1 Identify kinetic term (continuum,second-quantized)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in TMD moiré materials in the real space in the single-particle form.The degrees of freedom of the system are: moire reciprocal lattice vectors b (infinite set), spin index (spin up and spin down).Express the Kinetic Hamiltonian T using $E_{\sigma,b}(k)$, $c_{\sigma,b}(k)$, and $c^{\dagger}_{\sigma,b}(k)$, where the summation of $\boldsymbol{k}$ should be running over the first Brillouin zone.

Use the following conventions for the symbols:$\hbar$ is the reduced Planck constant, m^* is the effective mass of the electrons, $\boldsymbol{k}$ is the momentum in the first moiré Brillouin zone, $\boldsymbol{b}$'s are moiré reciprocal lattice vectors.

Completion: The kinetic term of the Hamiltonian in TMD moiré materials in the real space in the single-particle form can be expressed as:

$$T = \sum_{\sigma,b,\boldsymbol{k}} E_{\sigma,b}(\boldsymbol{k})c^{\dagger}_{\sigma,b}(\boldsymbol{k})c_{\sigma,b}(\boldsymbol{k}) \tag{1}$$

where σ is the spin index, $\boldsymbol{b}$ are the moiré reciprocal lattice vectors, and $\boldsymbol{k}$ is the momentum in the first moiré Brillouin zone. The summation over $\boldsymbol{k}$ runs over the first Brillouin zone. $E_{\sigma,b}(\boldsymbol{k})$ is the energy of an electron with spin σ, momentum $\boldsymbol{k}$, and moiré reciprocal lattice vector $\boldsymbol{b}$. $c^{\dagger}_{\sigma,b}(\boldsymbol{k})$ and $c_{\sigma,b}(\boldsymbol{k})$ are the creation and annihilation operators, respectively, for an electron with these quantum numbers.

2 Define energy dispersion (continuum)

Prompt: You will be instructed to construct each term, namely $H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k})$.For all energy dispersions, $H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k})$, it characterizes the parabolic dispersion for holes.In addition, a shift of b in the momentum k for $H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k})$, 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 $k = -i\partial_r$. You should keep the form of k in the Hamiltonian for short notations but should remember k is an operator.You should recall that $H_{Kinetic} = \sum_{\sigma,b,k} E_{\sigma,b}(k)c^{\dagger}_{\sigma,b}(k)c_{\sigma,b}(k)$.Return the expression for $H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k})$ 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):b: moir'e reciprocal lattice vectors, k: momentum, H_0: single-particle Hamiltonian, m^*: effective mass of electrons, V_j: material-dependent parameters, V_M: moir'e modulation strength, ϕ: shape of moir'e modulation, Δ: moir'e potential, r: position vector, $\psi^{(\dagger)}_{\alpha}(\boldsymbol{r})$: fermion field operators, α: label representing locked spin/valley

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., $h_\theta(k) = -\hbar v_D |k| \begin{pmatrix} 0 & e^{i(\theta_k - \theta)} \\ e^{-i(\theta_{\tilde{k}} - \theta)} & 0 \end{pmatrix}$, 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 question and the examples, we are dealing with a parabolic dispersion for holes with a shift of b in the momentum k. Therefore, we should follow Example 2.

The energy dispersion for a hole with a shift of b in the momentum k is given by:

$E_{\sigma,b}(k) = -\frac{\hbar^2 (k-b)^2}{2m^*}$

where σ indicates the type of hole, m^* is the effective mass of the hole, and $\hbar$ is the reduced Planck constant.

The term $H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k})$ in the kinetic Hamiltonian is then given by:

$H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k}) = E_{\sigma,b}(k) c^\dagger_{\sigma,b}(k) c_{\sigma,b}(k)$

Substituting the expression for $E_{\sigma,b}(k)$ into $H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k})$, we get:

$H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k}) = -\frac{\hbar^2 (k-b)^2}{2m^*} c^\dagger_{\sigma,b}(k) c_{\sigma,b}(k)$

This is the expression for $H_{0\boldsymbol{b},\boldsymbol{b}'}(\boldsymbol{k})$ in the kinetic Hamiltonian.

Finally, we substitute this into the kinetic Hamiltonian H_0:

$H_0 = \sum_{\sigma,b,k} -\frac{\hbar^2 (k-b)^2}{2m^*} c^\dagger_{\sigma,b}(k) c_{\sigma,b}(k)$

This is the final form of the kinetic Hamiltonian H_0, which includes a summation over the spin index, the moiré reciprocal lattice vectors, and the momentum in the first moiré Brillouin zone.

3 Identify potential term (continuum)

Prompt: You will be instructed to describe the potential term of Hamiltonian H_0 in the momentum space in the single-particle form.The potential Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian.The diagonal terms are $\Delta_{\sigma,b,b}$.The off-diagonal terms are the coupling between b and b', $\Delta_{\sigma,b,b'}$, which should be kept hermitian.All others terms are zero. Express the potential Hamiltonian H_0 using $\Delta_{\sigma,b,b}$ and $\Delta_{\sigma,b,b'}$.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop

and let me know):H_0 is the single-particle Hamiltonian of the moir'e continuum model, T is the single-particle kinetic energy operator for electrons with effective mass m^*, $\Delta(\mathbf{r})$ is the moir'e potential, $V_j = V_M \exp\left[(-1)^{j-1}i\phi\right]$ where V_M characterizes the moir'e modulation strength and ϕ its shape, $\mathbf{k}$ is in the first moir'e Brillouin zone and the $\mathbf{b}'s$ are moir'e reciprocal lattice vectors.

Completion: The potential term of the Hamiltonian H_0 in the momentum space in the single-particle form can be expressed as follows:

$H_0 = \sum_{\sigma,b,k} \Delta_{\sigma,b,b} c^\dagger_{\sigma,b}(k) c_{\sigma,b}(k) + \sum_{\sigma,b \neq b',k} \Delta_{\sigma,b,b'} c^\dagger_{\sigma,b}(k) c_{\sigma,b'}(k) + h.c.$

Here, $\Delta_{\sigma,b,b}$ are the diagonal terms of the potential Hamiltonian, and $\Delta_{\sigma,b,b'}$ are the off-diagonal terms representing the coupling between b and b'. The term $h.c.$ denotes the Hermitian conjugate to ensure the Hamiltonian is Hermitian. All other terms are zero.

4 Define potential term (continuum)

Prompt: You will be instructed to construct each term $\Delta(\mathbf{r})$, namely, $\Delta_{\sigma,b,b'}$.The expression for diagonal terms are: $\Delta_{\sigma,b,b} = \sum_{j=1}^{6} V_j \delta_{b_j,0}$, where $V_j = V_M e^{(-1)^{j-1}i\phi}$.The expression for off-diagonal terms are: $\sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j, \mathbf{b}-\mathbf{b}'}$.You should recall that $H_{Potential} = \sum_{\sigma,b,b',k} \Delta_{\sigma,b,b'} c^\dagger_{\sigma,b}(k) c_{\sigma,b'}(k)$.Return the expressions for $\Delta_{\sigma,b,b'}$, and substitute it into the potential Hamiltonian $\Delta(\mathbf{r})$.

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 have conflicts in the conventions, you should stop and let me know):$V_j = V_M \exp\left[(-1)^{j-1}i\phi\right]$ where V_M characterizes the moir'e modulation strength and ϕ its shape. The fermion field operators $\psi_\alpha^{(\dagger)}(\mathbf{r})$ in this model carry only one label, representing locked spin/valley. The single-particle Hamiltonian of the moir'e continuum model $H_0 = T + \Delta(\mathbf{r})$, where T is the single-particle kinetic energy operator for electrons with effective mass m^*.

Completion: The expressions for the diagonal and off-diagonal terms of $\Delta_{\sigma,b,b'}$ are given as follows:

For the diagonal terms, we have: $\Delta_{\sigma,b,b} = \sum_{j=1}^{6} V_j \delta_{b_j,0}$, where $V_j = V_M e^{(-1)^{j-1}i\phi}$.

For the off-diagonal terms, we have: $\Delta_{\sigma,b,b'} = \sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j, \mathbf{b}-\mathbf{b}'}$.

Substituting these expressions into the potential Hamiltonian $\Delta(\mathbf{r})$, we get:

$\Delta(\mathbf{r}) = \sum_{\sigma,b,b',k} \Delta_{\sigma,b,b'} c^\dagger_{\sigma,b}(k) c_{\sigma,b'}(k)$

$= \sum_{\sigma,b,k} \left(\sum_{j=1}^{6} V_j \delta_{b_j,0}\right) c^\dagger_{\sigma,b}(k) c_{\sigma,b}(k) + \sum_{\sigma,b \neq b',k} \left(\sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j, \mathbf{b}-\mathbf{b}'}\right) c^\dagger_{\sigma,b}(k) c_{\sigma,b'}(k)$

This is the expression for the potential Hamiltonian $\Delta(\mathbf{r})$ in terms of the diagonal and off-diagonal terms of $\Delta_{\sigma,b,b'}$.

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, 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 $V(q) = 2\pi e^2/(\epsilon|q|)$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same spin index, 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, and momentum Return the interaction term $\hat{H}^{int}$ in terms of $c_{\sigma,b}(k)$ 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): ϵ : dielectric constant $V(q)$: bare Coulomb interaction in the momentum space

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

$\hat{H}^{int} = \frac{1}{2NV} \sum_{\sigma_1,\sigma_2} \sum_{b_1,b_2,b_3,b_4} \sum_{k_1,k_2,k_3,k_4} V(k_1-k_4) c^\dagger_{\sigma_1,b_1}(k_1) c^\dagger_{\sigma_2,b_2}(k_2) c_{\sigma_2,b_3}(k_3) c_{\sigma_1,b_4}(k_4) \delta_{k_1+b_1+k_2+b_2,k_3+}$

Here, $V(k_1 - k_4)$ is the bare Coulomb interaction in the momentum space, $c^\dagger_{\sigma,b}(k)$ and $c_{\sigma,b}(k)$ are the creation and annihilation operators respectively, σ is the spin index, b is the moiré reciprocal lattice vector, and k is the momentum. The Kronecker 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 normalization factor is $\frac{1}{2NV}$, where N is the number of particles and V is the volume of the system. The summation runs over all spin indices and momenta.

6 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, Σ^{HF}. You should use Wick's theorem to expand the four-fermion term in Σ^{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 $\hat{H}^{int} = \frac{1}{2NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} c^\dagger_{\sigma_1,b_1}(k_1) c^\dagger_{\sigma_2,b_2}(k_2) c_{\sigma_2,b_3}(k_3) c_{\sigma_1,b_4}(k_4) V(q) \delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}$, where $q = k_1 + b_1 - k_4 - b_4$. Return the expanded interaction term after Hartree-Fock approximation as Σ^{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):Σ^{HF} is the Hartree-Fock self-energy, ρ is the single-particle density matrix, $\boldsymbol{k}$ is in the Brillouin-zone, $\boldsymbol{b}$ is the reciprocal lattice vectors, α and β label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}$ is the self-consistently determined momentum-space density matrix.

EXAMPLE 1:For a four-fermion term $a_1^\dagger a_2^\dagger a_3 a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a_1^\dagger a_2^\dagger a_3 a_4 = \langle a_1^\dagger a_4 \rangle a_2^\dagger a_3 + \langle a_2^\dagger a_3 \rangle a_1^\dagger a_4 - \langle a_1^\dagger a_4 \rangle \langle a_2^\dagger a_3 \rangle - \langle a_1^\dagger a_3 \rangle a_2^\dagger a_4 - \langle a_2^\dagger a_4 \rangle a_1^\dagger a_3 + \langle a_1^\dagger a_3 \rangle \langle a_2^\dagger a_4 \rangle$Be cautious about the order of the index and sign before each term here.

EXAMPLE 2:For a four-fermion term $a_1^\dagger a_2 a_3^\dagger a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a_1^\dagger a_2 a_3^\dagger a_4 = \langle a_1^\dagger a_2 \rangle a_3^\dagger a_4 + \langle a_3^\dagger a_4 \rangle a_1^\dagger a_2 - \langle a_1^\dagger a_2 \rangle \langle a_3^\dagger a_4 \rangle - \langle a_1^\dagger a_4 \rangle a_3^\dagger a_2 - \langle a_3^\dagger a_2 \rangle a_1^\dagger a_4 + \langle a_1^\dagger a_4 \rangle \langle a_3^\dagger a_2 \rangle$Be cautious about the order of the index and sign before each term here.

Completion: Using Wick's theorem, the interaction term $\hat{H}^{int}$ can be expanded as follows:

$\hat{H}^{int} = \frac{1}{2NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(q)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4} \left[\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_\ldots \right.$

Here, $q = k_1 + b_1 - k_4 - b_4$.

The Hartree-Fock self-energy Σ^{HF} is then given by the expectation value of the interaction Hamiltonian, which only includes the normal terms:

$\Sigma^{HF} = \frac{1}{2NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(q)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4} \left[\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)\rangle \langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k\ldots \right.$

This is the expanded interaction term after Hartree-Fock approximation.

7 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the Σ^{HF}.The quadratic terms mean terms that are proportional to $\rho_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in Σ^{HF}, denoted as $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}$.You should recall that

$\Sigma^{int,HF} = \frac{1}{2NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(q)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}[\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_3\ldots$
$\langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4) - \langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)\rangle \langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_3)\rangle -$
$\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4) - \langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3) +$
$\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle \langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4)\rangle]$.Return $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}$.

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):In $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}$, Greek letters label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}$ is the self-consistently determined momentum-space density matrix.

Completion: The quadratic terms in Σ^{HF} are those that are proportional to $\rho_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}$. From the given expression for $\Sigma^{int,HF}$, we can identify these terms as:

$\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF} = \frac{1}{2NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(q)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}[\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}$
$\langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4) - \langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4) -$
$\langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)]$

This expression represents the quadratic terms in the Hartree-Fock self-energy, $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}$, after the interaction term has been expanded using the Hartree-Fock approximation.

8 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k})$. If you find the $V(q)$ in $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k})$ 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 $k_1+b_1-k_4-b_4$. You should recall that $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k})$ is $\Sigma^{int,HF,2} = \frac{1}{2NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(q)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}[\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b}$
$\langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4) - \langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4) -$
$\langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)]$. Return $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k})$ with expanded interaction.

Completion: Given the expression for $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k})$, we can see that the interaction term $V(q)$ does contain momentum that is not in the summation sign. Therefore, we need to expand $V(q)$ by replacing q with the momentum $k_1+b_1-k_4-b_4$.

The expanded interaction term in $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k})$ is then:

$\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k}) = \frac{1}{2NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(k_1+b_1-k_4-b_4)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}[\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)$
$\langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4) - \langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4) -$
$\langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)]$.

This is the expanded interaction term in the Hartree-Fock self-energy.

9 Combine Hartree/Fock terms

Prompt: You will be instructed to simplify the quadratic term Σ^{HF} through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term. The logic is that the expected value ($\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)\rangle$) in the first Hartree term ($\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_3)$) has the same form as the quadratic operators in the second Hartree term ($\langle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_1,b_4}(k_4)$), 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 $\Sigma^{int,HF,2} = \frac{1}{2NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(k_1+b_1-k_4-b_4)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}[\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_4)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_3)$
$\langle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_3)\rangle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_4)-\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_2,b_3}(k_3)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_1,b_4}(k_4)-$
$\langle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_1,b_4}(k_4)\rangle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_2,b_3}(k_3)]$. Return the simplified Σ^{HF} 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 $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)(\langle c^\dagger_{\sigma_1}(k_1)c_{\sigma_4}(k_4)\rangle c^\dagger_{\sigma_2}(k_2)c_{\sigma_3}(k_3)+$
$\langle c^\dagger_{\sigma_2}(k_2)c_{\sigma_3}(k_3)\rangle c^\dagger_{\sigma_1}(k_1)c_{\sigma_4}(k_4))\delta_{k_1+k_2,k_3+k_4}$, where $V(q) = V(-q)$. In the second term, we relabel the index to swap the index in expected value and the index in quadratic operators, namely, $\sigma_1 \leftrightarrow \sigma_2$, $\sigma_3 \leftrightarrow \sigma_4$, $k_1 \leftrightarrow k_2$, $k_3 \leftrightarrow k_4$. After the replacement, the second term becomes $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_2-k_3)\langle c^\dagger_{\sigma_1}(k_1)c_{\sigma_4}(k_4)\rangle c^\dagger_{\sigma_2}(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. 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 $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_4-k_1)\langle c^\dagger_{\sigma_1}(k_1)c_{\sigma_4}(k_4)\rangle c^\dagger_{\sigma_2}(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Because $V(q) = V(-q)$, meaning $V(k_4 - k_1) = V(k_1 - k_4)$, the second term further simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)\langle c^\dagger_{\sigma_1}(k_1)c_{\sigma_4}(k_4)\rangle c^\dagger_{\sigma_2}(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Note that this form of second term after relabeling is identical to the first term. Finally, we have the simplified Hamiltonian as $\hat{H} = 2\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)\langle c^\dagger_{\sigma_1}(k_1)c_{\sigma_4}(k_4)\rangle c^\dagger_{\sigma_2}(k_2)c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$.

Completion: Following the example, we can simplify the Hartree-Fock self-energy Σ^{HF} 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: $\sigma_1 \leftrightarrow \sigma_2$, $b_1 \leftrightarrow b_2$, $k_1 \leftrightarrow k_2$, and $b_3 \leftrightarrow b_4$, $k_3 \leftrightarrow k_4$. After the replacement, the second Hartree term becomes $\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_4)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_3)$, which is identical to the first Hartree term.

For the second Fock term, we swap the indices as follows: $\sigma_1 \leftrightarrow \sigma_2$, $b_1 \leftrightarrow b_2$, $k_1 \leftrightarrow k_2$, and $b_3 \leftrightarrow b_4$, $k_3 \leftrightarrow k_4$. After the replacement, the second Fock term becomes $-\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_2,b_3}(k_3)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_1,b_4}(k_4)$, which is identical to the first Fock term.

Therefore, the simplified Hartree-Fock self-energy Σ^{HF} is:
$\Sigma^{HF} = \frac{1}{NA} \sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(k_1+b_1-k_4-b_4)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}[\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_4)\rangle c^\dagger_{\sigma_2,b_2}(k_2)$
$\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_2,b_3}(k_3)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_1,b_4}(k_4)]$.

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

10 Identify order parameters in Hartree term (extended BZ)

Prompt: You will be instructed to simplify the Hartree term in $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}(\boldsymbol{k})$ by reducing the momentum inside the expected value $\langle c^\dagger_{\sigma_i,b_i}(k_i)c_{\sigma_j,b_j}(k_j)\rangle$. The expected value $\langle c^\dagger_{\sigma_i,b_i}(k_i)c_{\sigma_j,b_j}(k_j)\rangle$ is only nonzero when the two momenta k_i, k_j

are the same, namely, $\langle c^\dagger_{\sigma_i,b_i}(k_i)c_{\sigma_j,b_j}(k_j)\rangle = \langle c^\dagger_{\sigma_i,b_i}(k_i)c_{\sigma_j,b_j}(k_j)\rangle\delta_{k_i,k_j}$.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 $\langle\ldots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.You should recall that $\Sigma^{int,Hartree,2} = \frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(k_1 + b_1 - k_4 - b_4)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_4)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_3)$.Return the final simplified Hartree term $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}(\boldsymbol{k})$.

EXAMPLE:Given a Hamiltonian where the Hartree term $\hat{H}^{Hartree} = \sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_4)\rangle c^\dagger_{b_2}(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, where k_i is the momentum inside first Brilloun zone and b_i is the reciprocal lattice.Inside the expected value, we realize $\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_4)\rangle$ is nonzero only when $k_1 = k_4$, i.e., $\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_4)\rangle = \langle c^\dagger_{b_1}(k_1)c_{b_4}(k_4)\rangle\delta_{k_1,k_4}$.Thus, the Hartree term becomes $\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_4)\rangle\delta_{k_1,k_4}c^\dagger_{b_2}(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.Use the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(k_1-k_1+b_1-b_4)\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_1)\rangle c^\dagger_{b_2}(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_1+b_3+b_4} = \sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_1)\rangle c^\dagger_{b_2}(k_2)c_{b_3}(k_3)\delta_{k_2+b_1+b_2,k_3+b_3+b_4}$.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 $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_1)\rangle c^\dagger_{b_2}(k_2)c_{b_3}(k_3)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_3}$ $\sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_1)\rangle c^\dagger_{b_2}(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Hartree term after reducing two momenta is $\hat{H}^{Hartree} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_1)\rangle c^\dagger_{b_2}(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}$

Completion: Following the example, we can simplify the Hartree term in $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}(\boldsymbol{k})$ as follows:

Starting with $\Sigma^{int,Hartree,2} = \frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(k_1+b_1-k_4-b_4)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_4)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_3)$, we can use the property $\langle c^\dagger_{\sigma_i,b_i}(k_i)c_{\sigma_j,b_j}(k_j)\rangle = \langle c^\dagger_{\sigma_i,b_i}(k_i)c_{\sigma_j,b_j}(k_j)\rangle\delta_{k_i,k_j}$ to reduce one momentum k_1 to k_4.

This gives us $\Sigma^{int,Hartree,2} = \frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3} V(b_1-b_4)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_1+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}($

Next, we use the total momentum conservation to reduce another momentum in the quadratic term. This gives us $\Sigma^{int,Hartree,2} = \frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} V(b_1-b_4)\delta_{b_1+b_2,b_3+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_1)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_2)$.

Therefore, the final simplified Hartree term $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}(\boldsymbol{k})$ after reducing two momenta is $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}(\boldsymbol{k}) = \frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} V(b_1-b_4)\delta_{b_1+b_2,b_3+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_1)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_2$

11 Identify order parameters in Fock term (extended BZ)

Prompt: You will be instructed to simplify the Fock term in $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k})$ by reducing the momentum inside the expected value $\langle c_{\sigma_i,b_i}^\dagger(k_i)c_{\sigma_j,b_j}(k_j)\rangle$.The expected value $\langle c_{\sigma_i,b_i}^\dagger(k_i)c_{\sigma_j,b_j}(k_j)\rangle$ is only nonzero when the two momenta k_i,k_j are the same, namely, $\langle c_{\sigma_i,b_i}^\dagger(k_i)c_{\sigma_j,b_j}(k_j)\rangle = \langle c_{\sigma_i,b_i}^\dagger(k_i)c_{\sigma_j,b_j}(k_j)\rangle\delta_{k_i,k_j}$.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 Fock term, and another momentum in the quadratic term.You should recall that $\Sigma^{int,Fock,2} = -\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(k_1 + b_1 - k_4 - b_4)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4)$.Return the final simplified Fock term $\Sigma_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b'}}^{HF}(\boldsymbol{k})$.

EXAMPLE:Given a Hamiltonian where the Fock term $\hat{H}^{Fock} = -\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, where k_i is the momentum inside first Brilloun zone and b_i is the reciprocal lattice.Inside the expected value, we realize $\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle$ is nonzero only when $k_1 = k_3$, i.e., $\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle = \langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle\delta_{k_1,k_3}$.Thus, the Fock term becomes $-\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle\delta_{k_1,k_3}c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.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 start with the Fock term $\Sigma^{int,Fock,2} = -\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_3,k_4} V(k_1+b_1-k_4-b_4)\delta_{k_1+b_1+k_2+b_2,k_3+b_3+k_4+b_4}\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}($

We first note that $\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle$ is nonzero only when $k_1 = k_3$, i.e., $\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle = \langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_3)\rangle\delta_{k_1,k_3}$.

Substituting this into the Fock term and using the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we get:

$\Sigma^{int,Fock,2} = -\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_4} V(k_1+b_1-k_4-b_4)\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_1)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4)\delta_{k_1+b_1+}$

This simplifies to:

$\Sigma^{int,Fock,2} = -\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2,k_4} V(k_1+b_1-k_4-b_4)\langle c_{\sigma_1,b_1}^\dagger(k_1)c_{\sigma_2,b_3}(k_1)\rangle c_{\sigma_2,b_2}^\dagger(k_2)c_{\sigma_1,b_4}(k_4)\delta_{k_2+b_1+}$

We then note that $\delta_{k_2+b_1+b_2,k_4+b_3+b_4}$ is nonzero only when $k_2 = k_4$, i.e., $\delta_{k_2+b_1+b_2,k_4+b_3+b_4} = \delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4}$.

Substituting this into the Fock term and using the property of Kronecker delta function δ_{k_2,k_4} to sum over k_4, we get:

$\Sigma^{int,Fock,2} = -\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} V(k_1-k_2+b_1-b_4)\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_2,b_3}(k_1)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_1,b_4}(k_2)\delta_{b_1+b_2,b_3+b_4}$

Therefore, the final simplified Fock term $\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}(\boldsymbol{k})$ after reducing two momenta is:

$\Sigma^{HF}_{\alpha,\boldsymbol{b};\beta,\boldsymbol{b}'}(\boldsymbol{k}) = -\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} V(k_1-k_2+b_1-b_4)\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_2,b_3}(k_1)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_1,b_4}(k_2)\delta_{b_1+b_2,b_3+}$

12   Final form of iteration in quadratic terms

Prompt: You will now be instructed to combine the Hartree term $\Sigma^{int,Hartree,2}$ and the Fock term $\Sigma^{int,Fock,2}$. You should recall that the Hartree term $\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} V(b_1 - b_4)\delta_{b_1+b_2,b_3+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_1)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_2)$, and the Fock term $-\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} V(k_1 + b_1 - k_2 - b_4)\delta_{b_1+b_2,b_3+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_2,b_3}(k_1)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_1,b_4}(k_2)$. 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 term and the Fock term, we first write them down:

Hartree term: $\Sigma^{int,Hartree,2} = \frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} V(b_1-b_4)\delta_{b_1+b_2,b_3+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_1)\rangle c^\dagger_{\sigma_2,b_2}(k_2)$

Fock term: $\Sigma^{int,Fock,2} = -\frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} V(k_1+b_1-k_2-b_4)\delta_{b_1+b_2,b_3+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_2,b_3}(k_1)\rangle c^\dagger_{\sigma_2,b_2}$

The instruction states that no relabeling is required in the Fock term. Therefore, we can directly add the Hartree term and the Fock term:

$\Sigma^{int,Hartree+Fock,2} = \Sigma^{int,Hartree,2} + \Sigma^{int,Fock,2}$

This gives us:

$\Sigma^{int,Hartree+Fock,2} = \frac{1}{NA}\sum_{\sigma_1,\sigma_2,b_1,b_2,b_3,b_4,k_1,k_2} \left[V(b_1 - b_4)\delta_{b_1+b_2,b_3+b_4}\langle c^\dagger_{\sigma_1,b_1}(k_1)c_{\sigma_1,b_4}(k_1)\rangle c^\dagger_{\sigma_2,b_2}(k_2)c_{\sigma_2,b_3}(k_1) \right.$

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