1 Identify kinetic term (continuum,first-quantized)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in ABC trilayer graphene in the momentum space in the single-particle form.The degrees of freedom of the system are: six sublattice sites labeled as A, B, A′, B′, A″, B″.Express the Kinetic Hamiltonian $H0$ using $\gamma0$, $\gamma1$, $\gamma2$, $\gamma3$, γN, f which are only on the diagonal terms, and arrange the basis in the order of A, B, A′, B′, A″, B″.

Use the following conventions for the symbols:f(k) = e^(i ky a / sqrt(3)) * (1 + 2 e^(-i 3 k{y} a / 2sqrt(3)) * cos(kx a / 2)), where $a = 2.46\ Å.\gamma0 = 3.12$ eV, $\gamma1 = 0.377\ eV$, $\gamma2 = 0.01$ eV, $\gamma3 = 0.3\ eV.\gamma N = \gamma N^0 * exp(- |k - K'| / kr)$, where kr = $\gamma1$ / ℏυ_F = 0.0573 Å^-1.

Completion: The kinetic term of the Hamiltonian in ABC trilayer graphene in the momentum space in the single-particle form can be written as a 6x6 matrix, with the basis ordered as A, B, A′, B′, A″, B″. The Hamiltonian H_0 is given by:

$$H_0 = [[0,_0, 0, 0, 0,_1 * f(k)], [_0, 0,_1, 0, 0, 0], [0,_1, 0,_0, 0, 0], [0, 0,_0, 0,_1, 0], [0, 0, 0,_1, 0,_3], [_1 * f(k), 0, 0, 0,_3, 0]]$$

where f(k) = e^(i ky a / sqrt(3)) * (1 + 2 e^(-i 3 k{y} a / 2sqrt(3)) * cos(kx a / 2)), and $a = 2.46\ Å$. The parameters $\gamma0$, $\gamma1$, $\gamma2$, $\gamma3$, and γN are given by the values specified in the question.

Note that the Hamiltonian is Hermitian, as required by quantum mechanics, and the off-diagonal terms represent the hopping energies between different sublattice sites. The diagonal terms are zero as there is no potential energy term in the kinetic Hamiltonian.

2 Define energy dispersion (continuum)

Prompt: You will be instructed to construct each term, namely $\gamma0$, $\gamma1$, $\gamma2$, $\gamma3$, γN, f.For all energy dispersions, $\gamma0$, $\gamma1$, $\gamma2$, $\gamma3$, γN, f, it characterizes the cos dispersion for electrons.

You should follow the EXAMPLE below to obtain correct energy dispersion, select the correct EXAMPLE by noticing the type of dispersion.Finally, in the real space, the momentum $k = -i\partial_r$. You should keep the form of k in the Hamiltonian for short notations but should remember k is an operator.You should recall that

$$\begin{pmatrix} 0 & \gamma_0 f & 0\%\gamma_4 f & \gamma_3 f^* + \gamma_N & 0 & \gamma_2 \\ \gamma_0 f^* & 0 & \gamma_1 & \%\gamma_4 f & 0 & 0 \\ \%\gamma_4 f^* 0 & \gamma_1 & 0 & \gamma_0 f & 0\%\gamma_4 f & \gamma_3 f^* \\ \gamma_3 f + \gamma_N^* & 0\%\gamma_4 f^* & \gamma_0 f^* & 0 & \gamma_1 & 0 \\ 0 & 0 & 0\%\gamma_4 f^* & \gamma_1 & 0 & \gamma_0 f \\ \gamma_2 & 0 & \gamma_3 f & 0 & \gamma_0 f^* & 0 \end{pmatrix}$$

.Return the expression for $\gamma0$, $\gamma1$, $\gamma2$, $\gamma3$, γN, f in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian {H}0 .

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):f(k) = e^(i ky a / sqrt(3)) * (1 + 2 e^(-i 3 k{y} a / 2sqrt(3)) * cos(kx a / 2)), where $a = 2.46\ Å.\gamma N = \gamma N^0 * exp(- |k - K'| / kr)$, where kr = $\gamma1$ / ℏυ_F = 0.0573 Å^-1.

EXAMPLE 1:A parabolic dispersion for electron is $E_\alpha = \frac{\hbar^2 k^2}{2m_\alpha}$, where α indicates the type of electron. If there is a further shift of q in the momentum k, the dispersion will become $E_\alpha = \frac{\hbar^2 (k-q)^2}{2m_\alpha}$.

EXAMPLE 2: A cos dispersion is $E_\alpha = -\cos(ka/2)$, where α indicates the type of particle. If there is a further shift of q in the momentum k, the dispersion will become $E_\alpha = -\cos((k-q)a/2)$. However, there could be more prefactors before cos depending on the geometry of the lattice.

EXAMPLE 3:A dirac dispersion for electron/hole is a 2 by 2 matrix, i.e., $h_\theta(k) = -\hbar v_D |k| \begin{pmatrix} 0 & e^{i(\theta_k - \theta)} \\ e^{-i(\theta_{\bar k} - \theta)} & 0 \end{pmatrix}$, where v_D is the Fermi velocity, θ is the twist angle, and θ_k indicates the azumith angle of k. If there is a further shift of K_θ in the momentum k, the dispersion will become $h_\theta(k) = -\hbar v_D |k - K_\theta| \begin{pmatrix} 0 & e^{i(\theta_{k-K_\theta} - \theta)} \\ e^{-i(\theta_{k-K_\theta} - \theta)} & 0 \end{pmatrix}$.

Completion: Given the cos dispersion for electrons, we can construct the terms $\gamma0$, $\gamma1$, $\gamma2$, $\gamma3$, γ_N, f as follows:

1. *$\gamma0$: This term represents the nearest-neighbor hopping energy. It can be expressed as $\gamma0$ = -cos(k a / 2), where a is the lattice constant.*

2. *$\gamma1$: This term represents the next-nearest-neighbor hopping energy. It can be expressed as $\gamma1$ = -cos((k-q) a / 2), where q is the shift in momentum.*

3. *γ2: This term represents the third-nearest-neighbor hopping energy. It can be expressed as* γ2 = -cos((k-2q) a / 2), *where 2q is the shift in momentum.*

4. *γ3: This term represents the fourth-nearest-neighbor hopping energy. It can be expressed as* γ3 = -cos((k-3q) a / 2), *where 3q is the shift in momentum.*

5. *γN: This term represents the Nth-nearest-neighbor hopping energy. It can be expressed as* γN = γN^0 * exp(- |k - K'| / kr), *where* kr = γ1 / ħυ_F = 0.0573 Å^-1.

6. f(k): This term represents the phase factor. It can be expressed as f(k) = e^(i ky *a / sqrt(3)) * (1 + 2 e^(-i 3 k{y} a / 2sqrt(3)) * cos(k_x a / 2)), where a = 2.46 Å.*

Substituting these expressions into the kinetic Hamiltonian, we get:

$$
\begin{pmatrix}
0 & -cos(ka/2)f & 0\%\gamma_4 f & -cos((k-3q)a/2)f^* + \,_N & 0 & -cos((k- \\
-cos(ka/2)f^* & 0 & -cos((k-q)a/2) & \%\gamma_4 f & 0 & 0 \\
\%\gamma_4 f^* 0 & -cos((k-q)a/2) & 0 & -cos(ka/2)f & 0\%\gamma_4 f & -cos((k- \\
-cos((k-3q)a/2)f + \,_N^* & 0\%\gamma_4 f^* & -cos(ka/2)f^* & 0 & -cos((k-q)a/2) & 0 \\
0 & 0 & 0\%\gamma_4 f^* & -cos((k-q)a/2) & 0 & -cos(k \\
-cos((k-2q)a/2) & 0 & -cos((k-3q)a/2)f & 0 & -cos(ka/2)f^* & 0
\end{pmatrix}
$$

This is the kinetic Hamiltonian with the terms γ0, γ1, γ2, γ3, γ_N, f substituted in.

3 Second-quantization (matrix)

Prompt: You will be instructed to construct the second quantized form of the total noninteracting Hamiltonian in the momentum space.The noninteracting Hamiltonian in the momentum space H_0 is the sum of Kinetic Hamiltonian H_0 and Potential Hamiltonian which is absent here.To construct the second quantized form of a Hamiltonian. You should construct the creation and annihilation operators from the basis explicitly. You should follow the EXAMPLE below to convert a Hamiltonian from the single-particle form to second-quantized form.Finally by "total", it means you need to take a summation over the momentum space position k.Return the second quantized form of the total noninteracting Hamiltonian $\hat{H}_0$

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):$f(\boldsymbol{k}) = e^{ik_y a/\sqrt{3}}\left(1 + 2e^{-i3k_y a/2\sqrt{3}}\cos\left(\frac{k_x a}{2}\right)\right).\gamma_N = \gamma_N^0 \exp\left(-\left|\boldsymbol{k}-\boldsymbol{K}^{(\prime)}\right|/k_r\right)$. The basis are six sublattice sites labeled as A, B, A', B', A'', B''

EXAMPLE:For a Hamiltonian H, where $H = \begin{pmatrix} H_{a,a} & H_{a,b} \\ H_{b,a} & H_{b,b} \end{pmatrix}$ and the order of basis is (a), (b), we can construct the creation operators $\psi_a^\dagger$ and $\psi_b^\dagger$, and the annihilation operator ψ_a and ψ_b.The corresponding second quantized form is $\hat{H} = \vec{\psi}^\dagger H \vec{\psi}$, where $\vec{\psi} = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$ and $\vec{\psi}^\dagger = \begin{pmatrix} \psi_a^\dagger & \psi_b^\dagger \end{pmatrix}$.

Completion: Given the Hamiltonian H, where H is a 6x6 matrix and the order of basis is (A), (B), (A'), (B'), (A''), (B''), we can construct the creation operators ψA†, ψB†, ψA'†, ψB'†, ψA''†, ψB''†, and the annihilation operators ψA, ψB, ψA', ψB', ψA'', ψB''.

The corresponding second quantized form is $\hat{H}_0 = \vec{\psi}^\dagger H \vec{\psi}$, where $\vec{\psi} = \begin{pmatrix} \psi_A \\ \psi_B \\ \psi'_A \\ \psi'_B \\ \psi''_A \\ \psi''_B \end{pmatrix}$ and $\vec{\psi}^\dagger =$

$\begin{pmatrix} \psi_A^\dagger & \psi_B^\dagger & \psi'_A & \psi'_B & \psi''_A & \psi''_B \end{pmatrix}$.
The total noninteracting Hamiltonian in the momentum space is then given by:
$\hat{H}_0 = \sum_k \vec{\psi}_k^\dagger H(k)\vec{\psi}_k$
where H(k) is the Hamiltonian matrix with the terms γ0, γ1, γ2, γ3, γ_N, f substituted in, and the sum is over all momentum space positions k.

4 Second-quantization (summation)

Prompt: You will be instructed to expand the second-quantized form Hamiltonian $\hat{H}_0$ using γ0, γ1, γ2, γ3, γN, f and c{k,\lambda}^\dagger. You should follow the EXAMPLE below to expand the Hamiltonian.You should use any previous knowledge to simplify it. For example, if any term of

$\gamma 0$, $\gamma 1$, $\gamma 2$, $\gamma 3$, γ_N, f is zero, you should remove it from the summation. You should recall that

$\hat{H}_0$ is $\vec{\psi}^\dagger = \begin{pmatrix} \psi_A^\dagger & \psi_B^\dagger & \psi_{A'}^\dagger & \psi_{B'}^\dagger & \psi_{A''}^\dagger & \psi_{B''}^\dagger \end{pmatrix}$ and the vector of annihilation operators $\vec{\psi} = \begin{pmatrix} \psi_A \\ \psi_B \\ \psi_{A'} \\ \psi_{B'} \\ \psi_{A''} \\ \psi_{B''} \end{pmatrix}$, and

$\hat{H}_0 = \sum_k \vec{\psi}_k^\dagger H_0(k) \vec{\psi}_k$. Return the expanded form of $\hat{H}_0$ after simplification.

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): $f(\boldsymbol{k}) = e^{ik_y a/\sqrt{3}}\left(1 + 2e^{-i3k_y a/2\sqrt{3}}\cos\left(\frac{k_x a}{2}\right)\right)$,

where $a = 2.46$. $\gamma_0 = 3.12\text{eV}$, $\gamma_1 = 0.377\text{eV}$, $\gamma_2 = 0.01\text{eV}$, $\gamma_3 = 0.3\text{eV}$. $\gamma_N = \gamma_N^0 \exp\left(-\left|\boldsymbol{k} - \boldsymbol{K}^{(\prime)}\right|/k_r\right)$, where $k_r = \gamma_1/\hbar v_F = 0.0573^{-1}$.

EXAMPLE: For a $\hat{H} = \vec{\psi}^\dagger H \vec{\psi}$, where $\vec{\psi} = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$ and $\vec{\psi}^\dagger = \begin{pmatrix} \psi_a^\dagger & \psi_b^\dagger \end{pmatrix}$, we can expand it as $\hat{H} = \sum_{i,j=\{a,b\}} \psi_i^\dagger H_{i,j} \psi_j$.

Completion: Given the Hamiltonian $\hat{H}_0 = \sum_k \vec{\psi}_k^\dagger H_0(k) \vec{\psi}_k$, where $\vec{\psi}_k^\dagger = \begin{pmatrix} \psi_{A,k}^\dagger & \psi_{B,k}^\dagger & \psi_{A',k}^\dagger & \psi_{B',k}^\dagger & \psi_{A'',k}^\dagger & \psi_{B'',k}^\dagger \end{pmatrix}$ and $\vec{\psi}_k = \begin{pmatrix} \psi_{A,k} \\ \psi_{B,k} \\ \psi_{A',k} \\ \psi_{B',k} \\ \psi_{A'',k} \\ \psi_{B'',k} \end{pmatrix}$, we can expand it as:

$\hat{H}_0 = \sum_k \sum_{i,j=\{A,B,A',B',A'',B''\}} \psi_{i,k}^\dagger H_{0,i,j}(k) \psi_{j,k}$

where $H_{0,i,j}(k)$ are the elements of the Hamiltonian matrix $H_0(k)$, which are functions of the parameters $\gamma 0$, $\gamma 1$, $\gamma 2$, $\gamma 3$, γ_N, f and the momentum k.

The explicit form of $H_{0,i,j}(k)$ depends on the specific form of the Hamiltonian matrix, which is not provided in the question. However, given the definitions of $\gamma 0$, $\gamma 1$, $\gamma 2$, $\gamma 3$, γ_N, f, and the fact that the Hamiltonian is Hermitian, we can write down the general form of the Hamiltonian matrix elements:

$H_{0,i,j}(k) = \gamma_0 \delta_{i,j} + \gamma_1 f(k)\delta_{i,j+1} + \gamma_2 f^2(k)\delta_{i,j+2} + \gamma_3 f^3(k)\delta_{i,j+3} + \gamma_N f^N(k)\delta_{i,j+N}$

where $\delta_{i,j}$ is the Kronecker delta function, which is 1 if i=j and 0 otherwise. The terms with f(k) represent the hopping terms between nearest, next-nearest, third-nearest, fourth-nearest, and Nth-nearest neighbors, respectively. The term with γ_0 represents the on-site energy.

Note that the indices i and j are cyclic, i.e., A+1=B, B+1=A', A'+1=B', B'+1=A", A"+1=B", B"+1=A.

The expanded form of $\hat{H}_0$ after simplification is then:

$\hat{H}_0 = \sum_k \left(\gamma_0 \sum_{i=\{A,B,A',B',A'',B''\}} \psi_{i,k}^\dagger \psi_{i,k} + \gamma_1 \sum_{i,j=\{A,B,A',B',A'',B''\}} f(k)\psi_{i,k}^\dagger \psi_{j+1,k} + \gamma_2 \sum_{i,j=\{A,B,A',B',A'',B''\}} f^2(k)\psi_{i,k}^\dagger \psi_{j+2} \right.$

This is the expanded form of the Hamiltonian $\hat{H}_0$ in terms of the creation and annihilation operators, the parameters $\gamma 0$, $\gamma 1$, $\gamma 2$, $\gamma 3$, γ_N, f, and the momentum k.

5 Identify interacting term (momentum space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian V_{HF} in the momentum space. The interaction Hamiltonian is a product of four parts. The first part is the product of four operators with two creation and two annihilation operators following the normal order, namely, creation operators are before annihilation operators. You should follow the order of $1, 2, 2, 1$ for the λ and λ', and $1, 2, 3, 4$ for the $\boldsymbol{k}$. The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators. The third part is the interaction form. You should use $V(q)$ with $V(q) = \widetilde{V}^{ll'}(\boldsymbol{q}) = 2\pi e^2/(|\boldsymbol{q}|\,\epsilon_r)$ when the sublattice indices l and l' refer to the atoms in the same layer, and $(2\pi e^2/(|\boldsymbol{q}|\epsilon_r))\exp\{-|\boldsymbol{q}|\,d\}$ when they refer to atoms in layers separated by a distance d, where q is the transferred total momentum between a creation operator and an annihilation operator with the same λ and λ', namely $q = k_1 - k_4$. The fourth part is the normalization factor, you should use $\frac{1}{2A}$ here. Finally, the summation should be running over all λ and λ', and $\boldsymbol{k}$ Return the interaction term V_{HF} in terms of $c_{\boldsymbol{k}\lambda}^\dagger$, $c_{\boldsymbol{k}\lambda}$ and $V(q)$ (with q expressed in terms of $\boldsymbol{k}$).

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): $c_{\boldsymbol{k}\lambda}^\dagger$, $c_{\boldsymbol{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgen}), $U_H^{ll'}$ and $U_X^{ll'}(\boldsymbol{q})$ involve sums over reciprocal lattice vectors $\boldsymbol{G}$. In these

equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

Completion: The interaction part of the Hamiltonian V_{HF} in the momentum space can be constructed as follows:

$V_{HF} = \frac{1}{2A} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_4) c^\dagger_{\boldsymbol{k}_1\lambda_1} c^\dagger_{\boldsymbol{k}_2\lambda_2} c_{\boldsymbol{k}_3\lambda_2} c_{\boldsymbol{k}_4\lambda_1}$

where $V(\boldsymbol{k}_1 - \boldsymbol{k}_4)$ is the interaction form, which is given by:

$V(q) = \widetilde{V}^{ll'}(\boldsymbol{q}) = 2\pi e^2/(|\boldsymbol{q}|\,\epsilon_r)$

when the sublattice indices l and l' refer to the atoms in the same layer, and

$(2\pi e^2/(|\boldsymbol{q}|\epsilon_r)) \exp\{-|\boldsymbol{q}|\,d]\}$

when they refer to atoms in layers separated by a distance d.

The summation is over all λ and λ', and $\boldsymbol{k}$, and the normalization factor is $\frac{1}{2A}$. The total momentum of all creation operators is the same as that of all annihilation operators, which is the constraint of total momentum conservation. The product of four operators with two creation and two annihilation operators follows the normal order, with creation operators before annihilation operators. The order of λ and λ' is $1,2,2,1$, and the order of $\boldsymbol{k}$ is $1,2,3,4$.

6 Wick's theorem expansion

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

$$V_{HF} = \frac{1}{2A} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_4) c^\dagger_{\boldsymbol{k}_1\lambda_1} c^\dagger_{\boldsymbol{k}_2\lambda_2} c_{\boldsymbol{k}_3\lambda_2} c_{\boldsymbol{k}_4\lambda_1} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4} \, .$$

Return the expanded interaction term after Hartree-Fock approximation as V_{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):$c^\dagger_{\boldsymbol{k}\lambda}$, $c_{\boldsymbol{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices.

EXAMPLE 1:For a four-fermion term $a^\dagger_1 a^\dagger_2 a_3 a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a^\dagger_1 a^\dagger_2 a_3 a_4 = \langle a^\dagger_1 a_4 \rangle a^\dagger_2 a_3 + \langle a^\dagger_2 a_3 \rangle a^\dagger_1 a_4 - \langle a^\dagger_1 a_4 \rangle \langle a^\dagger_2 a_3 \rangle - \langle a^\dagger_1 a_3 \rangle a^\dagger_2 a_4 - \langle a^\dagger_2 a_4 \rangle a^\dagger_1 a_3 + \langle a^\dagger_1 a_3 \rangle \langle a^\dagger_2 a_4 \rangle$Be cautious about the order of the index and sign before each term here.

EXAMPLE 2:For a four-fermion term $a^\dagger_1 a_2 a^\dagger_3 a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a^\dagger_1 a_2 a^\dagger_3 a_4 = \langle a^\dagger_1 a_2 \rangle a^\dagger_3 a_4 + \langle a^\dagger_3 a_4 \rangle a^\dagger_1 a_2 - \langle a^\dagger_1 a_2 \rangle \langle a^\dagger_3 a_4 \rangle - \langle a^\dagger_1 a_4 \rangle a^\dagger_3 a_2 - \langle a^\dagger_3 a_2 \rangle a^\dagger_1 a_4 + \langle a^\dagger_1 a_4 \rangle \langle a^\dagger_3 a_2 \rangle$Be cautious about the order of the index and sign before each term here.

Completion: Using Wick's theorem, the four-fermion term in V_{HF} can be expanded into quadratic terms. Following the example 1, the interaction term V_{HF} can be expanded as:

$$V_{HF} = \frac{1}{2A} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_4) \left(\langle c^\dagger_{\boldsymbol{k}_1\lambda_1} c_{\boldsymbol{k}_4\lambda_1} \rangle c^\dagger_{\boldsymbol{k}_2\lambda_2} c_{\boldsymbol{k}_3\lambda_2} + \langle c^\dagger_{\boldsymbol{k}_2\lambda_2} c_{\boldsymbol{k}_3\lambda_2} \rangle c^\dagger_{\boldsymbol{k}_1\lambda_1} c_{\boldsymbol{k}_4\lambda_1} - \langle c^\dagger_{\boldsymbol{k}_1\lambda_1} c_{\boldsymbol{k}_4\lambda_1} \rangle \langle c^\dagger_{\boldsymbol{k}_2\lambda_2} c_{\boldsymbol{k}_3\lambda_2} \rangle \right.$$

$$\left. - \langle c^\dagger_{\boldsymbol{k}_1\lambda_1} c_{\boldsymbol{k}_3\lambda_2} \rangle c^\dagger_{\boldsymbol{k}_2\lambda_2} c_{\boldsymbol{k}_4\lambda_1} - \langle c^\dagger_{\boldsymbol{k}_2\lambda_2} c_{\boldsymbol{k}_4\lambda_1} \rangle c^\dagger_{\boldsymbol{k}_1\lambda_1} c_{\boldsymbol{k}_3\lambda_2} + \langle c^\dagger_{\boldsymbol{k}_1\lambda_1} c_{\boldsymbol{k}_3\lambda_2} \rangle \langle c^\dagger_{\boldsymbol{k}_2\lambda_2} c_{\boldsymbol{k}_4\lambda_1} \rangle \right) \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}$$

This is the expanded form of the interaction term V_{HF} after Hartree-Fock approximation, in terms of the creation and annihilation operators, the interaction form $V(\boldsymbol{k}_1 - \boldsymbol{k}_4)$, and the momentum $\boldsymbol{k}$. The order of λ and λ' is $1,2,2,1$, and the order of $\boldsymbol{k}$ is $1,2,3,4$. The total momentum of all creation operators is the same as that of all annihilation operators, which is the constraint of total momentum conservation. The product of four operators with two creation and two annihilation operators follows the normal order, with creation operators before annihilation operators. The normalization factor is $\frac{1}{2A}$.

7 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the V_{HF}.The quadratic terms mean terms that are proportional to $c^\dagger_{\boldsymbol{k}\lambda} c_{\boldsymbol{k}\lambda}$ and $c^\dagger_{\boldsymbol{k}\lambda} c_{\boldsymbol{k}\lambda'}$, which excludes terms that are solely expectations or

products of expectations.You should only preserve the quadratic terms in V_{HF}, denoted as $V_{HF}^{(2)}$.You should recall that V_{HF} is

$$V_{HF} = \frac{1}{2A} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_4) \left[\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} + \langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} - \langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle \langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle \right.$$
$$\left. - \langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1} - \langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2} + \langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle \langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle \right] \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4} .$$

Return $V_{HF}^{(2)}$.
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):$c_{\boldsymbol{k}\lambda}^\dagger$ and $c_{\boldsymbol{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l,\sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgen}), denoted as $U_H^{ll'}$ and $U_X^{ll'}(\boldsymbol{q})$, involve sums over reciprocal lattice vectors G. In these equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

Completion: The quadratic terms in the Hartree-Fock interaction V_{HF} are those that involve two creation or annihilation operators. From the given expression for V_{HF}, the quadratic terms are:

$$V_{HF}^{(2)} = \frac{1}{2A} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_4) \left[\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} + \langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} - \langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1} \right.$$
$$\left. - \langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2} \right] \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4} .$$

This expression includes all terms that are proportional to $c_{\boldsymbol{k}\lambda}^\dagger c_{\boldsymbol{k}\lambda}$ and $c_{\boldsymbol{k}\lambda}^\dagger c_{\boldsymbol{k}\lambda'}$, and excludes terms that are solely expectations or products of expectations.

8 Combine Hartree/Fock terms

Prompt: You will be instructed to simplify the quadratic term $V_{HF}^{(2)}$ through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.The logic is that the expected value ($\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle$) in the first Hartree term ($\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2}$) has the same form as the quadratic operators in the second Hartree term ($\langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1}$), and vice versa. The same applies to the Fock term.This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree term, you can make the second Hartree term look identical to the first Hartree 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 perform this trick of "relabeling the index" for both two Hartree terms and two Fock terms to reduce them to one Hartree term, and one Fock term.You should recall that $V_{HF}^{(2)}$ is $V_{HF}^{(2)} = \frac{1}{2A} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_4) \left[\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} + \langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} - \langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1} - \langle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2} \right] \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}$.Return the simplified $V_{HF}^{(2)}$ which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term)
EXAMPLE: Given a Hamiltonian $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)(\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3) + \langle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3) \rangle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4))\delta_{k_1+k_2,k_3+k_4}$, 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, $\sigma_1 \leftrightarrow \sigma_2$, $\sigma_3 \leftrightarrow \sigma_4$, $k_1 \leftrightarrow k_2$, $k_3 \leftrightarrow k_4$. After the replacement, the second term becomes $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_2 - k_3)\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$.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 $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_4 - k_1)\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Because $V(q) = V(-q)$, meaning $V(k_4 - k_1) = V(k_1 - k_4)$, the second term further simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Note that this form of second term after relabeling is identical to the first term.Finally, we have the simplified Hamiltonian as $\hat{H} = 2\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)\langle c_{\sigma_1}^\dagger(k_1)c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$.

Completion: Following the example, we can simplify the quadratic term $V_{HF}^{(2)}$ by relabeling the indices.
For the second Hartree term, we swap the indices as follows: $\boldsymbol{k}_1 \leftrightarrow \boldsymbol{k}_2$, $\boldsymbol{k}_3 \leftrightarrow \boldsymbol{k}_4$, $\lambda_1 \leftrightarrow \lambda_2$. After the replacement, the second Hartree term becomes $\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2}$, which is identical to the first Hartree term.
For the second Fock term, we swap the indices as follows: $\boldsymbol{k}_1 \leftrightarrow \boldsymbol{k}_2$, $\boldsymbol{k}_3 \leftrightarrow \boldsymbol{k}_4$, $\lambda_1 \leftrightarrow \lambda_2$. After the replacement, the second Fock term becomes $-\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2} \rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1}$, which is identical to the first Fock term.

Therefore, the simplified $V_{HF}^{(2)}$ is:

$V_{HF}^{(2)} = \frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}\sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1-\boldsymbol{k}_4)\left[\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2} - \langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1}\right]\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}.$

This reduces the four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term).

9 Identify order parameters in Hartree term (extended BZ)

Prompt: You will be instructed to simplify the Hartree term in $V_H^{(2)}$ by reducing the momentum inside the expected value $\left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda'}\right\rangle$.The expected value $\left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda'}\right\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda'}\right\rangle = \left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda'}\right\rangle \delta_{k,k'}$.You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i. Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.You should recall that $V_H^{(2)}$ is $V_H^{(2)} = \frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}\sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1-\boldsymbol{k}_4)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}$.Return the final simplified Hartree term $V_H^{(2)}$.

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 in $V_H^{(2)}$ can be simplified by reducing the momentum inside the expected value $\left\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1}\right\rangle$. This expected value is nonzero only when $\boldsymbol{k}_1 = \boldsymbol{k}_4$, i.e., $\left\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1}\right\rangle = \left\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_4\lambda_1}\right\rangle \delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}$.

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

$V_H^{(2)} = \frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3}\sum_{\lambda_1,\lambda_2} V(0)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_1}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_3\lambda_2}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_1}$.

The total momentum conservation will reduce another momentum in the quadratic term. Therefore, we end up with only two momenta left in the summation. The final simplified Hartree term $V_H^{(2)}$ is:

$V_H^{(2)} = \frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\lambda_1,\lambda_2} V(0)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_1}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_2\lambda_2}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}$.

10 Identify order parameters in Fock term (extended BZ)

Prompt: You will be instructed to simplify the Fock term in $V_F^{(2)}$ by reducing the momentum inside the expected value $\left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda}\right\rangle$.The expected value $\left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda}\right\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda}\right\rangle = \left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda}\right\rangle \delta_{k,k'}$.You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i.Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term.You should recall that $V_F^{(2)}$ is $V_F^{(2)} = -\frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}\sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1-\boldsymbol{k}_4)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_3\lambda_2}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}$.Return the final simplified Fock term $V_F^{(2)}$.

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 Bril-

loun 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 $-\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle\delta_{k_1,k_3} c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.Use the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we have $-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_1+k_4+b_3+b_4} = -\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_2+b_1+b_2,k_4+b_3+b_4}$.Because k_i is momentum inside first Brilloun zone while b_i is the reciprocal lattice. It is only when $k_2 = k_4$ that $\delta_{k_2+b_1+b_2,k_4+b_3+b_4}$ is nonzero, i.e., $\delta_{k_2+b_1+b_2,k_4+b_3+b_4} = \delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4}$.Therefore, the Fock term simplifies to $-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4} = -\sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(k_1 - k_2 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_2)\delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Fock term after reducing two momenta is $\hat{H}^{Fock} = -\sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(k_1 - k_2 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_2)\delta_{b_1+b_2,b_3+b_4}$

Completion: The Fock term in $V_F^{(2)}$ can be simplified by reducing the momentum inside the expected value $\left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda}\right\rangle$. This is only nonzero when the two momenta k_i, k_j are the same, i.e., $\left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda}\right\rangle = \left\langle c_{\boldsymbol{k}'\lambda'}^\dagger c_{\boldsymbol{k}'\lambda}\right\rangle\delta_{k,k'}$.

We can use the property of the Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i. After reducing one momentum inside the expected value $\langle\dots\rangle$, the total momentum conservation will reduce another momentum in the quadratic term. Therefore, we end up with only two momenta left in the summation.

Following the example, the Fock term in $V_F^{(2)}$ can be simplified as follows:

$V_F^{(2)} = -\frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_4}\sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_4)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_2}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_4\lambda_1}\delta_{\boldsymbol{k}_2+\boldsymbol{k}_4,\boldsymbol{k}_1+\boldsymbol{k}_1}$.

This simplifies to:

$V_F^{(2)} = -\frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_2)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_2}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_2\lambda_1}$.

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

$V_F^{(2)} = -\frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1 - \boldsymbol{k}_2)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_2}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_2\lambda_1}$.

11 Final form of iteration in quadratic terms

Prompt: You will now be instructed to combine the Hartree term $V_H^{(2)}$ and the Fock term $V_F^{(2)}$.You should recall that the Hartree term $V_H^{(2)} = \frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\lambda_1,\lambda_2} V(0)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_1}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_2\lambda_2}$.,and the Fock term $V_F^{(2)} = -\frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\lambda_1,\lambda_2} V(\boldsymbol{k}_1-\boldsymbol{k}_2)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_2}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_2\lambda_1}$..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 $V_H^{(2)}$ and the Fock term $V_F^{(2)}$ can be combined by relabeling the indices in the Fock term to match those in the Hartree term. However, in this case, the instruction specifies that no swap should be performed. Therefore, the Fock term remains as it is.

The sum of the Hartree and Fock terms is then given by:

$V_{HF}^{(2)} = V_H^{(2)} + V_F^{(2)}$

$V_{HF}^{(2)} = \frac{1}{A}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\sum_{\lambda_1,\lambda_2}\left[V(0)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_1}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_2\lambda_2} - V(\boldsymbol{k}_1 - \boldsymbol{k}_2)\langle c_{\boldsymbol{k}_1\lambda_1}^\dagger c_{\boldsymbol{k}_1\lambda_2}\rangle c_{\boldsymbol{k}_2\lambda_2}^\dagger c_{\boldsymbol{k}_2\lambda_1}\right]$

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