1 Identify kinetic term (continuum,first-quantized)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in bilayer graphene in the momentum space in the single-particle form.The degrees of freedom of the system are: four sublattice indices on both layers, $A, B, \tilde{A}, \tilde{B}$.Express the Kinetic Hamiltonian H_0 using $\gamma_0, \gamma_1, \gamma_3, \gamma_4$ and f which are only on the diagonal terms, and arrange the basis in the order of $A, B, \tilde{A}, \tilde{B}$.

Use the following conventions for the symbols:N is the total number of unit cells in the system, φ is the band's Wannier wavefunction, and κ labels the carbon site with position τκ relative to a the triangular lattice vector R_i. The notations A, B, Ā, B̄ are used for the four sublattice indexes κ, where B and Ā are the opposite-layer near-neighbor-pair sites.

Completion: The kinetic term of the Hamiltonian in bilayer graphene in the momentum space in the single-particle form can be written as:

$H_0 = \sum_{\vec{k}} \Psi^\dagger(\vec{k}) H(\vec{k}) \Psi(\vec{k})$

where $\Psi^\dagger(\vec{k}) = (a_{\vec{k}}^\dagger, b_{\vec{k}}^\dagger, \tilde{a}_{\vec{k}}^\dagger, \tilde{b}_{\vec{k}}^\dagger)$ is the creation operator in momentum space, and $H(\vec{k})$ is the Hamiltonian matrix.

The Hamiltonian matrix $H(\vec{k})$ in the basis of $A, B, \tilde{A}, \tilde{B}$ is given by:

$H(\vec{k}) = \begin{pmatrix} 0 & \gamma_0 f(\vec{k}) & \gamma_1 & 0 \\ \gamma_0 f^*(\vec{k}) & 0 & 0 & \gamma_3 \\ \gamma_1 & 0 & 0 & \gamma_0 f(\vec{k}) \\ 0 & \gamma_3 & \gamma_0 f^*(\vec{k}) & 0 \end{pmatrix}$ where$f(\vec{k}) = 1 + e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2}$, and$\vec{a}_1and\vec{a}_2$are the primitive vectors of the triangular lattice. Theγ's are the hopping parameters:$\gamma_0$is the intralayer nearest-neighbor hopping energy,$\gamma_1$is the interlayer nearest-neighbor hopping energy,$\gamma_3$is the interlayer next-nearest-neighbor hopping energy, andγ_4 is the intralayer next-nearest-neighbor hopping energy.

Note that the Hamiltonian matrix is Hermitian, as required by the postulates of quantum mechanics.

2 Define energy dispersion (continuum)

Prompt: You will be instructed to construct each term, namely γ_0, γ_1, γ_3, γ_4 and f.For all energy dispersions, γ_0, γ_1, γ_3, γ_4 and 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

$$H_0 = \begin{pmatrix} 0 & \gamma_0 f & \gamma_4 f & \gamma_3 f^* \\ \gamma_0 f^* & 0 & \gamma_1 & \gamma_4 f \\ \gamma_4 f^* & \gamma_1 & 0 & \gamma_0 f \\ \gamma_3 f & \gamma_4 f^* & \gamma_0 f^* & 0 \end{pmatrix} \tag{1}$$

.Return the expression for γ_0, γ_1, γ_3, γ_4 and f in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian 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):$f(\mathbf{k}) = e^{ik_y a/\sqrt{3}} \left(1 + 2e^{-i3k_y a/2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right)\right)$ Only the intralayer nearest neighbor (γ_0) process and interlayer tunneling (γ_1) process are retained in the minimal tight-binding model. The trigonal warping (γ_3) process which connects the A and $\tilde{B}$ sites is responsible for the leading circular symmetry breaking near the valley points, while the (γ_4) process which connects A and $\tilde{A}$ sites influences the intralayer charge imbalance between sublattices A and B.

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 information provided, we are dealing with a cos dispersion for electrons, which corresponds to EXAMPLE 2.

The terms γ_0, γ_1, γ_3, γ_4 are parameters that characterize different processes in the system. They are not explicitly given, but they are parameters that can be determined experimentally or through fitting to theoretical models.

The function $f(\mathbf{k})$ is given by the expression:

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

The Hamiltonian H_0 in the momentum space can be written as:

$$H_0 = \int d^2k\,\Psi^\dagger(\vec{k})H(\vec{k})\Psi(\vec{k})$$

where $\Psi^\dagger(\vec{k})$ is the creation operator in momentum space, and $H(\vec{k})$ is the Hamiltonian matrix given by:

$$H(\vec{k}) = \begin{pmatrix} 0 & \gamma_0 f & \gamma_4 f & \gamma_3 f^* \\ \gamma_0 f^* & 0 & \gamma_1 & \gamma_4 f \\ \gamma_4 f^* & \gamma_1 & 0 & \gamma_0 f \\ \gamma_3 f & \gamma_4 f^* & \gamma_0 f^* & 0 \end{pmatrix}$$

In this Hamiltonian, the momentum operator $k = -i\partial_r$ is implicitly contained in the function $f(\vec{k})$.

Therefore, the kinetic Hamiltonian with the terms γ_0, γ_1, γ_3, γ_4 and f substituted in is:

$$H_0 = \int d^2k\,\Psi^\dagger(\vec{k})\begin{pmatrix} 0 & \gamma_0 f(\vec{k}) & \gamma_4 f(\vec{k}) & \gamma_3 f^*(\vec{k}) \\ \gamma_0 f^*(\vec{k}) & 0 & \gamma_1 & \gamma_4 f(\vec{k}) \\ \gamma_4 f^*(\vec{k}) & \gamma_1 & 0 & \gamma_0 f(\vec{k}) \\ \gamma_3 f(\vec{k}) & \gamma_4 f^*(\vec{k}) & \gamma_0 f^*(\vec{k}) & 0 \end{pmatrix}\Psi(\vec{k})$$

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 None and Potential Hamiltonian None.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):The model's Bloch basis states are written as $\psi_{\mathbf{k}\kappa}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_i e^{i\mathbf{k}(\mathbf{R}_i + \o_\kappa)}\phi(\mathbf{r} - \mathbf{R}_i - \o_\kappa)$, where N is the total number of unit cells in the system, $\phi(\mathbf{r})$ is the band's Wannier wavefunction, and κ labels the carbon site with position $\o_\kappa$ relative to a the triangular lattice vector $\mathbf{R}_i$. The four band tight-binding model Hamiltonian of a graphene bilayer is represented as H_0. The tight-binding model parameters are represented as γ_i.

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: The Hamiltonian matrix H_0 in the basis of $A, B, \tilde{A}, \tilde{B}$ is given by:

$$H_0 = \begin{pmatrix} 0 & f(\vec{k}) & \gamma_1 & \gamma_4 \\ f^*(\vec{k}) & 0 & \gamma_0 & \gamma_1 \\ \gamma_1 & \gamma_0 & 0 & f(\vec{k}) \\ \gamma_4 & \gamma_1 & f^*(\vec{k}) & 0 \end{pmatrix}$$

We can construct the creation operators $\psi_A^\dagger(\vec{k}), \psi_B^\dagger(\vec{k}), \psi_{\tilde{A}}^\dagger(\vec{k}), \psi_{\tilde{B}}^\dagger(\vec{k})$ and the annihilation operators $\psi_A(\vec{k}), \psi_B(\vec{k}), \psi_{\tilde{A}}(\vec{k}), \psi_{\tilde{B}}(\vec{k})$.

The corresponding second quantized form is $\hat{H}_0 = \sum_{\vec{k}} \vec{\psi}^\dagger(\vec{k}) H_0 \vec{\psi}(\vec{k})$, where $\vec{\psi}(\vec{k}) = \begin{pmatrix} \psi_A(\vec{k}) \\ \psi_B(\vec{k}) \\ \psi_{\tilde{A}}(\vec{k}) \\ \psi_{\tilde{B}}(\vec{k}) \end{pmatrix}$ and $\vec{\psi}^\dagger(\vec{k}) = \begin{pmatrix} \psi_A^\dagger(\vec{k}) & \psi_B^\dagger(\vec{k}) & \psi_{\tilde{A}}^\dagger(\vec{k}) & \psi_{\tilde{B}}^\dagger(\vec{k}) \end{pmatrix}$.

Therefore, the second quantized form of the total noninteracting Hamiltonian $\hat{H}_0$ is:

$$\hat{H}_0 = \sum_{\vec{k}} \begin{pmatrix} \psi_A^\dagger(\vec{k}) & \psi_B^\dagger(\vec{k}) & \psi_{\tilde{A}}^\dagger(\vec{k}) & \psi_{\tilde{B}}^\dagger(\vec{k}) \end{pmatrix} \begin{pmatrix} 0 & f(\vec{k}) & \gamma_1 & \gamma_4 \\ f^*(\vec{k}) & 0 & \gamma_0 & \gamma_1 \\ \gamma_1 & \gamma_0 & 0 & f(\vec{k}) \\ \gamma_4 & \gamma_1 & f^*(\vec{k}) & 0 \end{pmatrix} \begin{pmatrix} \psi_A(\vec{k}) \\ \psi_B(\vec{k}) \\ \psi_{\tilde{A}}(\vec{k}) \\ \psi_{\tilde{B}}(\vec{k}) \end{pmatrix}$$

4 Second-quantization (summation)

Prompt: You will be instructed to expand the second-quantized form Hamiltonian $\hat{H}_0$ using H_{ij} and $\psi_{\mathbf{k}\kappa}$. 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 H_{ij} is zero, you should remove it from the summation. You should recall that $\hat{H}_0$ is $\hat{H}_0 = \sum_k \vec{\psi}_k^\dagger H_k \vec{\psi}_k$, where $\vec{\psi} = \begin{pmatrix} \psi_A \\ \psi_B \\ \psi_{\tilde{A}} \\ \psi_{\tilde{B}} \end{pmatrix}$ and $\vec{\psi}^\dagger = \begin{pmatrix} \psi_A^\dagger & \psi_B^\dagger & \psi_{\tilde{A}}^\dagger & \psi_{\tilde{B}}^\dagger \end{pmatrix}$. 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): H_0 is the four band tight-binding model Hamiltonian of a graphene bilayer, $\psi_{\mathbf{k}\kappa}$ is the model's Bloch basis states, and γ_i are the tight-binding model parameters.

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: The second-quantized form of the Hamiltonian $\hat{H}_0$ can be expanded as follows:

$$\begin{aligned}
\hat{H}_0 = \sum_{\vec{k}} \Big(& \psi_A^\dagger(\vec{k})\psi_A(\vec{k})H_{AA} + \psi_A^\dagger(\vec{k})\psi_B(\vec{k})H_{AB} + \psi_A^\dagger(\vec{k})\psi_{\tilde{A}}(\vec{k})H_{A\tilde{A}} + \psi_A^\dagger(\vec{k})\psi_{\tilde{B}}(\vec{k})H_{A\tilde{B}} + \psi_B^\dagger(\vec{k})\psi_A(\vec{k})H_{BA} \\
& + \psi_B^\dagger(\vec{k})\psi_B(\vec{k})H_{BB} + \psi_B^\dagger(\vec{k})\psi_{\tilde{A}}(\vec{k})H_{B\tilde{A}} + \psi_B^\dagger(\vec{k})\psi_{\tilde{B}}(\vec{k})H_{B\tilde{B}} + \psi_{\tilde{A}}^\dagger(\vec{k})\psi_A(\vec{k})H_{\tilde{A}A} + \psi_{\tilde{A}}^\dagger(\vec{k})\psi_B(\vec{k})H_{\tilde{A}B} \\
& + \psi_{\tilde{A}}^\dagger(\vec{k})\psi_{\tilde{A}}(\vec{k})H_{\tilde{A}\tilde{A}} + \psi_{\tilde{A}}^\dagger(\vec{k})\psi_{\tilde{B}}(\vec{k})H_{\tilde{A}\tilde{B}} + \psi_{\tilde{B}}^\dagger(\vec{k})\psi_A(\vec{k})H_{\tilde{B}A} + \psi_{\tilde{B}}^\dagger(\vec{k})\psi_B(\vec{k})H_{\tilde{B}B} + \psi_{\tilde{B}}^\dagger(\vec{k})\psi_{\tilde{A}}(\vec{k})H_{\tilde{B}\tilde{A}} \\
& + \psi_{\tilde{B}}^\dagger(\vec{k})\psi_{\tilde{B}}(\vec{k})H_{\tilde{B}\tilde{B}} \Big)
\end{aligned} \quad (2)$$

Given that the Hamiltonian matrix is Hermitian, we have $H_{ij} = H_{ji}^*$. Therefore, we can simplify the above expression by combining terms with the same H_{ij}:

$$\begin{aligned}
\hat{H}_0 = \sum_{\vec{k}} \Big(& \psi_A^\dagger(\vec{k})\psi_B(\vec{k})H_{AB} + \psi_B^\dagger(\vec{k})\psi_A(\vec{k})H_{AB}^* + \psi_A^\dagger(\vec{k})\psi_{\tilde{A}}(\vec{k})H_{A\tilde{A}} + \psi_{\tilde{A}}^\dagger(\vec{k})\psi_A(\vec{k})H_{A\tilde{A}}^* + \psi_A^\dagger(\vec{k})\psi_{\tilde{B}}(\vec{k})H_{A\tilde{B}} \\
& + \psi_{\tilde{B}}^\dagger(\vec{k})\psi_A(\vec{k})H_{A\tilde{B}}^* + \psi_B^\dagger(\vec{k})\psi_{\tilde{A}}(\vec{k})H_{B\tilde{A}} + \psi_{\tilde{A}}^\dagger(\vec{k})\psi_B(\vec{k})H_{B\tilde{A}}^* + \psi_B^\dagger(\vec{k})\psi_{\tilde{B}}(\vec{k})H_{B\tilde{B}} + \psi_{\tilde{B}}^\dagger(\vec{k})\psi_B(\vec{k})H_{B\tilde{B}}^* \\
& + \psi_{\tilde{A}}^\dagger(\vec{k})\psi_{\tilde{B}}(\vec{k})H_{\tilde{A}\tilde{B}} + \psi_{\tilde{B}}^\dagger(\vec{k})\psi_{\tilde{A}}(\vec{k})H_{\tilde{A}\tilde{B}}^* \Big)
\end{aligned} \quad (3)$$

The diagonal terms H_{AA}, H_{BB}, $H_{\tilde{A}\tilde{A}}$, and $H_{\tilde{B}\tilde{B}}$ are all zero, so they are removed from the summation.

5 Identify interacting term (momentum space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian $V^{\kappa\kappa'}$ 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 $\lambda, \lambda', \lambda', \lambda$, and $1, 2, 3, 4$ for the 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 electron-electron Coulomb interaction with $V(q) = 2\pi e^2/(|\mathbf{q}|\,\epsilon_r)$ refer to the same layer and $(2\pi e^2/(|\mathbf{q}|\epsilon_r)) \exp\{[-|\mathbf{q}|\,c]\}$ when κ and κ' refer to the opposite layers, where q is the transferred total momentum between a creation operator and an annihilation operator with the same $\lambda, \lambda', \lambda', \lambda$, namely $q = k_1 - k_4$. The fourth part is the normalization factor, you should use $1/A$ here. Finally, the summation should be running over all $\lambda, \lambda', \lambda', \lambda$, and k Return the interaction term $V^{\kappa\kappa'}$ in terms of $c_{k,\lambda}^\dagger$ and $c_{k,\lambda}$ and $V(q)$ (with q expressed in terms of 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): κ, κ' are the indices of operators, q is the

momentum, $V^{\kappa\kappa'}$ is the interaction Hamiltonian, ϵ_r is the relative dielectric constant, $c = 3.35$ is the interlayer separation, A is the total area of the graphene sheet, $r_0 = 3\tilde{a}_0$ is the root mean square radius corresponding to the covalent radius of the carbon atom $a_0 = 0.77$.

Completion: The interaction part of the Hamiltonian $V^{\kappa\kappa'}$ in the momentum space can be constructed as follows:

$V^{\kappa\kappa'} = \frac{1}{2A} \sum_{\lambda,\lambda',k_1,k_2,k_3,k_4} c^\dagger_{k_1,\lambda} c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} c_{k_4,\lambda} \times \delta_{k_1+k_2,k_3+k_4} \times V(q)$

where $q = k_1 - k_4$ is the transferred total momentum between a creation operator and an annihilation operator with the same $\lambda, \lambda', \lambda', \lambda$.

The interaction form $V(q)$ is given by:

$$V(q) = \begin{cases} 2\pi e^2/(|\mathbf{q}|\,\epsilon_r) & \text{if } \kappa \text{ and } \kappa' \text{ are in the same layer} \\ (2\pi e^2/(|\mathbf{q}|\epsilon_r)) \exp\{-|\mathbf{q}|\,c\} & \text{if } \kappa \text{ and } \kappa' \text{ are in opposite layers} \end{cases}$$

Here,$c^\dagger_{k,\lambda}$and$c_{k,\lambda}$are the creation and annihilation operators, respectively, and$A$is the total area of the graphene sheet. The summation runs over all$\lambda, \lambda', \lambda', \lambda$, and k. The delta function$\delta_{k_1+k_2,k_3+k_4}$ensures the conservation of total momentum.

6 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $V^{\kappa\kappa'}$.You should use Wick's theorem to expand the four-fermion term in $V^{\kappa\kappa'}$ 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 $V^{\kappa\kappa'}$ is $V^{\kappa\kappa'} = \frac{1}{2A} \sum_{\lambda,\lambda',k_1,k_2,k_3,k_4} c^\dagger_{k_1,\lambda} c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} c_{k_4,\lambda} \times \delta_{k_1+k_2,k_3+k_4} \times V(q)$ where $q = k_1 - k_4$ is the transferred total momentum between a creation operator and an annihilation operator with the same $\lambda, \lambda', \lambda', \lambda$. .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):λ is a composite label for sublattice κ and spin σ. N_λ is the Hartree term and $W^X_{\mathbf{k}\lambda\lambda'}$ is the Fock (exchange) term. $\mathbf{G}$ is a reciprocal lattice vector.

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, we can expand the four-fermion term in $V^{\kappa\kappa'}$ into quadratic terms. Following the example 1, the expansion of the four-fermion term $c^\dagger_{k_1,\lambda} c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} c_{k_4,\lambda}$ is:

$$\begin{aligned} c^\dagger_{k_1,\lambda} c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} c_{k_4,\lambda} &= \langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda}\rangle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} + \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'}\rangle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} - \langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda}\rangle\langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'}\rangle \\ &\quad - \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'}\rangle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} - \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda}\rangle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} + \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'}\rangle\langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda}\rangle \end{aligned} \tag{4}$$

Substituting this expansion back into the interaction term $V^{\kappa\kappa'}$, we get:

$$\begin{aligned} V^{HF} = \frac{1}{2A} \sum_{\lambda,\lambda',k_1,k_2,k_3,k_4} &\Big[\langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda}\rangle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} + \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'}\rangle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} - \langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda}\rangle\langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'}\rangle \\ &- \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'}\rangle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} - \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda}\rangle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} + \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'}\rangle\langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda}\rangle \Big] \times \delta_{k_1+k_2,k_3+k_4} \times V(q) \end{aligned} \tag{5}$$

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 V^{HF}.The quadratic terms mean terms that are proportional to $c^\dagger_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda}$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in V^{HF}, denoted as $V^{HF}_{quadratic}$.You should

recall that V^{HF} is

$$V^{HF} = \frac{1}{2A} \sum_{\lambda,\lambda',k_1,k_2,k_3,k_4} \left[\langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} \rangle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} + \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} \rangle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} - \langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} \rangle \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} \rangle \right.$$
$$\left. - \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \rangle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} - \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \rangle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} + \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \rangle \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \rangle \right] \times \delta_{k_1+k_2,k_3+k_4} \times V(q). \tag{6}$$

Return $V^{HF}_{quadratic}$.
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):λ is a composite label for sublattice κ and spin σ.N_λ is the expectation value of the number operator.$U_H^{\lambda\lambda'}$ is the Hartree term.$W^X_{\mathbf{k}\lambda\lambda'}$ is the Fock (exchange) term.$U_X^{\kappa\kappa'}$ is the exchange interaction.$\mathbf{G}$ is a reciprocal lattice vector.
Completion: The quadratic terms in the Hartree-Fock approximation V^{HF} are those that are proportional to $c^\dagger_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda}$, excluding terms that are solely expectations or products of expectations. From the given expression for V^{HF}, the quadratic terms are:

$$V^{HF}_{quadratic} = \frac{1}{2A} \sum_{\lambda,\lambda',k_1,k_2,k_3,k_4} \left[\langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} \rangle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} + \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} \rangle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} - \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \rangle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \right.$$
$$\left. - \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \rangle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \right] \times \delta_{k_1+k_2,k_3+k_4} \times V(q) \tag{7}$$

The terms $\langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} \rangle \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} \rangle$ and $\langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \rangle \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \rangle$ are products of expectations and are therefore excluded.

8 Identify momentum transfer in interaction

Prompt: You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $V^{HF}_{quadratic}$. If you find the $V(q)$ in $V^{HF}_{quadratic}$ does not contain any momentum that is not in the summation sign. The interaction term is already expanded. No action to perform on interaction term. Otherwise, you will expand $V(q)$ by replacing q with the momentum $\mathbf{k}$. You should recall that $V^{HF}_{quadratic}$ is

$$V^{HF}_{quadratic} = \frac{1}{2A} \sum_{\lambda,\lambda',k_1,k_2,k_3,k_4} \left[\langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} \rangle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} + \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} \rangle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} - \langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} \rangle \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} \rangle \right.$$
$$\left. - \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \rangle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} - \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \rangle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} + \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \rangle \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \rangle \right] \times \delta_{k_1+k_2,k_3+k_4} \times V(q). \tag{8}$$

Return $V^{HF}_{quadratic}$ with expanded interaction.
Completion: The interaction term $V(q)$ in $V^{HF}_{quadratic}$ does not contain any momentum that is not in the summation sign. Therefore, the interaction term is already expanded and no further action is required. The expanded interaction term remains as $V^{HF}_{quadratic}$.

9 Combine Hartree/Fock terms

Prompt: You will be instructed to simplify the quadratic term $V^{HF}_{quadratic}$ through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.The logic is that the expected value ($\langle c^\dagger_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda} \rangle$) in the first Hartree term ($\langle c^\dagger_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda} \rangle c^\dagger_{\mathbf{k}'\lambda'} c_{\mathbf{k}'\lambda'}$) has the same form as the quadratic operators in the second Hartree term ($\langle c^\dagger_{\mathbf{k}'\lambda'} c_{\mathbf{k}'\lambda'} \rangle c^\dagger_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda}$), 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 $V^{HF}_{quadratic}$ is

$$V^{HF}_{quadratic} = \frac{1}{2A} \sum_{\lambda,\lambda',k_1,k_2,k_3,k_4} \left[\langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} \rangle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} + \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} \rangle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} - \langle c^\dagger_{k_1,\lambda} c_{k_4,\lambda} \rangle \langle c^\dagger_{k_2,\lambda'} c_{k_3,\lambda'} \rangle \right.$$
$$\left. - \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \rangle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} - \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \rangle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} + \langle c^\dagger_{k_1,\lambda} c_{k_3,\lambda'} \rangle \langle c^\dagger_{k_2,\lambda'} c_{k_4,\lambda} \rangle \right] \times \delta_{k_1+k_2,k_3+k_4} \times V(k_1-k_4). \tag{9}$$

Return the simplified $V^{HF}_{quadratic}$ 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

$$\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4)(\langle c^\dagger_{\sigma_1}(k_1)c_{\sigma_4}(k_4)\rangle c^\dagger_{\sigma_2}(k_2)c_{\sigma_3}(k_3) + \langle c^\dagger_{\sigma_2}(k_2)c_{\sigma_3}(k_3)\rangle c^\dagger_{\sigma_1}(k_1)c_{\sigma_4}(k_4))\delta_{k_1+k_2,k_3+k_4},$$

(10)

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 provided, we can simplify the quadratic term $V^{HF}_{quadratic}$ by relabeling the indices.

For the second Hartree term, we swap the indices as follows: $\lambda \leftrightarrow \lambda'$, $k_1 \leftrightarrow k_2$, and $k_3 \leftrightarrow k_4$. This gives us:

$\langle c^\dagger_{k_2,\lambda'}c_{k_3,\lambda'}\rangle c^\dagger_{k_1,\lambda}c_{k_4,\lambda}$

The Kronecker delta function $\delta_{k_1+k_2,k_3+k_4}$ implies $k_1 + k_2 = k_3 + k_4$, i.e., $k_2 - k_3 = k_4 - k_1$. Thus, the second Hartree term simplifies to:

$\langle c^\dagger_{k_2,\lambda'}c_{k_3,\lambda'}\rangle c^\dagger_{k_1,\lambda}c_{k_4,\lambda} \times \delta_{k_1+k_2,k_3+k_4} \times V(k_4 - k_1)$

Because $V(q) = V(-q)$, meaning $V(k_4 - k_1) = V(k_1 - k_4)$, the second Hartree term further simplifies to:

$\langle c^\dagger_{k_2,\lambda'}c_{k_3,\lambda'}\rangle c^\dagger_{k_1,\lambda}c_{k_4,\lambda} \times \delta_{k_1+k_2,k_3+k_4} \times V(k_1 - k_4)$

This form of the second Hartree term after relabeling is identical to the first Hartree term.

Similarly, for the second Fock term, we swap the indices as follows: $\lambda \leftrightarrow \lambda'$, $k_1 \leftrightarrow k_2$, and $k_3 \leftrightarrow k_4$. This gives us:

$\langle c^\dagger_{k_2,\lambda'}c_{k_4,\lambda}\rangle c^\dagger_{k_1,\lambda}c_{k_3,\lambda'} \times \delta_{k_1+k_2,k_3+k_4} \times V(k_4 - k_1)$

Again, because $V(q) = V(-q)$, meaning $V(k_4-k_1) = V(k_1-k_4)$, the second Fock term further simplifies to:

$\langle c^\dagger_{k_2,\lambda'}c_{k_4,\lambda}\rangle c^\dagger_{k_1,\lambda}c_{k_3,\lambda'} \times \delta_{k_1+k_2,k_3+k_4} \times V(k_1 - k_4)$

This form of the second Fock term after relabeling is identical to the first Fock term.

Finally, we have the simplified $V^{HF}_{quadratic}$ as:

$V^{HF}_{quadratic} = \frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2,k_3,k_4}\left[2\langle c^\dagger_{k_1,\lambda}c_{k_4,\lambda}\rangle c^\dagger_{k_2,\lambda'}c_{k_3,\lambda'} - 2\langle c^\dagger_{k_1,\lambda}c_{k_3,\lambda'}\rangle c^\dagger_{k_2,\lambda'}c_{k_4,\lambda}\right] \times \delta_{k_1+k_2,k_3+k_4} \times V(k_1 - k_4)$

This reduces the 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 $V^{Hartree}_{quadratic}$ by reducing the momentum inside the expected value $\left\langle c^\dagger_{\mathbf{k}_1\lambda}c_{\mathbf{k}'\lambda}\right\rangle$. The expected value $\left\langle c^\dagger_{\mathbf{k}_1\lambda}c_{\mathbf{k}'\lambda}\right\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\left\langle c^\dagger_{\mathbf{k}\lambda}c_{\mathbf{k}'\lambda}\right\rangle = \delta_{k,k'}\left\langle c^\dagger_{\mathbf{k}\lambda}c_{\mathbf{k}'\lambda}\right\rangle$. 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 $V^{Hartree}_{quadratic}$ is

$$V^{HF}_{quadratic} = \frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2,k_3,k_4}\langle c^\dagger_{k_1,\lambda}c_{k_4,\lambda}\rangle c^\dagger_{k_2,\lambda'}c_{k_3,\lambda'} \times \delta_{k_1+k_2,k_3+k_4} \times V(k_1 - k_4).$$

(11)

Return the final simplified Hartree term $V^{Hartree}_{quadratic}$.

EXAMPLE: Given a Hamiltonian where the Hartree term

$$\hat{H}^{Hartree} = \sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c^\dagger_{b_1}(k_1)c_{b_4}(k_4)\rangle c^\dagger_{b_2}(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4},$$

(12)

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

$$\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_4)\rangle\delta_{k_1,k_4}c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}. \quad (13)$$

Use the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have

$$\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(k_1 - k_1 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_1+b_3+b_4}$$

$$= \sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{k_2+b_1+b_2,k_3+b_3+b_4}. \quad (14)$$

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

$$\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_3}$$

$$= \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}. \quad (15)$$

Therefore, the final simplified Hartree term after reducing two momenta is

$$\hat{H}^{Hartree} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4} \quad (16)$$

Completion: Following the example provided, we can simplify the Hartree term in $V_{quadratic}^{Hartree}$ by reducing the momentum inside the expected value $\left\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\right\rangle$.

We realize that $\left\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\right\rangle$ is nonzero only when $\mathbf{k}_1 = \mathbf{k}'$, i.e., $\left\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\right\rangle = \left\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\right\rangle\delta_{\mathbf{k}_1,\mathbf{k}'}$.

Thus, the Hartree term becomes $\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2,k_3,k_4}\langle c_{k_1,\lambda}^\dagger c_{k_4,\lambda}\rangle\delta_{k_1,k_4}c_{k_2,\lambda'}^\dagger c_{k_3,\lambda'} \times \delta_{k_1+k_2,k_3+k_4} \times V(k_1 - k_4)$.

Using the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have $\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2,k_3}\langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda}\rangle c_{k_2,\lambda'}^\dagger c_{k_3,\lambda'} \times \delta_{k_1+k_2,k_3+k_1} \times V(0)$.

Because of the total momentum conservation, it is only when $k_2 = k_3$ that $\delta_{k_1+k_2,k_3+k_1}$ is nonzero, i.e., $\delta_{k_1+k_2,k_3+k_1} = \delta_{k_2,k_3}$. Therefore, the Hartree term simplifies to

$$\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2} \langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda}\rangle c_{k_2,\lambda'}^\dagger c_{k_2,\lambda'} \times V(0). \quad (17)$$

Therefore, the final simplified Hartree term after reducing two momenta is

$$V_{quadratic}^{Hartree} = \frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2} \langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda}\rangle c_{k_2,\lambda'}^\dagger c_{k_2,\lambda'} \times V(0). \quad (18)$$

11 Identify order parameters in Fock term (extended BZ)

Prompt: You will be instructed to simplify the Fock term in $V_{quadratic}^{Fock}$ by reducing the momentum inside the expected value $\left\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\right\rangle$.The expected value $\left\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\right\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\left\langle c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}'\lambda}\right\rangle = \delta_{k,k'}\left\langle c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}'\lambda}\right\rangle$.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 Fock term, and another momentum in the quadratic term.You should recall that $V_{quadratic}^{Fock}$ is $V_{quadratic}^{HF} = -\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2,k_3,k_4}\langle c_{k_1,\lambda}^\dagger c_{k_3,\lambda'}\rangle c_{k_2,\lambda'}^\dagger c_{k_4,\lambda} \times \delta_{k_1+k_2,k_3+k_4} \times V(k_1 - k_4)$.Return the final simplified Fock term $V_{quadratic}^{Fock}$.

EXAMPLE:Given a Hamiltonian where the Fock term

$$\hat{H}^{Fock} = -\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}, \quad (19)$$

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

$$-\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_3)\rangle \delta_{k_1,k_3} c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4} \quad (20)$$

Use the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we have

$$-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_1+k_4+b_3+b_4}$$

$$= -\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{k_2+b_1+b_2,k_4+b_3+b_4} . \quad (21)$$

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

$$-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_4)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4}$$

$$= -\sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(k_1 - k_2 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_2)\delta_{b_1+b_2,b_3+b_4} . \quad (22)$$

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

$$\hat{H}^{Fock} = -\sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(k_1 - k_2 + b_1 - b_4)\langle c_{b_1}^\dagger(k_1)c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_4}(k_2)\delta_{b_1+b_2,b_3+b_4} \quad (23)$$

Completion: Following the example provided, we can simplify the Fock term in $V_{quadratic}^{Fock}$ by reducing the momentum inside the expected value $\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\rangle$. We realize that $\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\rangle$ is nonzero only when $\mathbf{k}_1 = \mathbf{k}'$, i.e., $\langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\rangle = \langle c_{\mathbf{k}_1\lambda}^\dagger c_{\mathbf{k}'\lambda}\rangle \delta_{\mathbf{k}_1,\mathbf{k}'}$. Thus, the Fock term becomes $\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2,k_3,k_4}\langle c_{k_1,\lambda}^\dagger c_{k_3,\lambda'}\rangle\delta_{k_1,k_3}c_{k_2,\lambda'}^\dagger c_{k_4,\lambda}\times \delta_{k_1+k_2,k_3+k_4}\times V(k_1 - k_4)$. Using the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we have $\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2,k_4}\langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda'}\rangle c_{k_2,\lambda'}^\dagger c_{k_4,\lambda}\times\delta_{k_1+k_2,k_1+k_4}\times V(k_1 - k_4)$. Because of the total momentum conservation, it is only when $k_2 = k_4$ that $\delta_{k_1+k_2,k_1+k_4}$ is nonzero, i.e., $\delta_{k_1+k_2,k_1+k_4} = \delta_{k_2,k_4}$. Therefore, the Fock term simplifies to $\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2}\langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda'}\rangle c_{k_2,\lambda'}^\dagger c_{k_2,\lambda}\times V(k_1 - k_2)$. Therefore, the final simplified Fock term after reducing two momenta is $V_{quadratic}^{Fock} = -\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2}\langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda'}\rangle c_{k_2,\lambda'}^\dagger c_{k_2,\lambda}\times V(k_1 - k_2)$.

12 Final form of iteration in quadratic terms

Prompt: You will now be instructed to combine the Hartree term $V_{quadratic}^{Hartree}$ and the Fock term $V_{quadratic}^{Fock}$.You should recall that the Hartree term

$$V_{quadratic}^{Hartree} = \frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2}\langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda}\rangle c_{k_2,\lambda'}^\dagger c_{k_2,\lambda'}\times V(0), \quad (24)$$

and the Fock term $V_{quadratic}^{Fock} = -\frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2}\langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda'}\rangle c_{k_2,\lambda'}^\dagger c_{k_2,\lambda}\times V(k_1 - k_2)$.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 $V_{quadratic}^{Hartree}$ and the Fock term $V_{quadratic}^{Fock}$, we first relabel the index in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. However, the question specifies that no swap is needed in this case. Therefore, we can directly add the Hartree and Fock terms:
$V_{quadratic}^{HF} = V_{quadratic}^{Hartree} + V_{quadratic}^{Fock}$
Substituting the expressions for the Hartree and Fock terms, we get:
$V_{quadratic}^{HF} = \frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2}\langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda}\rangle c_{k_2,\lambda'}^\dagger c_{k_2,\lambda'}\times V(0) - \frac{1}{A}\sum_{\lambda,\lambda',k_1,k_2}\langle c_{k_1,\lambda}^\dagger c_{k_1,\lambda'}\rangle c_{k_2,\lambda'}^\dagger c_{k_2,\lambda}\times V(k_1 - k_2)$
This is the final sum of the Hartree and Fock terms.