)\cdot R_i} e^{-i(k_2-k_3)\cdot R_j} \end{aligned} \tag{11}$$

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

$$\begin{aligned} &\hat{H}^{int} \\ &= \frac{1}{N^2} \sum_{j,n} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(n) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) e^{-i(k_1-k_4)\cdot n} e^{-i(k_1-k_4+k_2-k_3)\cdot r_j} \end{aligned} \tag{12}$$

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,

$$\begin{aligned} \hat{H}^{int} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} \sum_{n} U(n) e^{-i(k_1-k_4)\cdot n} c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(k_1 \\ - k_4 + k_2 - k_3, G) \end{aligned} \tag{13}$$

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

$$\hat{H}^{int} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1 - k_4)c_s^\dagger(k_1)c_{s'}^\dagger(k_2)c_{s'}(k_3)c_s(k_4)\sum_G \delta(k_1 - k_4 + k_2 - k_3, G) \tag{14}$$

Completion: Following the example provided, we first express the number operators $n_s(R_i)$ and $n_{s'}(R_j)$ in terms of the creation and annihilation operators:

$$n_s(R_i) = c_s^\dagger(R_i)c_s(R_i) \tag{15}$$

$$n_{s'}(R_j) = c_{s'}^\dagger(R_j)c_{s'}(R_j) \tag{16}$$

Substituting these into the interacting Hamiltonian $\hat{H}^{int}$, we get:

$$\hat{H}^{int} = \frac{1}{2}\sum_{R_i,R_j}\sum_{s,s'=\uparrow,\downarrow} U(R_i - R_j)\, c_s^\dagger(R_i)c_s(R_i)c_{s'}^\dagger(R_j)c_{s'}(R_j) \tag{17}$$

Next, we apply the Fourier transformation to the creation and annihilation operators:

$$c_s^\dagger(R_i) = \frac{1}{\sqrt{N}}\sum_k c_s^\dagger(k)e^{-ik\cdot R_i} \tag{18}$$

$$c_s(R_i) = \frac{1}{\sqrt{N}}\sum_{k'} c_s(k')e^{ik'\cdot R_i} \tag{19}$$

$$c_{s'}^\dagger(R_j) = \frac{1}{\sqrt{N}}\sum_{k''} c_{s'}^\dagger(k'')e^{-ik''\cdot R_j} \tag{20}$$

$$c_{s'}(R_j) = \frac{1}{\sqrt{N}}\sum_{k'''} c_{s'}(k''')e^{ik'''\cdot R_j} \tag{21}$$

Substituting these into $\hat{H}^{int}$, we get:

$$\hat{H}^{int} = \frac{1}{2N^2}\sum_{R_i,R_j}\sum_{s,s'=\uparrow,\downarrow}\sum_{k,k',k'',k'''} U(R_i - R_j)\, c_s^\dagger(k)e^{-ik\cdot R_i}c_s(k')e^{ik'\cdot R_i}c_{s'}^\dagger(k'')e^{-ik''\cdot R_j}c_{s'}(k''')e^{ik'''\cdot R_j} \tag{22}$$

Simplifying, we get:

$$\hat{H}^{int} = \frac{1}{2N^2} \sum_{s,s'=\uparrow,\downarrow} \sum_{k,k',k'',k'''} \sum_{R_i,R_j} U(R_i - R_j)\, c_s^\dagger(k) c_s(k') c_{s'}^\dagger(k'') c_{s'}(k''') e^{-i(k-k')\cdot R_i} e^{-i(k''-k''')\cdot R_j} \tag{23}$$

Now, we define $n = R_i - R_j$ and make the replacement:

$$\hat{H}^{int} = \frac{1}{2N^2} \sum_{s,s'=\uparrow,\downarrow} \sum_{k,k',k'',k'''} \sum_{n} U(n)\, c_s^\dagger(k) c_s(k') c_{s'}^\dagger(k'') c_{s'}(k''') e^{-i(k-k')\cdot n} e^{-i(k''-k''')\cdot(n+R_j)} \tag{24}$$

Using the property of the Kronecker delta function, we get:

$$\hat{H}^{int} = \frac{1}{2N} \sum_{s,s'=\uparrow,\downarrow} \sum_{k,k',k'',k'''} \sum_{n} U(n)\, c_s^\dagger(k) c_s(k') c_{s'}^\dagger(k'') c_{s'}(k''') e^{-i(k-k')\cdot n} \sum_G \delta(k - k' + k'' - k''', G) \tag{25}$$

Finally, if we define the interaction in the momentum space as $U(k) = \sum_n U(n) e^{-ik\cdot n}$, the interacting Hamiltonian in the momentum space is:

$$\hat{H}^{int} = \frac{1}{2N} \sum_{s,s'=\uparrow,\downarrow} \sum_{k,k',k'',k'''} U(k-k')\, c_s^\dagger(k) c_s(k') c_{s'}^\dagger(k'') c_{s'}(k''') \sum_G \delta(k - k' + k'' - k''', G) \tag{26}$$

5 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $\hat{H}^{int}$.You should use Wick's theorem to expand the four-fermion term in $\hat{H}^{int}$ 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

$$\hat{H}^{int} = \frac{1}{2N} \sum_{s,s'} \sum_{k_1,k_2,k_3,k_4} U(k_1-k_4) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(k_1 - k_4 + k_2 - k_3, G)\,. \tag{27}$$

Return the expanded interaction term after Hartree-Fock approximation as $\hat{H}^{int,HF}$.

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):$\langle c_s^\dagger(k_1) c_{s'}(k_2)\rangle$: expectation of $c_s^\dagger(k_1) c_{s'}(k_2)$ over the many-body ground states.$\hat{H}^{int,HF}$: Interaction term after Hartree-Fock approximation

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 $\hat{H}^{int}$ into quadratic terms. The interaction term in the Hamiltonian is given by:

$$\hat{H}^{int} = \frac{1}{2N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(k_1 - k_4 + k_2 - k_3, G) \tag{28}$$

This term is similar to the four-fermion term in EXAMPLE 1, so we can expand it in a similar way:

$$\begin{aligned}\hat{H}^{int} = \frac{1}{2N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4) \Big[&\langle c_s^\dagger(k_1) c_s(k_4)\rangle c_{s'}^\dagger(k_2) c_{s'}(k_3) \\ &+ \langle c_{s'}^\dagger(k_2) c_{s'}(k_3)\rangle c_s^\dagger(k_1) c_s(k_4) - \langle c_s^\dagger(k_1) c_s(k_4)\rangle\langle c_{s'}^\dagger(k_2) c_{s'}(k_3)\rangle \\ &- \langle c_s^\dagger(k_1) c_{s'}(k_3)\rangle c_{s'}^\dagger(k_2) c_s(k_4) - \langle c_{s'}^\dagger(k_2) c_s(k_4)\rangle c_s^\dagger(k_1) c_{s'}(k_3) \\ &+ \langle c_s^\dagger(k_1) c_{s'}(k_3)\rangle\langle c_{s'}^\dagger(k_2) c_s(k_4)\rangle\Big] \sum_G \delta(k_1 - k_4 + k_2 - k_3, G)\end{aligned} \tag{29}$$

After the Hartree-Fock approximation, we only preserve the normal terms, which are the product of a creation operator and an annihilation operator. Therefore, the expanded interaction term after Hartree-Fock approximation is:

$$\begin{aligned}\hat{H}^{int,HF} = \frac{1}{2N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4) \Big[&\langle c_s^\dagger(k_1) c_s(k_4)\rangle c_{s'}^\dagger(k_2) c_{s'}(k_3) \\ &+ \langle c_{s'}^\dagger(k_2) c_{s'}(k_3)\rangle c_s^\dagger(k_1) c_s(k_4)\Big] \sum_G \delta(k_1 - k_4 + k_2 - k_3, G)\end{aligned} \tag{30}$$

6 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the $\hat{H}^{HF}$.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 $\hat{H}^{HF}$, denoted as $\hat{H}^{HF,2}$.You should recall that $\hat{H}^{HF}$ is

$$\hat{H}^{int,HF} = \frac{1}{2N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4)\Big(\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3) \\ + \langle c_{s'}^\dagger(k_2)c_{s'}(k_3)\rangle c_s^\dagger(k_1)c_s(k_4) - \langle c_s^\dagger(k_1)c_s(k_4)\rangle\langle c_{s'}^\dagger(k_2)c_{s'}(k_3)\rangle \\ - \langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle c_{s'}^\dagger(k_2)c_s(k_4) - \langle c_{s'}^\dagger(k_2)c_s(k_4)\rangle c_s^\dagger(k_1)c_{s'}(k_3) \\ + \langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle\langle c_{s'}^\dagger(k_2)c_s(k_4)\rangle\Big)\sum_G \delta(k_1-k_4+k_2-k_3,G).. \tag{31}$$

Return $\hat{H}^{HF,2}$.

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):$\hat{H}^{HF,2}$: the quadratic terms in $\hat{H}^{HF}$.

Completion: The quadratic terms in $\hat{H}^{HF}$, denoted as $\hat{H}^{HF,2}$, are those terms that are proportional to $c^\dagger c$. These terms exclude those that are solely expectations or products of expectations. From the given $\hat{H}^{int,HF}$, the quadratic terms are:

$$\hat{H}^{HF,2} = \frac{1}{2N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4)\Big[\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3) \\ + \langle c_{s'}^\dagger(k_2)c_{s'}(k_3)\rangle c_s^\dagger(k_1)c_s(k_4) - \langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle c_{s'}^\dagger(k_2)c_s(k_4) \\ - \langle c_{s'}^\dagger(k_2)c_s(k_4)\rangle c_s^\dagger(k_1)c_{s'}(k_3)\Big]\sum_G \delta(k_1-k_4+k_2-k_3,G) \tag{32}$$

This is the quadratic part of the Hartree-Fock Hamiltonian.

7 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $\hat{H}^{HF,2}$. If you find the $V(q)$ in $\hat{H}^{HF,2}$ 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_i. You should recall that $\hat{H}^{HF,2}$ is
$\hat{H}^{int,HF,2} = \frac{1}{2N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4)\Big(\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3) + \langle c_{s'}^\dagger(k_2)c_{s'}(k_3)\rangle c_s^\dagger(k_1)c_s(k_4) - \langle c_s^\dagger(k$
$k_4+k_2-k_3, G)$. Return $\hat{H}^{HF,2}$ with expanded interaction.

Completion: The interaction term $V(q)$ in $\hat{H}^{HF,2}$ is represented by $U(k_1-k_4)$. This term already contains momenta k_1 and k_4 that are in the summation sign. Therefore, the interaction term is already expanded and there is no need to replace q with any other momentum k_i.

So, the $\hat{H}^{HF,2}$ with the expanded interaction term remains the same:

$$
\begin{aligned}
\hat{H}^{HF,2} = \frac{1}{2N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4)\Big[&\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3) \\
&+\langle c_{s'}^\dagger(k_2)c_{s'}(k_3)\rangle c_s^\dagger(k_1)c_s(k_4) - \langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle c_{s'}^\dagger(k_2)c_s(k_4) \\
&-\langle c_{s'}^\dagger(k_2)c_s(k_4)\rangle c_s^\dagger(k_1)c_{s'}(k_3)\Big]\sum_G \delta(k_1-k_4+k_2-k_3,G)
\end{aligned}
\tag{33}
$$

8 Relabel the index

Prompt: You will be instructed to simplify the quadratic term $\hat{H}^{HF,2}$ through relabeling the index.The logic is that the expected value ($\langle c_s^\dagger(k_1)c_s(k_4)\rangle$) in the first Hartree term ($\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3)$) has the same form as the quadratic operators in the second Hartree term ($\langle c_{s'}^\dagger(k_2)c_{s'}(k_3)\rangle c_s^\dagger(k_1)c_s(k_4)$), and vice versa. The same applies to the Fock term.Namely, a replacement of 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 $\hat{H}^{HF,2}$ is $\hat{H}^{int,HF,2}=\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4}U(k_1-k_4)\left(\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3)-\langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle c_{s'}^\dagger(k_2)c_s(k_4)\right)\sum_G\delta(k_1-k_4+k_2-k_3,G)$ Return the simplified $\hat{H}^{HF,2}$.

EXAMPLE:Given a Hamiltonian $\hat{H}=\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4}V(k_1-k_4)(\langle c_{d,\sigma_1}^\dagger(k_1)c_{d,\sigma_4}(k_4)\rangle c_{p,\sigma_2}^\dagger(k_2)c_{p,\sigma_3}(k_3)$ $\langle c_{p,\sigma_2}^\dagger(k_2)c_{d,\sigma_3}(k_3)\rangle c_{d,\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4))\delta_{k_1+k_2,k_3+k_4}$, 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: To simplify the quadratic term $\hat{H}^{HF,2}$, we can relabel the indices in the second Hartree and Fock terms. We swap s and s', and k_1 with k_2, and k_3 with k_4. After the replacement, the second Hartree term becomes:

$$
\langle c_{s'}^\dagger(k_2)c_{s'}(k_3)\rangle c_s^\dagger(k_1)c_s(k_4) \tag{34}
$$

and the second Fock term becomes:

$$\langle c_{s'}^\dagger(k_2) c_s(k_1)\rangle c_s^\dagger(k_4) c_{s'}(k_3) \tag{35}$$

The Kronecker delta function $\delta(k_1-k_4+k_2-k_3,G)$ implies $k_1+k_2=k_3+k_4$, i.e., $k_2-k_3=k_4-k_1$. Thus, the interaction term $U(k_1-k_4)$ in the second Hartree and Fock terms can be rewritten as $U(k_2-k_3)$.

Because $U(q)=U(-q)$, meaning $U(k_2-k_3)=U(k_1-k_4)$, the second Hartree and Fock terms can be simplified to:

$$U(k_1-k_4)\langle c_{s'}^\dagger(k_2) c_{s'}(k_3)\rangle c_s^\dagger(k_1) c_s(k_4) \tag{36}$$

and

$$U(k_1-k_4)\langle c_{s'}^\dagger(k_2) c_s(k_1)\rangle c_s^\dagger(k_4) c_{s'}(k_3) \tag{37}$$

respectively.

Therefore, the simplified $\hat{H}^{HF,2}$ is:

$$\begin{aligned}\hat{H}^{HF,2} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4)\Big(&\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3) \\ &+\langle c_{s'}^\dagger(k_2)c_{s'}(k_3)\rangle c_s^\dagger(k_1)c_s(k_4) - \langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle c_{s'}^\dagger(k_2)c_s(k_4) \\ &-\langle c_{s'}^\dagger(k_2)c_s(k_1)\rangle c_s^\dagger(k_4)c_{s'}(k_3)\Big)\sum_G \delta(k_1-k_4+k_2-k_3,G)\end{aligned} \tag{38}$$

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 $\langle c_s^\dagger(k_1)c_s(k_4)\rangle$.The expected value $\langle c_s^\dagger(k_1)c_s(k_4)\rangle$ is only nonzero when the two momenta k_i,k_j are the same, namely, $\langle c_s^\dagger(k_1)c_s(k_4)\rangle = \langle c_s^\dagger(k_1)c_s(k_4)\rangle\delta_{k_1,k_4}$.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 Hartree term, and another momentum in the quadratic term.You should recall that H_{Hartree} is $\hat{H}^{int,HF,2} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4)\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3)\sum_G \delta(k_1-k_4+k_2-k_3,G)$.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 $\sum_{k_1,k_2,k_3,s_1,s_2}V(k_1-k_1)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3)\sum_G\delta_{k_1+k_2-k_3-k_1,G}=\sum_{k_1,k_2,k_3,s_1,s_2}V(0)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3)\sum_G\delta_k$ 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 $\sum_{k_1,k_2,k_3,s_1,s_2}V(0)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3)\delta_{k_2-k_3,0}=\sum_{k_1,k_2,s_1,s_2}V(0)\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1)\rangle c_{s_2}^\dagger(k_2$ fore, 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:

$$H_{\text{Hartree}}=\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4}U(k_1-k_4)\langle c_s^\dagger(k_1)c_s(k_4)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3)\sum_G\delta(k_1-k_4+k_2-k_3,G) \tag{39}$$

We know that $\langle c_s^\dagger(k_1)c_s(k_4)\rangle$ is nonzero only when $k_1=k_4$, i.e., $\langle c_s^\dagger(k_1)c_s(k_4)\rangle=\langle c_s^\dagger(k_1)c_s(k_4)\rangle\delta_{k_1,k_4}$.

Substituting this into the Hartree term, we get:

$$H_{\text{Hartree}}=\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4}U(k_1-k_4)\langle c_s^\dagger(k_1)c_s(k_4)\rangle\delta_{k_1,k_4}c_{s'}^\dagger(k_2)c_{s'}(k_3)\sum_G\delta(k_1-k_4+k_2-k_3,G) \tag{40}$$

Using the property of the Kronecker delta function δ_{k_1,k_4} to sum over k_4, we get:

$$H_{\text{Hartree}}=\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3}U(0)\langle c_s^\dagger(k_1)c_s(k_1)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3)\sum_G\delta(k_1-k_1+k_2-k_3,G) \tag{41}$$

Simplifying further, we get:

$$H_{\text{Hartree}}=\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3}U(0)\langle c_s^\dagger(k_1)c_s(k_1)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_3)\sum_G\delta(k_2-k_3,G) \tag{42}$$

Since k_2 and k_3 are momenta inside the first Brillouin zone, the difference between k_2 and k_3 cannot exceed the first shell of the reciprocal lattice vector. Therefore, G can only take the value of the origin point in the reciprocal lattice, and $\sum_G\delta(k_2-k_3,G)=\delta_{k_2,k_3}$.

Substituting this into the Hartree term, we get:

$$H_{\text{Hartree}}=\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2}U(0)\langle c_s^\dagger(k_1)c_s(k_1)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_2) \tag{43}$$

Therefore, the final simplified Hartree term after reducing one momentum is:

$$H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2} U(0)\langle c_s^\dagger(k_1)c_s(k_1)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_2) \tag{44}$$

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 $\langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle$.The expected value $\langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle = \langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle\delta_{k_1,k_3}$.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 $\hat{H}^{int,HF,2} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1-k_4)\langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle c_{s'}^\dagger(k_2)c_s(k_4)\sum_G \delta(k_1-k_4+k_2-k_3, G)$.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: To simplify the Fock term in H_{Fock}, we first note that the expectation value $\langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle$ is nonzero only when $k_1 = k_3$, i.e., $\langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle = \langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle\delta_{k_1,k_3}$.

Substituting this into the Fock term, we get:

$$\begin{split} H_{\text{Fock}} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4} U(k_1 \\ - k_4)\langle c_s^\dagger(k_1)c_{s'}(k_3)\rangle\delta_{k_1,k_3}c_{s'}^\dagger(k_2)c_s(k_4)\sum_G \delta(k_1-k_4+k_2-k_3, G) \end{split} \tag{45}$$

Using the property of the Kronecker delta function δ_{k_1,k_3} to sum over k_3, we get:

$$H_{\text{Fock}} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_4} U(k_1-k_4)\langle c_s^\dagger(k_1)c_{s'}(k_1)\rangle c_{s'}^\dagger(k_2)c_s(k_4)\sum_G \delta(k_1 - k_4 + k_2 - k_1, G) \tag{46}$$

Simplifying the delta function $\sum_G \delta(k_1 - k_4 + k_2 - k_1, G)$, we get δ_{k_2,k_4}, as the difference between k_2 and k_4 cannot exceed the first shell of reciprocal lattice vector.

Therefore, the Fock term simplifies to:

$$H_{\text{Fock}} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2} U(k_1-k_2)\langle c_s^\dagger(k_1)c_{s'}(k_1)\rangle c_{s'}^\dagger(k_2)c_s(k_2) \tag{47}$$

This is the final simplified Fock term after reducing one momentum.

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

$$H_{\text{Hartree}} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2} U(0)\langle c_s^\dagger(k_1)c_s(k_1)\rangle c_{s'}^\dagger(k_2)c_{s'}(k_2) \tag{48}$$

and

$$H_{\text{Fock}} = -\frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2} U(k_1-k_2)\langle c_s^\dagger(k_1)c_{s'}(k_1)\rangle c_{s'}^\dagger(k_2)c_s(k_2) \tag{49}$$

To make the quadratic operators in the Fock term the same as those in the Hartree term, we can relabel the indices in the Fock term. However, in this case, the instruction specifies that no swap should be performed. Therefore, the Fock term remains the same.

Adding the Hartree term and the Fock term, we get:

$$
\begin{aligned}
H_{\mathrm{HF}} &= H_{\mathrm{Hartree}} + H_{\mathrm{Fock}} \\
&= \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} \big[U(0) \langle c_s^\dagger(k_1) c_s(k_1) \rangle \\
&\qquad\qquad - U(k_1 - k_2) \langle c_s^\dagger(k_1) c_{s'}(k_1) \rangle \big] \, c_{s'}^\dagger(k_2) c_{s'}(k_2)
\end{aligned}
\tag{50}
$$

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