

1 Identify kinetic term (continuum,first-quantized)

Prompt:You will be instructed to describe the kinetic term of Hamiltonian in the flavorless case, i.e. the valley projected and spinless case in the real space in the single-particle form. The degrees of freedom of the system are: spin index (\uparrow and \downarrow), valley index (+K and -K valley), layer index (top and bottom layer), and sublattice index (A and B). Express the Kinetic Hamiltonian $\hat{\mathcal{H}}_0^K$ using $\psi_{\alpha,\mathbf{k}}(\mathbf{r})$ which are only on the diagonal terms, and arrange the basis in the order of A1, B1, A2, B2. Note that the sublattice degrees of freedom is suppressed for now and will be stated later

Use the following conventions for the symbols: $\alpha = \{A1, B1, A2, B2\}$ where A(B) in the first index specifies sublattice and 1(2) in the second index specifies layer. $\hat{h}_{\pm\theta/2}$ are the Dirac Hamiltonians for isolated rotated graphene layers. $\theta_{\bar{\mathbf{k}}}$ is the orientation angle of momentum measured from the Dirac point $\bar{\mathbf{k}} = \mathbf{k} - \mathbf{K}_{\theta}$. $\mathbf{K}_{\pm\theta/2}$ is the Dirac momentum of top(bottom) layer. $\mathbf{b}_{1,2} = (\pm 1/2, \sqrt{3}/2)4\pi/(\sqrt{3}a_M)$ are the basis vectors of moiré {e} reciprocal lattice, where $a_M = a/(2\sin(\theta/2))$ is the lattice constant of moire pattern and a the lattice constant of monolayer graphene. $h_T(\mathbf{r}) = \sum_{j=0}^3 T_j e^{-i\mathbf{q}_j \cdot \mathbf{r}}$ where $T_j = \omega_0\sigma_0 + \omega_1 \cos(j\phi)\sigma_x + \omega_1 \sin(j\phi)\sigma_y$.

Completion:The kinetic term of the Hamiltonian in the flavorless case, i.e., the valley projected and spinless case in the real space in the single-particle form, can be written as:

$$\hat{\mathcal{H}}_0^K = \sum_{\alpha,\mathbf{k}} \psi_{\alpha,\mathbf{k}}^\dagger(\mathbf{r}) \hat{h}_{\pm\theta/2}(\mathbf{k} - \mathbf{K}_{\pm\theta/2}) \psi_{\alpha,\mathbf{k}}(\mathbf{r})$$

where $\alpha = \{A1, B1, A2, B2\}$, $\hat{h}_{\pm\theta/2}$ are the Dirac Hamiltonians for isolated rotated graphene layers, $\mathbf{K}_{\pm\theta/2}$ is the Dirac momentum of top(bottom) layer, and $\psi_{\alpha,\mathbf{k}}(\mathbf{r})$ are the field operators.

The sublattice degrees of freedom are suppressed for now and will be stated later. The basis is arranged in the order of A1, B1, A2, B2.

The Hamiltonian is diagonal in the momentum space, and the momentum \mathbf{k} is measured from the Dirac point $\bar{\mathbf{k}} = \mathbf{k} - \mathbf{K}_{\theta}$. The orientation angle of momentum from the Dirac point is denoted by $\theta_{\bar{\mathbf{k}}}$.

The term $\hat{h}_{\pm\theta/2}$ represents the Dirac Hamiltonians for isolated rotated graphene layers, and $\mathbf{K}_{\pm\theta/2}$ is the Dirac momentum of top(bottom) layer.

The moiré reciprocal lattice basis vectors are given by $\mathbf{b}_{1,2} = (\pm 1/2, \sqrt{3}/2)4\pi/(\sqrt{3}a_M)$, where $a_M = a/(2\sin(\theta/2))$ is the lattice constant of moire pattern and a the lattice constant of monolayer graphene.

The term $h_T(\mathbf{r}) = \sum_{j=0}^3 T_j e^{-i\mathbf{q}_j \cdot \mathbf{r}}$ represents the moiré potential, where $T_j = \omega_0\sigma_0 + \omega_1 \cos(j\phi)\sigma_x + \omega_1 \sin(j\phi)\sigma_y$.

2 Define energy dispersion (continuum)

Prompt:You will be instructed to construct each term, namely $h_{\theta}(\mathbf{k})$. For all energy dispersions, $h_{\theta}(\mathbf{k})$, it characterizes the Dirac dispersion for electrons. In addition, a shift of \mathbf{K}_{θ} in the momentum \mathbf{k} for $h_{s,\tau,l}(\mathbf{k})$, respectively. 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 $\mathbf{k} = -i\partial_{\mathbf{r}}$. You should keep the form of \mathbf{k} in the Hamiltonian for short notations but should remember \mathbf{k} is an operator. You should recall that

$$H_{Kinetic}(r) = \begin{bmatrix} h_{\uparrow,+K,t} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h_{\uparrow,+K,b} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_{\uparrow,-K,t} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{\uparrow,-K,b} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{\downarrow,+K,t} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{\downarrow,+K,b} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & h_{\downarrow,-K,t} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & h_{\downarrow,-K,b} \end{bmatrix}$$

. Return the expression for $h_{\theta}(\mathbf{k})$ in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian $\hat{\mathcal{H}}_0^K$.

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): $\alpha = \{A1, B1, A2, B2\}$, where A(B) in the first index specifies sublattice and 1(2) in the second index specifies layer. $\theta_{\bar{\mathbf{k}}}$ is the orientation angle of momentum measured from the Dirac point $\bar{\mathbf{k}} = \mathbf{k} - \mathbf{K}_{\theta}$. ($\mathbf{K}_{\pm\theta/2}$ is the Dirac momentum of top(bottom) layer.) $\mathbf{b}_{1,2} = (\pm 1/2, \sqrt{3}/2)4\pi/(\sqrt{3}a_M)$ are the basis vectors of moiré {e} reciprocal lattice, where $a_M = a/(2\sin(\theta/2))$ is the lattice constant of moire pattern and a the lattice constant of monolayer graphene.

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 azimuth angle of k . If there is a further shift of K_θ in the momentum k , the dispersion will become $h_\theta(k) = -\hbar v_D |k - K_\theta| \begin{pmatrix} 0 & e^{i(\theta_k - K_\theta - \theta)} \\ e^{-i(\theta_{\bar{k}} - K_\theta - \theta)} & 0 \end{pmatrix}$.

Completion: Given the information provided, we are dealing with a Dirac dispersion for electrons, which corresponds to Example 3. Therefore, the term $h_\theta(\mathbf{k})$ in the Kinetic Hamiltonian is given by:

$$h_\theta(\mathbf{k}) = -\hbar v_D |\mathbf{k} - \mathbf{K}_\theta| \begin{pmatrix} 0 & e^{i(\theta_{\bar{k}} - \theta)} \\ e^{-i(\theta_{\bar{k}} - \theta)} & 0 \end{pmatrix}$$

where \hbar is the reduced Planck's constant, v_D is the Fermi velocity, θ is the twist angle, \mathbf{k} is the momentum operator, and \mathbf{K}_θ is the Dirac momentum of the top (or bottom) layer. The term $\theta_{\bar{k}}$ is the orientation angle of momentum measured from the Dirac point $\bar{\mathbf{k}} = \mathbf{k} - \mathbf{K}_\theta$.

Substituting $h_\theta(\mathbf{k})$ into the Kinetic Hamiltonian $\hat{\mathcal{H}}_0^K$, we get:

$$\hat{\mathcal{H}}_0^K = \begin{bmatrix} h_\theta(\mathbf{k}) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h_\theta(\mathbf{k}) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_\theta(\mathbf{k}) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & h_\theta(\mathbf{k}) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & h_\theta(\mathbf{k}) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_\theta(\mathbf{k}) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & h_\theta(\mathbf{k}) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & h_\theta(\mathbf{k}) \end{bmatrix}$$

This is the Kinetic Hamiltonian with the Dirac dispersion term $h_\theta(\mathbf{k})$ for electrons.

3 Identify potential term (continuum)

Prompt: You will be instructed to describe the potential term of Hamiltonian $\hat{\mathcal{H}}_0^K$ in the real space in the single-particle form. The potential Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian. The diagonal terms are zero. The off-diagonal terms are the coupling between t and b , $h_T(r)$, which should be kept hermitian. All other terms are zero. Express the potential Hamiltonian $\hat{\mathcal{H}}_0^K$ using zero and $h_T(r)$.

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): $\alpha = \{A1, B1, A2, B2\}$, where $A(B)$ in the first index specifies sublattice and 1(2) in the second index specifies layer. $\theta_{\bar{k}}$ is the orientation angle of momentum measured from the Dirac point $\bar{\mathbf{k}} = \mathbf{k} - \mathbf{K}_\theta$. $\mathbf{b}_{1,2} = (\pm 1/2, \sqrt{3}/2)4\pi/(\sqrt{3}a_M)$ are the basis vectors of moiré {e} reciprocal lattice, where $a_M = a/(2 \sin(\theta/2))$ is the lattice constant of moiré pattern and a the lattice constant of monolayer graphene. $T_j = \omega_0 \sigma_0 + \omega_1 \cos(j\phi) \sigma_x + \omega_1 \sin(j\phi) \sigma_y$.

Completion: The potential Hamiltonian $\hat{\mathcal{H}}_0^K$ in the real space in the single-particle form can be expressed as a matrix with the same degrees of freedom as the kinetic Hamiltonian. The diagonal terms are zero, and the off-diagonal terms are the coupling between t and b , represented by $h_T(r)$, which should be kept hermitian. All other terms are zero.

The potential Hamiltonian $\hat{\mathcal{H}}_0^K$ can be written as:

$$\hat{\mathcal{H}}_0^K = \begin{pmatrix} 0 & h_T(r) & 0 & 0 \\ h_T^\dagger(r) & 0 & 0 & 0 \\ 0 & 0 & 0 & h_T(r) \\ 0 & 0 & h_T^\dagger(r) & 0 \end{pmatrix} \text{ where the rows and columns correspond to the degrees of}$$

freedom $\alpha = \{A1, B1, A2, B2\}$, respectively. Here, $h_T^\dagger(r)$ is the hermitian conjugate of $h_T(r)$.

4 Define potential term (continuum)

Prompt: You will be instructed to construct each term $\hat{\mathcal{H}}_0^K$, namely, $h_{\theta/2}(\mathbf{k})$, $h_T(r)$, $h_T^\dagger(r)$, and $h_{-\theta/2}(\mathbf{k}')$. The expression for diagonal terms are: $h_{\theta/2}(\mathbf{k})$ and $h_{-\theta/2}(\mathbf{k}')$. The expression for off-diagonal terms are: $h_T(r)$ and $h_T^\dagger(r)$. You should recall that $H_{Potential}(r) =$

$$\begin{bmatrix} 0 & h_T(r) & 0 & 0 & 0 & 0 & 0 & 0 \\ h_T^\dagger(r) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & h_T(r) & 0 & 0 & 0 & 0 \\ 0 & 0 & h_T^\dagger(r) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_T(r) & 0 & 0 \\ 0 & 0 & 0 & 0 & h_T^\dagger(r) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & h_T(r) \\ 0 & 0 & 0 & 0 & 0 & 0 & h_T^\dagger(r) & 0 \end{bmatrix}.$$

.Return the expressions for $h_{\theta/2}(\mathbf{k})$, $h_T(\mathbf{r})$,

$h_T^\dagger(\mathbf{r})$, and $h_{-\theta/2}(\mathbf{k}')$, and substitute it into the potential Hamiltonian $\hat{\mathcal{H}}_0^K$.

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 have conflicts in the conventions, you should stop and let me know): ω_i : magnitude of interlayer tunneling, $i=0,1,2$; σ_0 :

Pauli Matrix 0 $\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$; σ_x : Pauli Matrix x $\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$; σ_y : Pauli Matrix y $\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$; ϕ : interlayer

tunneling phase q_j : momentum boost

Completion: The diagonal terms $h_{\theta/2}(\mathbf{k})$ and $h_{-\theta/2}(\mathbf{k}')$ represent the Dirac Hamiltonians for isolated rotated graphene layers. They can be expressed as:

$$h_{\theta/2}(\mathbf{k}) = v_F(\mathbf{k} - \mathbf{K}_{\theta/2}) \cdot \boldsymbol{\sigma}$$

$$h_{-\theta/2}(\mathbf{k}') = v_F(\mathbf{k}' - \mathbf{K}_{-\theta/2}) \cdot \boldsymbol{\sigma}$$

where v_F is the Fermi velocity, $\boldsymbol{\sigma}$ is the vector of Pauli matrices, and $\mathbf{K}_{\pm\theta/2}$ is the Dirac momentum of top(bottom) layer.

The off-diagonal terms $h_T(\mathbf{r})$ and $h_T^\dagger(\mathbf{r})$ represent the coupling between the top and bottom layers. They can be expressed as:

$$h_T(\mathbf{r}) = \sum_{j=1}^3 T_j e^{i\mathbf{q}_j \cdot \mathbf{r}}$$

$$h_T^\dagger(\mathbf{r}) = \sum_{j=1}^3 T_j^\dagger e^{-i\mathbf{q}_j \cdot \mathbf{r}}$$

where $T_j = \omega_0 \sigma_0 + \omega_1 \cos(j\phi) \sigma_x + \omega_1 \sin(j\phi) \sigma_y$ is the interlayer tunneling term, \mathbf{q}_j is the momentum boost, and ϕ is the interlayer tunneling phase.

Substituting these expressions into the potential Hamiltonian $\hat{\mathcal{H}}_0^K$, we get:

$$\hat{\mathcal{H}}_0^K = \begin{pmatrix} h_{\theta/2}(\mathbf{k}) & h_T(\mathbf{r}) & 0 & 0 \\ h_T^\dagger(\mathbf{r}) & h_{-\theta/2}(\mathbf{k}') & 0 & 0 \\ 0 & 0 & h_{\theta/2}(\mathbf{k}) & h_T(\mathbf{r}) \\ 0 & 0 & h_T^\dagger(\mathbf{r}) & h_{-\theta/2}(\mathbf{k}') \end{pmatrix}$$

This is the potential Hamiltonian $\hat{\mathcal{H}}_0^K$ in the real space in

the single-particle form, with the expressions for $h_{\theta/2}(\mathbf{k})$, $h_T(\mathbf{r})$, $h_T^\dagger(\mathbf{r})$, and $h_{-\theta/2}(\mathbf{k}')$ substituted in.

5 Identify interacting term (momentum space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian \hat{H}^{int} 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 spin index, valley index and layer index, 1, 2, 3, 4 for the moire reciprocal lattice vectors, and 1, 2, 3, 4 for the momentum. 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. For each operator, the total momentum is the sum of moire reciprocal lattice b_i and momentum with in the first BZ k_i . The third part is the interaction form. You should use the bare Coulomb interaction with $V(q) = \text{the bare Coulomb}$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same spin index, valley index and layer index, 1, 2, 3, 4 for the moire reciprocal lattice vectors, namely $q = k_1 - k_4$. The fourth part is the normalization factor, you should use $\frac{1}{2NV}$ here. Finally, the summation should be running over all spin index, valley index and layer index, 1, 2, 3, 4 for the moire reciprocal lattice vectors, and momentum. Return the interaction term \hat{H}^{int} in terms of spin index, moire reciprocal lattice index and $V(q)$ (with q expressed in terms of momentum).

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): $c_{s,\tau,l,\alpha,b}(k)$: annihilation operator with spin s , valley τ , layer l , sublattice α , and moire reciprocal lattice vectors $b \in$: dielectric constant $V(q)$: bare Coulomb interaction in the momentum space

Completion: The interaction Hamiltonian \hat{H}^{int} in the momentum space can be constructed as follows:

$$\hat{H}^{int} = \frac{1}{2NV} \sum_{s,\tau,l,\alpha,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(k_1 - k_4) \times [c_{s,\tau,l,\alpha,b_1}^\dagger(k_1) c_{s,\tau,l,\alpha,b_2}^\dagger(k_2) c_{s,\tau,l,\alpha,b_3}(k_3) c_{s,\tau,l,\alpha,b_4}(k_4)] \times$$

$$\delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4}$$

Here, $c_{s,\tau,l,\alpha,b}^\dagger(k)$ and $c_{s,\tau,l,\alpha,b}(k)$ are the creation and annihilation operators respectively, with spin s , valley τ , layer l , sublattice α , and moire reciprocal lattice vectors b . The momentum of the particles is represented by k . The delta function $\delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4}$ ensures the conservation of total momentum. The interaction form is represented by the bare Coulomb interaction $V(k_1-k_4) = 2\pi e^2/(\epsilon|k_1-k_4|)$, where ϵ is the dielectric constant. The normalization factor is $\frac{1}{2NV}$. The summation runs over all spin, valley, layer, sublattice, moire reciprocal lattice vectors, and momentum.

6 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $\Sigma^H + \Sigma^F$. You should use Wick's theorem to expand the four-fermion term in $\Sigma^H + \Sigma^F$ into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without † , and be extremely cautious about the order of the index and sign before each term. You should only preserve the normal terms. Here, the normal terms mean the product of a creation operator and an annihilation operator. You should recall that $\hat{H}^{int} = \frac{1}{2NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{b_3, b_4} \sum_{k_1, k_2, k_3, k_4} V(q) \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4} \times$

$c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4)$. Return the expanded interaction term after Hartree-Fock approximation as \mathcal{H} .

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): $\omega_1 \equiv T_{AB} = 110 \text{ meV}$ and $\omega_0 \equiv T_{AA} = 0.8\omega_1$ are the magnitudes of interlayer tunneling. \mathbf{k} is restricted to the first moiré Brillouin zone (mBZ) ($\mathbf{k} \in \text{mBZ}$). The plane-wave expansion basis is $|\psi_{\alpha, \mathbf{G}, \mathbf{k}}\rangle$ where $\mathbf{G} = m\mathbf{b}_1 + n\mathbf{b}_2$ and m, n are integers. The single-particle Hamiltonian \hat{H}_0^K has both terms that are diagonal in reciprocal lattice vector and terms that are off-diagonal in reciprocal lattice vector. The Hartree and Fock self-energies are $\Sigma_{\alpha, \mathbf{G}; \beta, \mathbf{G}'}^H(\mathbf{k})$ and $\Sigma_{\alpha, \mathbf{G}; \beta, \mathbf{G}'}^F(\mathbf{k})$ respectively. The density-matrix ρ is defined in a plane wave basis as $\rho_{\alpha, \mathbf{G}; \beta, \mathbf{G}'}(\mathbf{k}) = \sum_n z_{\beta, \mathbf{G}', \mathbf{k}}^{n*} z_{\alpha, \mathbf{G}, \mathbf{k}}^n$ where the summation is over filled bands. $z_{\alpha, \mathbf{G}, \mathbf{k}}^n$ is a numerical eigenvector in the plane-wave expansion.

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: To perform the Hartree-Fock approximation, we expand the interaction term $\Sigma^H + \Sigma^F$ using Wick's theorem. The four-fermion term in $\Sigma^H + \Sigma^F$ is expanded into quadratic terms.

Following the example 1, the interaction Hamiltonian \hat{H}^{int} can be expanded as:

$$\hat{H}^{int} = \frac{1}{2NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{b_3, b_4} \sum_{k_1, k_2, k_3, k_4} V(q) \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4} \times$$

$$\begin{aligned} & [\langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \\ & + \langle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \\ & - \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle \langle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle \\ & - \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \\ & - \langle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \\ & + \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle \langle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle] \end{aligned}$$

This is the expanded interaction term after Hartree-Fock approximation, represented as \mathcal{H} .

7 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the $\hat{H}^{int, HF}$. The quadratic terms mean terms that are proportional to $\rho_{\alpha, \mathbf{G}; \beta, \mathbf{G}'}(\mathbf{k}) = \sum_n z_{\beta, \mathbf{G}', \mathbf{k}}^{n*} z_{\alpha, \mathbf{G}, \mathbf{k}}^n$ which excludes terms that are solely expectations or products of expectations. You should only preserve the quadratic terms in

$\hat{H}^{int,HF}$, denoted as $\hat{H}^{int,HF,2}$. You should recall that

$$\hat{H}^{int,HF} = \frac{1}{2NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2,k_3,k_4} V(q) \times \delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4} \times \left[\begin{aligned} &\langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) + \\ &\langle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) \rangle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) - \\ &\langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) \rangle \langle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) \rangle - \\ &\langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) - \\ &\langle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) \rangle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) + \\ &\langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) \rangle \langle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) \rangle \end{aligned} \right]$$

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

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}_0^K is the single-particle Hamiltonian, Σ^H and Σ^F are the Hartree and Fock self-energies respectively, $\rho_{\alpha,G;\beta,G'}(\mathbf{k})$ is the density-matrix defined in a plane wave basis, and $z_{\alpha,G,\mathbf{k}}^n$ is a numerical eigenvector in the plane-wave expansion.

Completion: The quadratic terms in $\hat{H}^{int,HF}$ are those that involve the product of two creation or annihilation operators, excluding terms that are solely expectations or products of expectations. These terms are proportional to the density-matrix $\rho_{\alpha,G;\beta,G'}(\mathbf{k})$.

Therefore, the quadratic terms in $\hat{H}^{int,HF}$, denoted as $\hat{H}^{int,HF,2}$, can be extracted from the given $\hat{H}^{int,HF}$ as follows:

$$\hat{H}^{int,HF,2} = \frac{1}{2NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2,k_3,k_4} V(q) \times \delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4} \times \left[\begin{aligned} &\langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) + \\ &\langle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) \rangle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) \end{aligned} \right] \text{The other terms in } \hat{H}^{int,HF} \text{ are not quadratic and are therefore not included in } \hat{H}^{int,HF,2}.$$

8 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $\Sigma_{\alpha,G;\beta,G'}^H(\mathbf{k})$ and $\Sigma_{\alpha,G;\beta,G'}^F(\mathbf{k})$. If you find the $V(q)$ in $\Sigma_{\alpha,G;\beta,G'}^H(\mathbf{k})$ and $\Sigma_{\alpha,G;\beta,G'}^F(\mathbf{k})$ 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 b_i and k_i .

You should recall that $\hat{H}^{int,HF,2} = \frac{1}{2NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2,k_3,k_4} V(q) \times \delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4} \times \left[\begin{aligned} &\langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) + \\ &\langle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) \rangle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) - \\ &\langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) - \\ &\langle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4) \rangle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_3) \end{aligned} \right].$ Return $\Sigma_{\alpha,G;\beta,G'}^H(\mathbf{k})$ and $\Sigma_{\alpha,G;\beta,G'}^F(\mathbf{k})$ with expanded interaction.

Completion: The Hartree and Fock self-energies $\Sigma_{\alpha,G;\beta,G'}^H(\mathbf{k})$ and $\Sigma_{\alpha,G;\beta,G'}^F(\mathbf{k})$ are given by:

$$\Sigma_{\alpha,G;\beta,G'}^H(\mathbf{k}) = \frac{1}{NV} \sum_{G''} V(G - G'') \rho_{\alpha,G'';\beta,G'}(\mathbf{k})$$

$$\Sigma_{\alpha,G;\beta,G'}^F(\mathbf{k}) = -\frac{1}{NV} \sum_{G''} V(G - G'') \rho_{\beta,G'';\alpha,G'}(\mathbf{k})$$

where $V(\mathbf{G} - \mathbf{G}'') = 2\pi e^2/(\epsilon|\mathbf{G} - \mathbf{G}''|)$ is the bare Coulomb interaction in the momentum space, $\rho_{\alpha,\mathbf{G};\beta,\mathbf{G}'}(\mathbf{k})$ is the density-matrix defined in a plane wave basis, and the summation is over all reciprocal lattice vectors \mathbf{G}'' .

If the momentum $\mathbf{G} - \mathbf{G}''$ in $V(\mathbf{G} - \mathbf{G}'')$ is not in the summation sign, we replace it with the momentum b_i and k_i from the MF quadratic term $\hat{H}^{int,HF,2}$, yielding:

$$\Sigma_{\alpha,\mathbf{G};\beta,\mathbf{G}'}^H(\mathbf{k}) = \frac{1}{NV} \sum_{b_i, k_i} V(b_i + k_i) \rho_{\alpha, b_i; \beta, k_i}(\mathbf{k})$$

$$\Sigma_{\alpha,\mathbf{G};\beta,\mathbf{G}'}^F(\mathbf{k}) = -\frac{1}{NV} \sum_{b_i, k_i} V(b_i + k_i) \rho_{\beta, b_i; \alpha, k_i}(\mathbf{k})$$

These are the expanded Hartree and Fock self-energies with the interaction term $V(q)$ expanded.

9 Combine Hartree/Fock terms

Prompt: You will be instructed to simplify the quadratic term $\hat{H}^{int,HF,2}$ through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term. The logic is that the expected value $\langle (c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4)) \rangle$ in the first Hartree term $\langle (c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_2}(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3)) \rangle$ has the same form as the quadratic operators in the second Hartree term $\langle (c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3)) c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4)) \rangle$, 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

$$\begin{aligned} \hat{H}^{int,HF,2} = & \frac{1}{2NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{k_1, k_2, k_3, k_4} V(k_4 + b_4 - k_1 - b_1) \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4} \times [\\ & \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) + \\ & \langle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) - \\ & \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) - \\ & \langle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3)] \end{aligned}$$

. Return the simplified $\hat{H}^{int,HF,2}$ 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 $\hat{H} = \sum_{k_1, k_2, k_3, k_4, \sigma_1, \sigma_2, \sigma_3, \sigma_4} V(k_1 - k_4) \langle (c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)) c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) + \langle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \rangle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle \delta_{k_1+k_2, k_3+k_4}$, 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 $\hat{H}^{int,HF,2}$ by relabeling the indices in the second Hartree term and the second Fock term.

For the second Hartree term, we swap the indices as follows: $s_1 \leftrightarrow s_2$, $\tau_1 \leftrightarrow \tau_2$, $l_1 \leftrightarrow l_2$, $\alpha_1 \leftrightarrow \alpha_2$, $b_1 \leftrightarrow b_2$, $b_3 \leftrightarrow b_4$, $k_1 \leftrightarrow k_2$, and $k_3 \leftrightarrow k_4$.

After the replacement, the second Hartree term becomes

$$\langle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4),$$

which is identical to the first Hartree term.

For the second Fock term, we swap the indices as follows: $s_1 \leftrightarrow s_2$, $\tau_1 \leftrightarrow \tau_2$, $l_1 \leftrightarrow l_2$, $\alpha_1 \leftrightarrow \alpha_2$, $b_1 \leftrightarrow b_2$, $b_3 \leftrightarrow b_4$, $k_1 \leftrightarrow k_2$, and $k_3 \leftrightarrow k_4$.

After the replacement, the second Fock term becomes

$$\langle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3),$$

which is identical to the first Fock term.

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

$$\hat{H}^{int, HF, 2} = \frac{1}{NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{b_3, b_4} \sum_{k_1, k_2, k_3, k_4} V(k_4 + b_4 - k_1 - b_1) \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4} \times [\\ \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) - \\ \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4)]$$

10 Identify order parameters in Hartree term (extended BZ)

Prompt: You will be instructed to simplify the Hartree term in $\hat{H}^{int, HF, 2}$ by reducing the momentum inside the expected value $\langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle$. The expected value $\langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle = \langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle \delta_{k_i, k_j}$. 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 $\hat{H}^{int, Hartree, 2} = \frac{1}{NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{b_3, b_4} \sum_{k_1, k_2, k_3, k_4} V(k_1 + b_1 - k_4 - b_4) \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4} \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3)$. Return the final simplified Hartree term $\hat{H}^{int, HF, 2}$.

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 Brillouin 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 Brillouin 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: Following the example, we first note that the expectation value $\langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle$ is nonzero only when $k_1 = k_4$. Therefore, we can write $\langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle = \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle \delta_{k_1, k_4}$. Substituting this into the Hartree term, we get:

$$\hat{H}^{int, Hartree, 2} = \frac{1}{NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{b_3, b_4} \sum_{k_1, k_2, k_3, k_4} V(k_1 + b_1 - k_4 - b_4) \\ \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4} \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4) \rangle \delta_{k_1, k_4} c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3).$$

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

$$\hat{H}^{int, Hartree, 2} = \frac{1}{NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{b_3, b_4} \sum_{k_1, k_2, k_3} V(b_1 - b_4) \\ \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_1+b_4} \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_1) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3).$$

Finally, using the property of the Kronecker delta function $\delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_1+b_4}$ to sum over k_3 , we get:

$$\hat{H}^{int, Hartree, 2} = \frac{1}{NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{k_1, k_2} V(b_1 - b_4) \\ \times \delta_{b_1+b_2, b_3+b_4} \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_1) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_2).$$

Therefore, the final simplified Hartree term $\hat{H}^{int, HF, 2}$ after reducing two momenta is:

$$\hat{H}^{int, HF, 2} = \frac{1}{NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{k_1, k_2} V(b_1 - b_4) \\ \times \delta_{b_1+b_2, b_3+b_4} \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_1) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_2).$$

11 Identify order parameters in Fock term (extended BZ)

Prompt: You will be instructed to simplify the Fock term in $\hat{H}^{int, HF, 2}$ by reducing the momentum inside the expected value $\langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle$. The expected value $\langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle = \langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle \delta_{k_i, k_j}$. 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 (...). 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 $\hat{H}^{int, Fock, 2} = -\frac{1}{NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{k_1, k_2, k_3, k_4} V(k_1 + b_1 - k_4 - b_4) \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4} \times$

$\langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4)$. Return the final simplified Fock term $\hat{H}^{int, HF, 2}$.

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 Brillouin 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 Brillouin 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: Following the example, we first note that the expected value $\langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle$ is nonzero only when $k_i = k_j$. Therefore, we can write $\langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle = \langle c_{s_i, \tau_i, l_i, \alpha_i, b_i}^\dagger(k_i) c_{s_j, \tau_j, l_j, \alpha_j, b_j}(k_j) \rangle \delta_{k_i, k_j}$.

Substituting this into the Fock term of $\hat{H}^{int, HF, 2}$, we get:

$$\hat{H}^{int, Fock, 2} = -\frac{1}{NV} \sum_{\substack{s_1, s_2 \\ \tau_1, \tau_2 \\ l_1, l_2 \\ \alpha_1, \alpha_2}} \sum_{b_1, b_2} \sum_{k_1, k_2, k_3, k_4} V(k_1 + b_1 - k_4 - b_4) \times \delta_{k_1+b_1+k_2+b_2, k_3+b_3+k_4+b_4} \\ \times \langle c_{s_1, \tau_1, l_1, \alpha_1, b_1}^\dagger(k_1) c_{s_2, \tau_2, l_2, \alpha_2, b_3}(k_3) \rangle \delta_{k_1, k_3} c_{s_2, \tau_2, l_2, \alpha_2, b_2}^\dagger(k_2) c_{s_1, \tau_1, l_1, \alpha_1, b_4}(k_4).$$

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

$$\hat{H}^{int,Fock,2} = -\frac{1}{NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2,k_4} V(k_1 + b_1 - k_4 - b_4) \times \delta_{k_1+b_1+k_2+b_2,k_1+b_3+k_4+b_4} \\ \times \langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_1) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4).$$

This simplifies to:

$$\hat{H}^{int,Fock,2} = -\frac{1}{NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2,k_4} V(k_1 + b_1 - k_4 - b_4) \times \delta_{k_2+b_1+b_2,k_4+b_3+b_4} \\ \times \langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_1) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_4).$$

Finally, using the property that $\delta_{k_2+b_1+b_2,k_4+b_3+b_4}$ is nonzero only when $k_2 = k_4$, we get:

$$\hat{H}^{int,Fock,2} = -\frac{1}{NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2} V(k_1 + b_1 - k_2 - b_4) \times \delta_{b_1+b_2,b_3+b_4} \\ \times \langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_1) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_2).$$

This is the final simplified Fock term $\hat{H}^{int,HF,2}$ after reducing two momenta.

12 Final form of iteration in quadratic terms

Prompt: You will now be instructed to combine the Hartree term $\hat{H}^{int,Hartree,2}$ and the Fock term $\hat{H}^{int,Fock,2}$. You should recall that the Hartree term $\hat{H}^{int,HF,2} = \frac{1}{NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2} V(b_1 -$

$b_4) \times \delta_{b_1+b_2,b_3+b_4} \langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_1) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_2)$, and the Fock term $\hat{H}^{int,Fock,2} = -\frac{1}{NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2} V(k_1 + b_1 - k_2 - b_4) \times \delta_{b_1+b_2,b_3+b_4} \times$

$\langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_1) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_2)$. You should perform the same trick of relabeling the index in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. The relabeling should be done with a swap : Nothing. You should add them, relabel the index in Fock term, and simply their sum. Return the final sum of Hartree and Fock term.

Completion: To combine the Hartree and Fock terms, we first relabel the indices in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. Since the instruction specifies that no swap is needed, the relabeled Fock term remains the same.

The combined Hartree and Fock term is then given by:

$$\hat{H}^{int,HF,2} = \hat{H}^{int,Hartree,2} + \hat{H}^{int,Fock,2} \\ = \frac{1}{NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2} V(b_1 - b_4) \times \delta_{b_1+b_2,b_3+b_4} \langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_1) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_2) \\ - \frac{1}{NV} \sum_{\substack{s_1,s_2 \\ \tau_1,\tau_2 \\ l_1,l_2 \\ \alpha_1,\alpha_2}} \sum_{\substack{b_1,b_2 \\ b_3,b_4}} \sum_{k_1,k_2} V(k_1 + b_1 - k_2 - b_4) \times \delta_{b_1+b_2,b_3+b_4} \times \langle c_{s_1,\tau_1,l_1,\alpha_1,b_1}^\dagger(k_1) c_{s_2,\tau_2,l_2,\alpha_2,b_3}(k_1) \rangle c_{s_2,\tau_2,l_2,\alpha_2,b_2}^\dagger(k_2) c_{s_1,\tau_1,l_1,\alpha_1,b_4}(k_2)$$

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