1 Identify kinetic term (lattice)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in TBG in the real space in the second-quantized form.The degrees of freedom of the system are: spin and sublatticeThe kinetic term is a tight-binding model composed of the following hopping process: site i and site j with the amplitude $h_{\alpha\beta}(R_i - R_j)$

The summation should be taken over all spin and sublattice and all real space positions.Return the Kinetic Hamiltonian H_0.

Use the following conventions for the symbols:$d_{\alpha,i,\sigma}$ is the annihilation operator of an electron with spin $=\uparrow,\downarrow$ on sublattice of unit cell i, and $h_{\alpha\beta}(R_i - R_j)$ is the corresponding tight-binding matrix element between sublattices and located in unit cells centered at R_i and R_j respectively.

Completion: The kinetic term of the Hamiltonian in the second-quantized form can be written as:

$H_0 = \sum_{i,j} \sum_{\alpha,\beta} \sum_{\sigma} h_{\alpha\beta}(R_i - R_j) d^{\dagger}_{\alpha,i,\sigma} d_{\beta,j,\sigma}$

Here, the first sum is over all unit cells i and j, the second sum is over all sublattices and , and the third sum is over all spin states . The operator $d^{\dagger}_{\alpha,i,\sigma}$ creates an electron with spin on sublattice of unit cell i, and $d_{\beta,j,\sigma}$ annihilates an electron with spin on sublattice of unit cell j. The matrix element $h_{\alpha\beta}(R_i - R_j)$ represents the hopping amplitude between these sites.

2 Identify interacting term (real space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian, $\mathcal{H}_{\mathrm{C}}$ in the real space in the second-quantized form.The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian H_0.The interaction is a density-density interaction composed of the following process: site i and site j with the interaction strength $V_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j)$ The summation should be taken over all $\alpha\beta$ and all real space positions.Return the interaction term $\mathcal{H}_{\mathrm{C}}$ in terms of $\hat{n}_{\alpha,i}$.

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): $\hat{n}_{\alpha,i} = \sum_{\sigma} d^{\dagger}_{\alpha,i,\sigma} d_{\alpha,i,\sigma}$ is the local density operator and $V_{\alpha\beta}(\mathbf{R}) = e^2/(\varepsilon\xi) \sum_{m=-\infty}^{\infty} (-1)^m [(|\boldsymbol{\tau}_\alpha - \boldsymbol{\phi}_\beta + \mathbf{R}|/\xi)^2 + m^2]^{-\frac{1}{2}}$ is the screened form of the interaction in the presence of symmetric gates located at the top and bottom of the TBG heterostructure.

Completion: The interaction part of the Hamiltonian, $\mathcal{H}_{\mathrm{C}}$, in real space in the second-quantized form can be constructed as follows:

$\mathcal{H}_{\mathrm{C}} = \frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta} V_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) \hat{n}_{\alpha,i} \hat{n}_{\beta,j}$

Here, the factor of 1/2 is introduced to avoid double counting of interactions. The summations are over all sites i and j, and over all α and β. The interaction strength $V_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j)$ is given by the screened form of the interaction. The

local density operators $\hat{n}_{\alpha,i}$ and $\hat{n}_{\beta,j}$ are defined as $\hat{n}_{\alpha,i} = \sum_\sigma d^\dagger_{\alpha,i,\sigma} d_{\alpha,i,\sigma}$ and $\hat{n}_{\beta,j} = \sum_\sigma d^\dagger_{\beta,j,\sigma} d_{\beta,j,\sigma}$ respectively.

3 Fourier transform noninteracting term to momentum space (lattice)

Prompt: You will be instructed to convert the noninteracting Hamiltonian $\mathcal{H}_0$ in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to $d^\dagger_{\alpha,i,\sigma}$ in the real space to the $d^\dagger_{\alpha,\mathbf{k},\sigma}$ in the momentum space, which is defined as $d^\dagger_{\alpha,\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_i d^\dagger_{\alpha,i,\sigma} e^{ik \cdot R_i}$, 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 $\mathcal{H}_0$ is $H_0 = \sum_{i,j} \sum_{\alpha,\beta} \sum_\sigma h_{\alpha\beta}(R_i - R_j) d^\dagger_{\alpha,i,\sigma} d_{\beta,j,\sigma}$ Express the total noninteracting Hamiltonian $\mathcal{H}_0$ in terms of $d^\dagger_{\alpha,\mathbf{k},\sigma}$. 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): $d_{\alpha,\mathbf{k},\sigma}$: annihilation operator at momentum k, spin s , sublattice α $d^\dagger_{\alpha,\mathbf{k},\sigma}(k)$: creation operator at momentum k, spin s , sublattice α N : 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

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

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

$$\hat{H} = \frac{1}{N} \sum_{i,n} \sum_{k_1,k_2} c^\dagger(k_1) c(k_2) t(n) e^{-i(k_1 - k_2) \cdot R_i} e^{-ik_2 \cdot n} \tag{2}$$

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

$$\hat{H} = \sum_{k_1,k_2} \sum_n t(n) e^{-ik_2 \cdot n} c^\dagger(k_1) c(k_2) \delta(k_1, k_2) \tag{3}$$

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

$$\hat{H} = \sum_{k_1} \sum_n t(n) e^{-ik_1 \cdot n} c^\dagger(k_1) c(k_1) \tag{4}$$

For simplicity, we replace k_1 with k, we obtain

$$\hat{H} = \sum_k \sum_n t(n) e^{-ik \cdot n} c^\dagger(k) c(k) \tag{5}$$

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

$$\hat{H} = \sum_k E(k) c^\dagger(k) c(k) \tag{6}$$

Completion: Following the example, we first define the Fourier transformation for the creation and annihilation operators:

$d^\dagger_{\alpha,i,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} d^\dagger_{\alpha,\mathbf{k},\sigma} e^{-i\mathbf{k}\cdot\mathbf{R}_i}$

$d_{\beta,j,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} d_{\beta,\mathbf{k}',\sigma} e^{i\mathbf{k}'\cdot\mathbf{R}_j}$

Substitute these into $\mathcal{H}_0$:

$\mathcal{H}_0 = \sum_{i,j} \sum_{\alpha,\beta} \sum_\sigma h_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} d^\dagger_{\alpha,\mathbf{k},\sigma} e^{-i\mathbf{k}\cdot\mathbf{R}_i} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} d_{\beta,\mathbf{k}',\sigma} e^{i\mathbf{k}'\cdot\mathbf{R}_j}$

This simplifies to:

$\mathcal{H}_0 = \frac{1}{N} \sum_{i,j} \sum_{\alpha,\beta} \sum_\sigma \sum_{\mathbf{k},\mathbf{k}'} h_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) d^\dagger_{\alpha,\mathbf{k},\sigma} d_{\beta,\mathbf{k}',\sigma} e^{-i\mathbf{k}\cdot\mathbf{R}_i} e^{i\mathbf{k}'\cdot\mathbf{R}_j}$

Now, make a replacement by defining $\mathbf{n} = \mathbf{R}_i - \mathbf{R}_j$:

$\mathcal{H}_0 = \frac{1}{N} \sum_{i,\mathbf{n}} \sum_{\alpha,\beta} \sum_\sigma \sum_{\mathbf{k},\mathbf{k}'} h_{\alpha\beta}(\mathbf{n}) d^\dagger_{\alpha,\mathbf{k},\sigma} d_{\beta,\mathbf{k}',\sigma} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} e^{-i\mathbf{k}'\cdot\mathbf{n}}$

Because $\frac{1}{N} \sum_i e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} = \delta(\mathbf{k},\mathbf{k}')$, where $\delta(\mathbf{k},\mathbf{k}')$ is the Kronecker delta function, we have:

$\mathcal{H}_0 = \sum_{\mathbf{k},\mathbf{k}'} \sum_{\alpha,\beta} \sum_\sigma \sum_{\mathbf{n}} h_{\alpha\beta}(\mathbf{n}) d^\dagger_{\alpha,\mathbf{k},\sigma} d_{\beta,\mathbf{k}',\sigma} e^{-i\mathbf{k}'\cdot\mathbf{n}} \delta(\mathbf{k},\mathbf{k}')$

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

$\mathcal{H}_0 = \sum_{\mathbf{k}} \sum_{\alpha,\beta} \sum_\sigma \sum_{\mathbf{n}} h_{\alpha\beta}(\mathbf{n}) d^\dagger_{\alpha,\mathbf{k},\sigma} d_{\beta,\mathbf{k},\sigma} e^{-i\mathbf{k}\cdot\mathbf{n}}$

If we define energy dispersion $E_{\alpha\beta}(\mathbf{k}) = \sum_{\mathbf{n}} h_{\alpha\beta}(\mathbf{n}) e^{-i\mathbf{k}\cdot\mathbf{n}}$, where $\mathbf{n}$ is the summation of all hopping pairs, the noninteracting Hamiltonian in the momentum space is:

$\mathcal{H}_0 = \sum_{\mathbf{k}} \sum_{\alpha,\beta} \sum_\sigma E_{\alpha\beta}(\mathbf{k}) d^\dagger_{\alpha,\mathbf{k},\sigma} d_{\beta,\mathbf{k},\sigma}$

4 Fourier transform interacting term to momentum space (lattice)

Prompt: You will be instructed to convert the interacting Hamiltonian, $\mathcal{H}_C$, 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 $d^\dagger_{\alpha,i,\sigma}$ in the real space to the $d^\dagger_{\alpha,\mathbf{k},\sigma}$ in the momentum space, which is defined as $d^\dagger_{\alpha,\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_i d^\dagger_{\alpha,i,\sigma} e^{ik\cdot R_i}$, where i is integrated over all sites in the entire real space, and $\mathbf{q}$ is defined within the first Brillouin zone. You should follow the

EXAMPLE below to apply the Fourier transformation.You should recall that $\mathcal{H}_\text{C}$ is $\mathcal{H}_\text{C} = \frac{1}{2}\sum_{i,j}\sum_{\alpha,\beta}V_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j)\hat{n}_{\alpha,i}\hat{n}_{\beta,j}$. Express $\mathcal{H}_\text{C}$ in terms of $d^\dagger_{\alpha,\mathbf{k},\sigma}$. Simplify any summation index if possible.

EXAMPLE:Write an interacting Hamiltonian $\hat{H}^{int}$ in the second quantized form in the real space, $\hat{H}^{int} = \sum_{s,s'}\sum_{i,j}U(R_i - R_j)c^\dagger_s(R_i)c^\dagger_{s'}(R_j)c_{s'}(R_j)c_s(R_i)$, where i,j are summed over the entire real space.Define the Fourier transformation $c^\dagger_s(k) = \frac{1}{\sqrt{N}}\sum_i c^\dagger_s(R_i)e^{ik\cdot R_i}$, 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 $c^\dagger_s(R_i) = \frac{1}{\sqrt{N}}\sum_k c^\dagger_s(k)e^{-ik\cdot R_i}$, 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

$$\hat{H}^{int} = \sum_{s,s'}\sum_{i,j}U(R_i \tag{7}$$

$$- R_j)\frac{1}{\sqrt{N}}\sum_{k_1}c^\dagger_s(k_1)e^{-ik_1\cdot R_i}\frac{1}{\sqrt{N}}\sum_{k_2}c^\dagger_{s'}(k_2)e^{-ik_2\cdot R_j}\frac{1}{\sqrt{N}}\sum_{k_3}c_{s'}(k_3)e^{ik_3\cdot R_j}\frac{1}{\sqrt{N}}\sum_{k_4}c_s(k_4)e^{ik_4\cdot R_i}$$

$$= \sum_{s,s'}\sum_{i,j}\frac{1}{N^2}\sum_{k_1,k_2,k_3,k_4}U(R_i$$

$$- R_j)c^\dagger_s(k_1)c^\dagger_{s'}(k_2)c_{s'}(k_3)c_s(k_4)e^{-i(k_1-k_4)\cdot R_i}e^{-i(k_2-k_3)\cdot R_j}$$

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

$$\hat{H}^{int} \tag{8}$$

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

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,

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

$$- k_4 + k_2 - k_3, G) \tag{9}$$

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

$$\hat{H}^{int} = \frac{1}{N}\sum_{s,s'}\sum_{k_1,k_2,k_3,k_4}U(k_1 - k_4)c^\dagger_s(k_1)c^\dagger_{s'}(k_2)c_{s'}(k_3)c_s(k_4)\sum_G\delta(k_1 \tag{10}$$

$$- k_4 + k_2 - k_3, G)$$

Completion: Following the example, we first apply the Fourier transformation to the creation and annihilation operators in $\mathcal{H}_\text{C}$. The Fourier transformation of the creation operator is given by $d^\dagger_{\alpha,\mathbf{k},\sigma} = \frac{1}{\sqrt{N}}\sum_i d^\dagger_{\alpha,i,\sigma}e^{ik\cdot R_i}$,

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and the inverse Fourier transformation of the annihilation operator is $d_{\alpha,i,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} d_{\alpha,\mathbf{k},\sigma} e^{-i\mathbf{k}\cdot R_i}$.

Substituting these into $\mathcal{H}_C$, we get:

$\mathcal{H}_C = \frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta} V_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) \sum_\sigma \frac{1}{N} \sum_{\mathbf{k}_1} d^\dagger_{\alpha,\mathbf{k}_1,\sigma} e^{i\mathbf{k}_1\cdot R_i} \frac{1}{N} \sum_{\mathbf{k}_2} d_{\alpha,\mathbf{k}_2,\sigma} e^{-i\mathbf{k}_2\cdot R_i} \sum_{\sigma'} \frac{1}{N} \sum_{\mathbf{k}_3} d^\dagger_{\beta,\mathbf{k}_3,\sigma'} e^{i\mathbf{k}_3\cdot R_j} \frac{1}{N}$

Simplifying, we get:

$\mathcal{H}_C = \frac{1}{2N^2} \sum_{i,j} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) d^\dagger_{\alpha,\mathbf{k}_1,\sigma} d_{\alpha,\mathbf{k}_2,\sigma} d^\dagger_{\beta,\mathbf{k}_3,\sigma'} d_{\beta,\mathbf{k}_4,\sigma'} e^{i(\mathbf{k}_1-\mathbf{k}_2)\cdot R_i} e^{i(\mathbf{k}_3-\mathbf{k}_4)\cdot R_j}$.

Now, we make a replacement by defining $\mathbf{n} = \mathbf{R}_i - \mathbf{R}_j$:

$\mathcal{H}_C = \frac{1}{2N^2} \sum_{j,\mathbf{n}} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{n}) d^\dagger_{\alpha,\mathbf{k}_1,\sigma} d_{\alpha,\mathbf{k}_2,\sigma} d^\dagger_{\beta,\mathbf{k}_3,\sigma'} d_{\beta,\mathbf{k}_4,\sigma'} e^{i(\mathbf{k}_1-\mathbf{k}_2)\cdot \mathbf{n}} e^{i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{k}_3-\mathbf{k}_4)\cdot R_j}$.

Using the property $\frac{1}{N} \sum_i e^{-i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{k}_3-\mathbf{k}_4)\cdot R_i} = \sum \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})$, where $\delta(..,..)$ is the Kronecker delta function, and $\mathbf{G}$ is the all reciprocal lattices in the momentum space, we get:

$\mathcal{H}_C = \frac{1}{2N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \sum_{\mathbf{n}} V_{\alpha\beta}(\mathbf{n}) d^\dagger_{\alpha,\mathbf{k}_1,\sigma} d_{\alpha,\mathbf{k}_2,\sigma} d^\dagger_{\beta,\mathbf{k}_3,\sigma'} d_{\beta,\mathbf{k}_4,\sigma'} e^{i(\mathbf{k}_1-\mathbf{k}_2)\cdot \mathbf{n}} \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})$.

Finally, if we define the interaction in the momentum space $V_{\alpha\beta}(\mathbf{k}) = \sum_{\mathbf{n}} V_{\alpha\beta}(\mathbf{n}) e^{-i\mathbf{k}\cdot\mathbf{n}}$, where $\mathbf{n}$ is the summation of all hopping pairs, the interacting Hamiltonian in the momentum space is:

$\mathcal{H}_C = \frac{1}{2N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1-\mathbf{k}_2) d^\dagger_{\alpha,\mathbf{k}_1,\sigma} d_{\alpha,\mathbf{k}_2,\sigma} d^\dagger_{\beta,\mathbf{k}_3,\sigma'} d_{\beta,\mathbf{k}_4,\sigma'} \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})$.

5 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $\mathcal{H}_C$.You should use Wick's theorem to expand the four-fermion term in $\mathcal{H}_C$ 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 $\mathcal{H}_C$ is $\mathcal{H}_C = \frac{1}{2N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) d^\dagger_{\alpha,\mathbf{k}_1,\sigma} d_{\alpha,\mathbf{k}_2,\sigma} d^\dagger_{\beta,\mathbf{k}_3,\sigma'} d_{\beta,\mathbf{k}_4,\sigma'} \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})$.Return the expanded interaction term after Hartree-Fock approximation as $\mathcal{H}_{HF}$.

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):$\mathcal{H}_{HF}$ is the Hartree-Fock Hamiltonian, $\bar{h}_{\alpha\beta}(\mathbf{k}, \sigma)$ is the renormalized matrix elements due to both Hartree and Fock contributions, $\rho_{\alpha\beta}(\mathbf{k}, \sigma)$ is the zero-temperature density matrix for a given momentum and spin, and $\phi^{(n)}_{\alpha,\mathbf{k}}(\sigma)$ are the exact eigenvectors of $\mathcal{H}_{HF}$. $\rho_{\alpha\beta}(\mathbf{k}, \sigma) = \sum_n^{\text{occupied}} \phi^{(n)}_{\alpha,\mathbf{k}}(\sigma) \phi^{(n)*}_{\beta,\mathbf{k}}(\sigma)$

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: Applying Wick's theorem to the interaction term $\mathcal{H}_C$ and preserving only the normal terms, we can expand the four-fermion term as follows:

$\mathcal{H}_C = \frac{1}{2N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})$

$[\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle -$
$\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle]$

The Hartree-Fock Hamiltonian $\mathcal{H}_{HF}$ is then obtained by replacing the expectation values of the normal-ordered products of the creation and annihilation operators with the zero-temperature density matrix elements $\rho_{\alpha\beta}(\mathbf{k}, \sigma)$:

$\mathcal{H}_{HF} = \frac{1}{2N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})$

$[\rho_{\alpha\alpha}(\mathbf{k}_1 - \mathbf{k}_2, \sigma) d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \rho_{\beta\beta}(\mathbf{k}_3 - \mathbf{k}_4, \sigma') d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \rho_{\alpha\alpha}(\mathbf{k}_1 - \mathbf{k}_2, \sigma)\rho_{\beta\beta}(\mathbf{k}_3 - \mathbf{k}_4, \sigma') - \rho_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_4, \sigma) d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \rho_{\beta\alpha}(\mathbf{k}_3 - \mathbf{k}_2, \sigma') d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \rho_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_4, \sigma)\rho_{\beta\alpha}(\mathbf{k}_3 - \mathbf{k}_2, \sigma')]$

This is the Hartree-Fock approximation of the interaction term $\mathcal{H}_C$.

6 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the $\mathcal{H}_{HF}$.The quadratic terms mean terms that are proportional to $d_{\alpha,\mathbf{k},\sigma}^\dagger d_{\beta,\mathbf{k},\sigma}$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in $\mathcal{H}_{HF}$, denoted as $\mathcal{H}_{HF,2}$.You should recall that $\mathcal{H}_{HF}$ is $\mathcal{H}_C = \frac{1}{2N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})[\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle - \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle]$.Return $\mathcal{H}_{HF,2}$.

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):$\mathcal{H}_{HF}$ is the Hartree-Fock term, $\bar{h}_{\alpha\beta}(\mathbf{k}, \sigma)$ is the renormalized matrix elements due to both Hartree and Fock contributions, $d_{\alpha,\mathbf{k},\sigma}^\dagger$ and $d_{\beta,\mathbf{k},\sigma}$ are creation and annihilation operators respectively, and $\rho_{\alpha\beta}(\mathbf{k}, \sigma)$ is the zero-temperature density matrix for a given momentum and spin.

Completion: The quadratic terms in the Hartree-Fock Hamiltonian, $\mathcal{H}_{HF}$, are those that are proportional to $d_{\alpha,\mathbf{k},\sigma}^\dagger d_{\beta,\mathbf{k},\sigma}$. From the given expression for $\mathcal{H}_C$, we can identify these terms as:

$\mathcal{H}_{HF,2} = \frac{1}{2N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})[\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} \rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}]$

This expression includes all terms that are proportional to $d_{\alpha,\mathbf{k},\sigma}^\dagger d_{\beta,\mathbf{k},\sigma}$ and excludes terms that are solely expectations or products of expectations.

7 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $\mathcal{H}_{\mathrm{HF},2}$. If you find the $V(q)$ in $\mathcal{H}_{\mathrm{HF},2}$ 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 $\mathbf{k}$. You should recall that $\mathcal{H}_{\mathrm{HF},2}$ is $\mathcal{H}_{\mathrm{HF},2} = \frac{1}{2N}\sum_{\alpha,\beta}\sum_{\sigma,\sigma'}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2)\sum_{\mathbf{G}}\delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})[\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}]$. Return $\mathcal{H}_{\mathrm{HF},2}$ with expanded interaction.

Completion: The interaction term $V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2)$ in $\mathcal{H}_{\mathrm{HF},2}$ is already in momentum space and does not contain any momentum that is not in the summation sign. Therefore, the interaction term is already expanded and there is no need to perform any further action on it.

So, the $\mathcal{H}_{\mathrm{HF},2}$ with expanded interaction is:

$\mathcal{H}_{\mathrm{HF},2} = \frac{1}{2N}\sum_{\alpha,\beta}\sum_{\sigma,\sigma'}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2)\sum_{\mathbf{G}}\delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})[\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}]$.

8 Relabel the index

Prompt: You will be instructed to simplify the quadratic term $\mathcal{H}_{\mathrm{HF},2}$ through relabeling the index.The logic is that the expected value $(\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle)$ in the first Hartree term $(\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'})$ has the same form as the quadratic operators in the second Hartree term $(\langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma})$, and vice versa. The same applies to the Fock term.Namely, a replacement of α and β, σ and σ', $\mathbf{k}_1$ and $\mathbf{k}_3$, $\mathbf{k}_2$ and $\mathbf{k}_4$ 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 $\mathcal{H}_{\mathrm{HF},2}$ is $\mathcal{H}_{\mathrm{HF},2} = \frac{1}{2N}\sum_{\alpha,\beta}\sum_{\sigma,\sigma'}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2)\sum_{\mathbf{G}}\delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})[\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'} + \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma} - \langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}]$ Return the simplified $\mathcal{H}_{\mathrm{HF},2}$.

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: Following the example, we can simplify $\mathcal{H}_{\text{HF},2}$ by relabeling the indices in the second Hartree and Fock terms.

For the second Hartree term, we swap α with β, σ with σ', $\mathbf{k}_1$ with $\mathbf{k}_3$, and $\mathbf{k}_2$ with $\mathbf{k}_4$. This gives us:

$\langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}$

which simplifies to:

$\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}$

For the second Fock term, we swap α with β, σ with σ', $\mathbf{k}_1$ with $\mathbf{k}_3$, and $\mathbf{k}_2$ with $\mathbf{k}_4$. This gives us:

$\langle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}$

which simplifies to:

$\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}$

Therefore, the simplified $\mathcal{H}_{\text{HF},2}$ is:

$\mathcal{H}_{\text{HF},2} = \frac{1}{2N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 -$ $\mathbf{k}_4, \mathbf{G})[\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}+\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}-\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}-$ $\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\beta,\mathbf{k}_4,\sigma'}\rangle d_{\beta,\mathbf{k}_3,\sigma'}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}]$

9   Identify order parameters in Hartree term

Prompt: You will be instructed to simplify the Hartree term, $h_{\alpha\beta}^{\text{H}}(\mathbf{k},\sigma)$, by reducing the momentum inside the expected value $\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle$.The expected value $\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle = \delta_{k_1,k_2}\langle d_{\alpha,\mathbf{k}_1,\sigma}^\dagger d_{\alpha,\mathbf{k}_2,\sigma}\rangle$.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 $h_{\alpha\beta}^{\mathrm{H}}(\mathbf{k}, \sigma)$ is $\mathcal{H}_{\mathrm{HF},2} = \frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G}) \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_2,\sigma} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^{\dagger} d_{\beta,\mathbf{k}_4,\sigma'}$.Return the final simplified Hartree term $h_{\alpha\beta}^{\mathrm{H}}(\mathbf{k}, \sigma)$.

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: Following the example, we can simplify the Hartree term $h_{\alpha\beta}^{\mathrm{H}}(\mathbf{k}, \sigma)$ by reducing the momentum inside the expected value $\langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_2,\sigma} \rangle$.

We know that $\langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_2,\sigma} \rangle$ is nonzero only when $\mathbf{k}_1 = \mathbf{k}_2$, i.e., $\langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_2,\sigma} \rangle = \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_2,\sigma} \rangle \delta_{\mathbf{k}_1,\mathbf{k}_2}$.

Substituting this into the Hartree term, we get:

$\mathcal{H}_{\mathrm{HF},2} = \frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G}) \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_2,\sigma} \rangle \delta_{\mathbf{k}_1,\mathbf{k}_2} d_{\beta,\mathbf{k}_3,\sigma'}^{\dagger} d_{\beta,\mathbf{k}}$

Using the property of Kronecker delta function $\delta_{\mathbf{k}_1,\mathbf{k}_2}$ to sum over $\mathbf{k}_2$, we get:

$\mathcal{H}_{\mathrm{HF},2} = \frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(0) \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_1,\sigma} \rangle \sum_{\mathbf{G}} \delta(\mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G}) d_{\beta,\mathbf{k}_3,\sigma'}^{\dagger} d_{\beta,\mathbf{k}_4,\sigma'}$.

We can further simplify $\sum_{\mathbf{G}} \delta(\mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G})$ to $\delta_{\mathbf{k}_3,\mathbf{k}_4}$, because the difference between $\mathbf{k}_3$ and $\mathbf{k}_4$ cannot exceed the first shell of reciprocal lattice vector.

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

$h_{\alpha\beta}^{\mathrm{H}}(\mathbf{k}, \sigma) = \frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_3} V_{\alpha\beta}(0) \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_1,\sigma} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^{\dagger} d_{\beta,\mathbf{k}_3,\sigma'}$.

10 Identify order parameters in Fock term

Prompt: You will be instructed to simplify the Fock term in $h_{\alpha\beta}^{\mathrm{F}}(\mathbf{k}, \sigma)$ by reducing the momentum inside the expected value $\langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\beta,\mathbf{k}_4,\sigma'} \rangle$.The expected value $\langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\beta,\mathbf{k}_4,\sigma'} \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\beta,\mathbf{k}_4,\sigma'} \rangle = \delta_{k_1,k_4} \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\beta,\mathbf{k}_4,\sigma'} \rangle$.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 Fock term, and another momentum in the quadratic term.You should recall that $h^{\mathrm{F}}_{\alpha\beta}(\mathbf{k}, \sigma)$ is $\mathcal{H}_{\mathrm{HF},2} = -\frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G}) \langle d^{\dagger}_{\alpha,\mathbf{k}_1,\sigma} d_{\beta,\mathbf{k}_4,\sigma'} \rangle d^{\dagger}_{\beta,\mathbf{k}_3,\sigma'} d_{\alpha,\mathbf{k}_2,\sigma}$.Return the final simplified Fock term $h^{\mathrm{F}}_{\alpha\beta}(\mathbf{k}, \sigma)$.

EXAMPLE:Given a Hamiltonian where the Fock term $\hat{H}^{Fock} = -\sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4) \langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_3) \rangle c^{\dagger}_{s_2}(k_2) c_{s_1}(k_4) \sum_{G} \delta_{k_1+k_2-k_3-k_4,G}$, 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 $\langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_3) \rangle$ is nonzero only when $k_1 = k_3$, i.e., $\langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_3) \rangle = \langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_3) \rangle \delta_{k_1,k_3}$.Thus, the Fock term becomes $-\sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4) \langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_3) \rangle \delta_{k_1,k_3} c^{\dagger}_{s_2}(k_2) c_{s_1}(k_4) \sum_{G} \delta_{k_1+k_2-k_3-k_4,G}$.Use the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we have $-\sum_{k_1,k_2,k_4,s_1,s_2} V(k_1 - k_4) \langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_1) \rangle c^{\dagger}_{s_2}(k_2) c_{s_1}(k_4) \sum_{G} \delta_{k_2-k_4,G}$.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 $-\sum_{k_1,k_2,k_4,s_1,s_2} V(k_1 - k_4) \langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_1) \rangle c^{\dagger}_{s_2}(k_2) c_{s_1}(k_4) \delta_{k_2-k_4,0} = -\sum_{k_1,k_2,s_1,s_2} V(k_1 - k_2) \langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_1) \rangle c^{\dagger}_{s_2}(k_2) c_{s_1}(k_2)$.Therefore, the final simplified Fock term after reducing one momentum is $\hat{H}^{Fock} = -\sum_{k_1,k_2,s_1,s_2} V(k_1 - k_2) \langle c^{\dagger}_{s_1}(k_1) c_{s_2}(k_1) \rangle c^{\dagger}_{s_2}(k_2) c_{s_1}(k_2)$

Completion: Following the example, we can simplify the Fock term $h^{\mathrm{F}}_{\alpha\beta}(\mathbf{k}, \sigma)$ in the Hamiltonian $\mathcal{H}_{\mathrm{HF},2}$.

First, we use the property of the expected value $\langle d^{\dagger}_{\alpha,\mathbf{k}_1,\sigma} d_{\beta,\mathbf{k}_4,\sigma'} \rangle$ to reduce one momentum. This expected value is nonzero only when $\mathbf{k}_1 = \mathbf{k}_4$, $\alpha = \beta$, and $\sigma = \sigma'$, i.e., $\langle d^{\dagger}_{\alpha,\mathbf{k}_1,\sigma} d_{\beta,\mathbf{k}_4,\sigma'} \rangle = \delta_{\mathbf{k}_1,\mathbf{k}_4} \langle d^{\dagger}_{\alpha,\mathbf{k}_1,\sigma} d_{\beta,\mathbf{k}_4,\sigma'} \rangle$.

Substituting this into $\mathcal{H}_{\mathrm{HF},2}$, we get:

$\mathcal{H}_{\mathrm{HF},2} = -\frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4, \mathbf{G}) \delta_{\mathbf{k}_1,\mathbf{k}_4} \langle d^{\dagger}_{\alpha,\mathbf{k}_1,\sigma} d_{\beta,\mathbf{k}_4,\sigma'} \rangle d^{\dagger}_{\beta,\mathbf{k}_3,\sigma'} d_{\alpha,\mathbf{k}_2,\sigma}$.

Using the property of the Kronecker delta function $\delta_{\mathbf{k}_1,\mathbf{k}_4}$ to sum over $\mathbf{k}_4$, we get:

$\mathcal{H}_{\mathrm{HF},2} = -\frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \sum_{\mathbf{G}} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_1, \mathbf{G}) \langle d^{\dagger}_{\alpha,\mathbf{k}_1,\sigma} d_{\beta,\mathbf{k}_1,\sigma'} \rangle d^{\dagger}_{\beta,\mathbf{k}_3,\sigma'} d_{\alpha,\mathbf{k}_2,\sigma}$.

Simplifying the delta function $\delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_1, \mathbf{G})$ to $\delta(\mathbf{k}_2 - \mathbf{k}_3, \mathbf{G})$, and noting that $\mathbf{G}$ can only take the value of the origin point in the reciprocal lattice, we get $\delta(\mathbf{k}_2 - \mathbf{k}_3, 0)$.

Therefore, the final simplified Fock term $h^{\mathrm{F}}_{\alpha\beta}(\mathbf{k}, \sigma)$ is:

$h^{\mathrm{F}}_{\alpha\beta}(\mathbf{k}, \sigma) = -\frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \langle d^{\dagger}_{\alpha,\mathbf{k}_1,\sigma} d_{\beta,\mathbf{k}_1,\sigma'} \rangle d^{\dagger}_{\beta,\mathbf{k}_2,\sigma'} d_{\alpha,\mathbf{k}_2,\sigma}$.

11   Final form of iteration in quadratic terms

Prompt: You will now be instructed to combine the Hartree term $h_{\alpha\beta}^{\mathrm{H}}(\mathbf{k}, \sigma)$ and the Fock term $h_{\alpha\beta}^{\mathrm{F}}(\mathbf{k}, \sigma)$.You should recall that the Hartree term $h_{\alpha\beta}^{\mathrm{H}}(\mathbf{k}, \sigma) = \frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_3} V_{\alpha\beta}(0) \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_1,\sigma} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^{\dagger} d_{\beta,\mathbf{k}_3,\sigma'}$,and the Fock term $h_{\alpha\beta}^{\mathrm{F}}(\mathbf{k}, \sigma) = -\frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\beta,\mathbf{k}_1,\sigma'} \rangle d_{\beta,\mathbf{k}_2,\sigma'}^{\dagger} d_{\alpha,\mathbf{k}_2,\sigma}$.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 and the Fock term can be combined as follows:

$h_{\alpha\beta}^{\mathrm{HF}}(\mathbf{k}, \sigma) = h_{\alpha\beta}^{\mathrm{H}}(\mathbf{k}, \sigma) + h_{\alpha\beta}^{\mathrm{F}}(\mathbf{k}, \sigma)$

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

$h_{\alpha\beta}^{\mathrm{HF}}(\mathbf{k}, \sigma) = \frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_3} V_{\alpha\beta}(0) \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\alpha,\mathbf{k}_1,\sigma} \rangle d_{\beta,\mathbf{k}_3,\sigma'}^{\dagger} d_{\beta,\mathbf{k}_3,\sigma'} - \frac{1}{N} \sum_{\alpha,\beta} \sum_{\sigma,\sigma'} \sum_{\mathbf{k}_1,\mathbf{k}_2} V_{\alpha\beta}(\mathbf{k}_1 - \mathbf{k}_2) \langle d_{\alpha,\mathbf{k}_1,\sigma}^{\dagger} d_{\beta,\mathbf{k}_1,\sigma'} \rangle d_{\beta,\mathbf{k}_2,\sigma'}^{\dagger} d_{\alpha,\mathbf{k}_2,\sigma}$

Since the question specifies that no relabeling is required, the final sum of the Hartree and Fock terms is as above.