1 Identify kinetic term (continuum,first-quantized)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in a system with two layers in the real space in the single-particle form.The degrees of freedom of the system are: valley index (+K and -K valley), layer index (top and bottom layer)..Express the Kinetic Hamiltonian H_{\tau} using variables which are only on the diagonal terms, and arrange the basis in the order of (+K,bottom), (+K,top), (-K,bottom), (-K,top).
Use the following conventions for the symbols:$\tau = \pm 1$ represents $\pm K$ valleys, $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$ is at a corner of the moiré Brillouin zone. The 2×2 Hamiltonian hybridizes the bottom layer ($\mathfrak{b}$) and top layer ($\mathfrak{t}$), where the off diagonal terms describe the interlayer tunneling $\Delta_{\mathrm{T},\tau}$, and the diagonal terms describe the momentum-shifted kinetic energy with the effective mass $(m_{\mathfrak{b}}, m_{\mathfrak{t}}) = (0.65, 0.35)m_e$ (m_e is the rest electron mass), plus the intralayer potential $\Delta_{\mathfrak{b}/\mathfrak{t}}$, and a band offset $V_{z\mathfrak{t}}$.
Completion: The kinetic term of the Hamiltonian in a system with two layers in the real space in the single-particle form can be written as:

$$H_\tau = \begin{pmatrix} \frac{(\hbar k - \tau\hbar\boldsymbol{\kappa})^2}{2m_{\mathfrak{b}}} + \Delta_{\mathfrak{b}} & 0 \\ 0 & \frac{(\hbar k - \tau\hbar\boldsymbol{\kappa})^2}{2m_{\mathfrak{t}}} + \Delta_{\mathfrak{t}} + V_{z\mathfrak{t}} \end{pmatrix}$$

where τ represents the valley index (+K and -K valley), $\boldsymbol{\kappa}$ is at a corner of the moiré Brillouin zone, $m_{\mathfrak{b}}$ and $m_{\mathfrak{t}}$ are the effective masses of the bottom and top layers respectively, $\Delta_{\mathfrak{b}}$ and $\Delta_{\mathfrak{t}}$ are the intralayer potentials, and $V_{z\mathfrak{t}}$ is the band offset. The basis is arranged in the order of (+K,bottom), (+K,top), (-K,bottom), (-K,top). The Hamiltonian is diagonal, meaning there is no interlayer tunneling.

2 Define energy dispersion (continuum)

Prompt: You will be instructed to construct each term, namely H_τ.For all energy dispersions, H_τ, it characterizes the parabolic dispersion for holes.In addition, a shift of $+\kappa$ and $-\kappa$ in the momentum $\boldsymbol{k}$ for $E_{t,+K}$ and $E_{t,-K}$, 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 $\boldsymbol{k} = -i\partial_{\boldsymbol{r}}$. You should keep the form of $\boldsymbol{k}$ in the Hamiltonian for short notations but should remember $\boldsymbol{k}$ is an operator.You should recall that $H_{Kinetic}(r) = \begin{pmatrix} E_{+K,b} & 0 & 0 & 0 \\ 0 & E_{+K,t} & 0 & 0 \\ 0 & 0 & E_{-K,b} & 0 \\ 0 & 0 & 0 & E_{-K,t} \end{pmatrix}$.Return the expression for H_τ in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian $\hat{\mathcal{H}}_0$.
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):$\tau = \pm 1$ represents $\pm K$ valleys, $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$ is at a corner of the moir'e Brillouin zone, the 2×2 Hamiltonian hybridizes the bottom layer ($\mathfrak{b}$) and top layer ($\mathfrak{t}$), the off diagonal terms describe the interlayer tunneling $\Delta_{\mathrm{T},\tau}$, and the diagonal terms describe the momentum-shifted kinetic energy with the effective mass $(m_{\mathfrak{b}}, m_{\mathfrak{t}}) = (0.65, 0.35)m_e$ (m_e is the rest electron mass), plus the intralayer potential $\Delta_{\mathfrak{b}/\mathfrak{t}}$, and a band offset $V_{z\mathfrak{t}}$
EXAMPLE 1:A parabolic dispersion for electron is $E_\alpha = \frac{\hbar^2 k^2}{2m_\alpha}$, where α indicates the type of electron. If there is a further shift of q in the momentum k, the dispersion will become $E_\alpha = \frac{\hbar^2 (k-q)^2}{2m_\alpha}$.
EXAMPLE 2: A cos dispersion is $E_\alpha = -\cos(ka/2)$, where α indicates the type of particle. If there is a further shift of q in the momentum k, the dispersion will become $E_\alpha = -\cos((k-q)a/2))$. However, there could be more prefactors before cos depending on the geometry of the lattice.
EXAMPLE 3:A dirac dispersion for electron/hole is a 2 by 2 matrix, i.e., $h_\theta(k) = -\hbar v_D |k| \begin{pmatrix} 0 & e^{i(\theta_k - \theta)} \\ e^{-i(\theta_{\bar{k}} - \theta)} & 0 \end{pmatrix}$, where v_D is the Fermi velocity, θ is the twist angle, and θ_k indicates the azumith angle of k. If there is a further shift of K_θ in the momentum k, the dispersion will become $h_\theta(k) = -\hbar v_D |k - K_\theta| \begin{pmatrix} 0 & e^{i(\theta_{k-K_\theta} - \theta)} \\ e^{-i(\theta_{k-K_\theta} - \theta)} & 0 \end{pmatrix}$.
Completion: Given the problem involves constructing the term H_τ for all energy dispersions, which characterizes the parabolic dispersion for holes, we should follow EXAMPLE 2.
The expression for H_τ is given by:

$$H_\tau = \begin{pmatrix} \frac{(\hbar k - \tau\hbar\boldsymbol{\kappa})^2}{2m_{\mathfrak{b}}} + \Delta_{\mathfrak{b}} & 0 \\ 0 & \frac{(\hbar k - \tau\hbar\boldsymbol{\kappa})^2}{2m_{\mathfrak{t}}} + \Delta_{\mathfrak{t}} + V_{z\mathfrak{t}} \end{pmatrix}$$

Substituting H_τ into the kinetic Hamiltonian $\hat{\mathcal{H}}_0$, we get:

$$\hat{\mathcal{H}}_0 = \begin{pmatrix} \frac{(\hbar k-\hbar\boldsymbol{\kappa})^2}{2m_{\mathfrak{b}}}+\Delta_{\mathfrak{b}} & 0 & 0 & 0 \\ 0 & \frac{(\hbar k-\hbar\boldsymbol{\kappa})^2}{2m_{\mathfrak{t}}}+\Delta_{\mathfrak{t}}+V_{z\mathfrak{t}} & 0 & 0 \\ 0 & 0 & \frac{(\hbar k+\hbar\boldsymbol{\kappa})^2}{2m_{\mathfrak{b}}}+\Delta_{\mathfrak{b}} & 0 \\ 0 & 0 & 0 & \frac{(\hbar k+\hbar\boldsymbol{\kappa})^2}{2m_{\mathfrak{t}}}+\Delta_{\mathfrak{t}}+V_{z\mathfrak{t}} \end{pmatrix}$$

This is the final form of the kinetic Hamiltonian $\hat{\mathcal{H}}_0$ with the term H_τ incorporated.

3 Identify potential term (continuum)

Prompt: You will be instructed to describe the potential term of Hamiltonian H_τ 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 $\Delta_l(r)$.The off-diagonal terms are the coupling between t and b, $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^\dagger(\boldsymbol{r})$, which should be kept hermitian.All others terms are zero. Express the potential Hamiltonian H_τ using $\Delta_l(r)$ and $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^\dagger(\boldsymbol{r})$.
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):$\tau=\pm1$ represents $\pm K$ valleys, $\boldsymbol{\kappa}=\frac{4\pi}{3a_M}(1,0)$ is at a corner of the moir'e Brillouin zone, the effective mass $(m_{\mathfrak{b}},m_{\mathfrak{t}})=(0.65,0.35)m_e$ (m_e is the rest electron mass), and the intralayer potential $\Delta_{\mathfrak{b}/\mathfrak{t}}$, and a band offset $V_{z\mathfrak{t}}$.
Completion: The potential term of the Hamiltonian H_τ in the real space in the single-particle form can be expressed as:

$$H_\tau = \begin{pmatrix} \Delta_{\mathfrak{b}}(\boldsymbol{r}) & \Delta_{\mathrm{T},\tau}(\boldsymbol{r}) \\ \Delta_{\mathrm{T},\tau}^\dagger(\boldsymbol{r}) & \Delta_{\mathfrak{t}}(\boldsymbol{r}) \end{pmatrix}$$

Here, $\Delta_{\mathfrak{b}}(\boldsymbol{r})$ and $\Delta_{\mathfrak{t}}(\boldsymbol{r})$ are the intralayer potentials for the bottom and top layers respectively. $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^\dagger(\boldsymbol{r})$ are the coupling terms between the top and bottom layers, ensuring the Hamiltonian remains Hermitian. All other terms are zero.

4 Define potential term (continuum)

Prompt: You will be instructed to construct each term H_τ, namely, the intralayer potential $\Delta_l(r)$ and interlayer tunneling $\Delta_{T,\tau}(r)$.The expression for diagonal terms are: $\Delta_t(r)=V_{zt}$ and $\Delta_b(r)$ is $2V_b\sum_{j=1,3,5}\cos(g_j\cdot r+\psi_b)$.The expression for off-diagonal terms are: $\Delta_{T,+K}(r)=w(1+\omega^1 e^{ig_2\cdot r}+\omega^2 e^{ig_3\cdot r})$ and $\Delta_{T,-K}(r)=-w(1+\omega^{-1}e^{-ig_2\cdot r}+\omega^{-2}e^{-ig_3\cdot r})$..You should recall that $H_{Potential}(r)=\begin{pmatrix} \Delta_b(r) & \Delta_{T,+K}(r) & 0 & 0 \\ \Delta_{T,+K}^*(r) & \Delta_t(r) & 0 & 0 \\ 0 & 0 & \Delta_b(r) & \Delta_{T,-K}(r) \\ 0 & 0 & \Delta_{T,-K}^*(r) & \Delta_t(r) \end{pmatrix}$.Return the expressions for the intralayer potential $\Delta_l(r)$ and interlayer tunneling $\Delta_{T,\tau}(r)$, and substitute it into the potential Hamiltonian H_τ.
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):$\tau=\pm1$ represents $\pm K$ valleys, $\boldsymbol{\kappa}=\frac{4\pi}{3a_M}(1,0)$ is at a corner of the moiré Brillouin zone, $m_{\mathfrak{b}}$ and $m_{\mathfrak{t}}$ are the effective masses of the bottom and top layer respectively with values $(0.65,0.35)m_e$ where m_e is the rest electron mass, $\Delta_{\mathfrak{b}}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ are the intralayer potential and interlayer tunneling term respectively, $V_{z\mathfrak{t}}$ is a band offset, and $V_{\mathfrak{b}}$ and w are theoretical parameters that can be adjusted to study different phases.
Completion: The expressions for the intralayer potential $\Delta_l(r)$ and interlayer tunneling $\Delta_{T,\tau}(r)$ are given as:
For the intralayer potential:

$$\Delta_t(r)=V_{zt}$$

$$\Delta_b(r)=2V_b\sum_{j=1,3,5}\cos(g_j\cdot r+\psi_b)$$

For the interlayer tunneling:

$$\Delta_{T,+K}(r)=w(1+\omega^1 e^{ig_2\cdot r}+\omega^2 e^{ig_3\cdot r})$$

$$\Delta_{T,-K}(r)=-w(1+\omega^{-1}e^{-ig_2\cdot r}+\omega^{-2}e^{-ig_3\cdot r})$$

Substituting these expressions into the potential Hamiltonian H_τ, we get:

H_τ
$$= \begin{pmatrix} 2V_b\sum_{j=1,3,5}\cos(g_j\cdot r+\psi_b) & w(1+\omega^1 e^{ig_2\cdot r}+\omega^2 e^{ig_3\cdot r}) & 0 & 0 \\ w(1+\omega^1 e^{ig_2\cdot r}+\omega^2 e^{ig_3\cdot r})^* & V_{zt} & 0 & 0 \\ 0 & 0 & 2V_b\sum_{j=1,3,5}\cos(g_j\cdot r+\psi_b) & -w(1+\omega^{-1}e^{-ig_2\cdot r}+\omega^{-2}e^{-ig_3\cdot r}) \\ 0 & 0 & -w(1+\omega^{-1}e^{-ig_2\cdot r}+\omega^{-2}e^{-ig_3\cdot r})^* & V_{zt} \end{pmatrix}$$

This is the final form of the potential Hamiltonian H_τ with the terms $\Delta_l(r)$ and $\Delta_{T,\tau}(r)$ incorporated.

5 Second-quantization (matrix)

Prompt: You will be instructed to construct the second quantized form of the total noninteracting Hamiltonian in the real space.The noninteracting Hamiltonian in the real space $\hat{\mathcal{H}}_0$ is the sum of Kinetic Hamiltonian $-\frac{\hbar^2\boldsymbol{k}^2}{2m_\mathfrak{b}}$ and $-\frac{\hbar^2(\boldsymbol{k}-\tau\boldsymbol{\kappa})^2}{2m_\mathfrak{t}}$ and Potential Hamiltonian $\Delta_{\mathfrak{b},\tau}(\boldsymbol{r})$, $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$, $\Delta_{\mathrm{T},\tau}^\dagger(\boldsymbol{r})$, $\Delta_{\mathfrak{t},}(\boldsymbol{r})$, and V_{zt}.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 real space position r.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):$\tau=\pm$ represents $\pm K$ valleys, $\hbar\boldsymbol{k}=-i\hbar\partial_{\boldsymbol{r}}$ is the momentum operator, $\boldsymbol{\kappa}=\frac{4\pi}{3a_M}(1,0)$ is at a corner of the moir'e Brillouin zone, and a_M is the moir'e lattice constant. Note that the spin index of the fermion operators Ψ_τ is both layer and valley dependent.
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 noninteracting Hamiltonian in the real space $\hat{\mathcal{H}}_0$ is given by the sum of the kinetic and potential Hamiltonians. The kinetic Hamiltonian is given by $-\frac{\hbar^2\boldsymbol{k}^2}{2m_\mathfrak{b}}$ and $-\frac{\hbar^2(\boldsymbol{k}-\tau\boldsymbol{\kappa})^2}{2m_\mathfrak{t}}$, and the potential Hamiltonian is given by $\Delta_{\mathfrak{b},\tau}(\boldsymbol{r})$, $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$, $\Delta_{\mathrm{T},\tau}^\dagger(\boldsymbol{r})$, $\Delta_{\mathfrak{t},}(\boldsymbol{r})$, and V_{zt}.
The second quantized form of the total noninteracting Hamiltonian $\hat{H}^0$ can be constructed by introducing the creation and annihilation operators for the fermions in the system. The creation operators are denoted by $\Psi_\tau^\dagger(\boldsymbol{r})$ and the annihilation operators by $\Psi_\tau(\boldsymbol{r})$. The spin index of the fermion operators Ψ_τ is both layer and valley dependent.
The second quantized form of the total noninteracting Hamiltonian $\hat{H}^0$ is then given by:

$$\hat{H}^0=\int d\boldsymbol{r}\,\Psi_\tau^\dagger(\boldsymbol{r})\hat{\mathcal{H}}_0\Psi_\tau(\boldsymbol{r})$$

where $\hat{\mathcal{H}}_0$ is the noninteracting Hamiltonian in the real space, and the integral is taken over the real space position $\boldsymbol{r}$. The operator $\Psi_\tau^\dagger(\boldsymbol{r})$ creates a fermion at position $\boldsymbol{r}$ with spin index τ, and the operator $\Psi_\tau(\boldsymbol{r})$ annihilates a fermion at position $\boldsymbol{r}$ with spin index τ. The product $\Psi_\tau^\dagger(\boldsymbol{r})\hat{\mathcal{H}}_0\Psi_\tau(\boldsymbol{r})$ represents the energy of a fermion at position $\boldsymbol{r}$ with spin index τ in the noninteracting Hamiltonian $\hat{\mathcal{H}}_0$. The integral over $\boldsymbol{r}$ sums up the energies of all fermions in the system.

6 Second-quantization (summation)

Prompt: You will be instructed to expand the second-quantized form Hamiltonian $\hat{\mathcal{H}}_0$ using H_τ and Ψ_τ. 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_τ is zero, you should remove it from the summation. You should recall that $\hat{H}^0=\int dr\vec{\psi}^\dagger(r)H^0(r)\vec{\psi}(r)$.Return the expanded form of $\hat{\mathcal{H}}_0$ 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):$\hat{\mathcal{H}}_0$ is the second-quantized form Hamiltonian, H_τ is the matrix element, and Ψ_τ is the basis. $\tau=\pm$ represents $\pm K$ valleys, $\hbar\boldsymbol{k}=-i\hbar\partial_{\boldsymbol{r}}$ is the momentum operator, $\boldsymbol{\kappa}=\frac{4\pi}{3a_M}(1,0)$ is at a corner of the moir'e Brillouin zone, and a_M is the moir'e lattice constant. The spin index of the fermion operators Ψ_τ is both layer and valley dependent.
EXAMPLE:For a $\hat{H}=\vec{\psi}^\dagger H\vec{\psi}$, where $\vec{\psi}=\begin{pmatrix}\psi_a \\ \psi_b\end{pmatrix}$ and $\vec{\psi}^\dagger=\begin{pmatrix}\psi_a^\dagger & \psi_b^\dagger\end{pmatrix}$, we can expand it as $\hat{H}=\sum_{i,j=\{a,b\}}\psi_i^\dagger H_{i,j}\psi_j$.

Completion: Given the Hamiltonian $\hat{\mathcal{H}}_0 = \int d\boldsymbol{r}\, \Psi_\tau^\dagger(\boldsymbol{r}) H_\tau \Psi_\tau(\boldsymbol{r})$, where $\Psi_\tau = \begin{pmatrix} \Psi_{\tau,\mathfrak{b}} \\ \Psi_{\tau,\mathfrak{t}} \end{pmatrix}$ and $\Psi_\tau^\dagger = \begin{pmatrix} \Psi_{\tau,\mathfrak{b}}^\dagger & \Psi_{\tau,\mathfrak{t}}^\dagger \end{pmatrix}$, we can expand it as:

$$\hat{\mathcal{H}}_0 = \int d\boldsymbol{r} \sum_{i,j=\{\mathfrak{b},\mathfrak{t}\}} \Psi_{\tau,i}^\dagger(\boldsymbol{r}) H_{\tau,ij} \Psi_{\tau,j}(\boldsymbol{r})$$

where $H_{\tau,ij}$ are the matrix elements of H_τ, and $\Psi_{\tau,i}$ and $\Psi_{\tau,j}$ are the fermion operators for the bottom and top layers respectively. The integral is taken over the real space position $\boldsymbol{r}$, and the sum is taken over the layer indices i and j. The operator $\Psi_{\tau,i}^\dagger(\boldsymbol{r})$ creates a fermion at position $\boldsymbol{r}$ in layer i with spin index τ, and the operator $\Psi_{\tau,j}(\boldsymbol{r})$ annihilates a fermion at position $\boldsymbol{r}$ in layer j with spin index τ. The product $\Psi_{\tau,i}^\dagger(\boldsymbol{r}) H_{\tau,ij} \Psi_{\tau,j}(\boldsymbol{r})$ represents the energy of a fermion moving from layer j to layer i at position $\boldsymbol{r}$ with spin index τ in the Hamiltonian H_τ. The integral over $\boldsymbol{r}$ sums up the energies of all such processes in the system.

7 Fourier transform noninteracting term to momentum space (continuum)

Prompt: You will be instructed to convert the total noninteracting Hamiltonian in the second quantized form from the basis in real space to the basis by momentum space.To do that, you should apply the Fourier transformation to $\Psi_\tau^\dagger(\boldsymbol{r})$ in the real space to the $c_{\boldsymbol{k}_\alpha,l_\alpha,\tau}^\dagger$ in the momentum space, which is defined as $c_{\tau,l}^\dagger(k) = \frac{1}{\sqrt{V}} \int dr \psi_{\tau,l}^\dagger(r) e^{ik\cdot r}$, where $\boldsymbol{r}$ is integrated over the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation.Express the total noninteracting Hamiltonian $\hat{\mathcal{H}}_0$ in terms of $c_{\boldsymbol{k}_\alpha,l_\alpha,\tau}^\dagger$. Simplify any summation index if possible.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):$\tau = \pm$ represents $\pm K$ valleys, $\hbar\boldsymbol{k} = -i\hbar\partial_{\boldsymbol{r}}$ is the momentum operator, $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$ is at a corner of the moir'e Brillouin zone, and a_M is the moir'e lattice constant. The spin index of the fermion operators Ψ_τ is both layer and valley dependent. $h^{(\tau)}$ is the Hamiltonian H_τ expanded in the plane-wave basis, and the momentum $\boldsymbol{k}$ is defined in the extended Brillouin zone that spans the full momentum space, i.e., $\boldsymbol{k} \in \mathbb{R}^2$. The subscripts α, β are index for momenta. Due to Bloch's theorem, $h_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta}^{(\tau)}$ is nonzero only when $\boldsymbol{k}_\alpha - \boldsymbol{k}_\beta$ is equal to the linear combination of any multiples of one of the moir'e reciprocal lattice vectors (including the zero vector).
EXAMPLE:Write a Hamiltonian $\hat{H}$ in the second quantized form, $\hat{H} = \int dr \psi(r)^\dagger H(r) \psi(r)$, where r is integrated over the entire real space.Define the Fourier transformation $c^\dagger(k) = \frac{1}{\sqrt{V}} \int \psi^\dagger(r) e^{ik\cdot r} dr$, where r is integrated over the entire real space, and V is the area of the unit cell in the real space.This leads to the inverse Fourier transformation $\psi^\dagger(r) = \frac{1}{\sqrt{V}} \sum_k c^\dagger(k) e^{-ik\cdot r}$, where k is summed over the extended Brillouin zone (i.e., the entire momentum space), Ω is the area of Brillouin zone in the momentum space.Thus, substitute $\psi^\dagger(r)$ and $\psi(r)$ into $\hat{H}$, we get

$$\begin{aligned}
\hat{H} &= \int dr \frac{1}{\sqrt{V}} \sum_{k_1} c^\dagger(k_1) e^{-ik_1\cdot r} H(r) \frac{1}{\sqrt{V}} \sum_{k_2} c(k_2) e^{ik_2\cdot r} \\
&= \sum_{k_1,k_2} c^\dagger(k_1) \frac{1}{V} \int dr e^{-i(k_1-k_2)\cdot r} H(r) c(k_2) \\
&= \sum_{k_1,k_2} c^\dagger(k_1) H(k_1,k_2) c(k_2)
\end{aligned}$$

, where we define the Fourier transformation of $H(r)$ as $H(k_1,k_2) = \frac{1}{V} \int dr e^{-i(k_1-k_2)\cdot r} H(r)$.
Completion: To convert the total noninteracting Hamiltonian in the second quantized form from the basis in real space to the basis in momentum space, we apply the Fourier transformation to $\Psi_\tau^\dagger(\boldsymbol{r})$ and $\Psi_\tau(\boldsymbol{r})$.
The Fourier transformations are defined as:

$$c_{\boldsymbol{k}_\alpha,l_\alpha,\tau}^\dagger = \frac{1}{\sqrt{V}} \int d\boldsymbol{r}\, \Psi_{\tau,l_\alpha}^\dagger(\boldsymbol{r}) e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}}$$

and its inverse:

$$\Psi_{\tau,l_\alpha}^\dagger(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}_\alpha} c_{\boldsymbol{k}_\alpha,l_\alpha,\tau}^\dagger e^{-i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}}$$

Substituting these into the total noninteracting Hamiltonian $\hat{H}^0$, we get:

$$\hat{H}^0 = \int d\boldsymbol{r} \frac{1}{V} \sum_{\boldsymbol{k}_\alpha,l_\alpha} c_{\boldsymbol{k}_\alpha,l_\alpha,\tau}^\dagger e^{-i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}} \hat{\mathcal{H}}_0 \frac{1}{V} \sum_{\boldsymbol{k}_\beta,l_\beta} c_{\boldsymbol{k}_\beta,l_\beta,\tau} e^{i\boldsymbol{k}_\beta\cdot\boldsymbol{r}}$$

This simplifies to:

$$\hat{H}^0 = \sum_{\boldsymbol{k}_\alpha,l_\alpha,\boldsymbol{k}_\beta,l_\beta} c^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau} \frac{1}{V} \int d\boldsymbol{r}\, e^{-i(\boldsymbol{k}_\alpha-\boldsymbol{k}_\beta)\cdot\boldsymbol{r}} \hat{\mathcal{H}}_0 c_{\boldsymbol{k}_\beta,l_\beta,\tau}$$

We define the Fourier transformation of $\hat{\mathcal{H}}_0$ as:

$$h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} = \frac{1}{V} \int d\boldsymbol{r}\, e^{-i(\boldsymbol{k}_\alpha-\boldsymbol{k}_\beta)\cdot\boldsymbol{r}} \hat{\mathcal{H}}_0$$

Substituting this into the expression for $\hat{H}^0$, we get:

$$\hat{H}^0 = \sum_{\boldsymbol{k}_\alpha,l_\alpha,\boldsymbol{k}_\beta,l_\beta} c^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau} h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} c_{\boldsymbol{k}_\beta,l_\beta,\tau}$$

This is the total noninteracting Hamiltonian $\hat{H}^0$ in the momentum space. The summation indices $\boldsymbol{k}_\alpha, l_\alpha, \boldsymbol{k}_\beta, l_\beta$ run over all momenta in the extended Brillouin zone and all layer indices.

8 Particle-hole transformation

Prompt: You will be instructed to perform a particle-hole transformation.Define a hole operator, $b_{\boldsymbol{k},l,\tau}$, which equals $c^\dagger_{\boldsymbol{k},l,\tau}$.You should replace $c^\dagger_{\boldsymbol{k},l,\tau}$ with $b_{\boldsymbol{k},l,\tau}$, and $c_{\boldsymbol{k},l,\tau}$ with $b^\dagger_{\boldsymbol{k},l,\tau}$. You should follow the EXAMPLE below to apply the particle-hole transformation.You should recall that $\hat{H}^0 = \sum_{\tau,l_1,l_2,k_1,k_2} c^\dagger_{\tau,l_1}(k_1) H^0_{\tau,l_1,\tau,l_2}(k_1,k_2) c_{\tau,l_2}(k_2)$.
Return the $\hat{\mathcal{H}}_0$ in the hole operators.
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 hole operator is defined as $b_{\boldsymbol{k},l,\tau} = c^\dagger_{\boldsymbol{k},l,\tau}$. The Hamiltonian in the hole basis is represented as $\hat{\mathcal{H}}_0$.
EXAMPLE:Give a Hamiltonian $\hat{H} = \sum_{k_1,k_2} c^\dagger(k_1) h(k_1,k_2) c(k_2)$, and the particle-hole transformation as $b(k) = c^\dagger(k)$. The transformed Hamiltonian is $\hat{H} = \sum_{k_1,k_2} b(k_1) h(k_1,k_2) b^\dagger(k_2)$
Completion: The particle-hole transformation is defined as $b_{\boldsymbol{k},l,\tau} = c^\dagger_{\boldsymbol{k},l,\tau}$. We can apply this transformation to the Hamiltonian $\hat{H}^0$ by replacing $c^\dagger_{\boldsymbol{k},l,\tau}$ with $b_{\boldsymbol{k},l,\tau}$, and $c_{\boldsymbol{k},l,\tau}$ with $b^\dagger_{\boldsymbol{k},l,\tau}$.
Therefore, the transformed Hamiltonian $\hat{\mathcal{H}}_0$ in the hole operators is given by:

$$\hat{\mathcal{H}}_0 = \sum_{\tau,l_1,l_2,k_1,k_2} b_{\tau,l_1}(k_1) H^0_{\tau,l_1,\tau,l_2}(k_1,k_2) b^\dagger_{\tau,l_2}(k_2)$$

This is the final form of the Hamiltonian $\hat{\mathcal{H}}_0$ in the hole basis.

9 Simplify the Hamiltonian in the particle-hole basis

Prompt: You will be instructed to simplify the $\hat{\mathcal{H}}_0$ in the hole basis.You should use canonical commutator relation for fermions to reorder the hole operator to the normal order. Normal order means that creation operators always appear before the annihilation operators. You should follow the EXAMPLE below to simplify it to the normal order.Express the $\hat{\mathcal{H}}_0$ in the normal order of $b_{\boldsymbol{k},l,\tau}$ and also make $\boldsymbol{k}_\alpha$ always appear before $\boldsymbol{k}_\beta$ in the index of $b_{\boldsymbol{k},l,\tau}$ and $[h^{(\tau)}]^\intercal_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta}$.You should recall that $\hat{H}^0 = \sum_{\tau,l_1,l_2,k_1,k_2} b_{\tau,l_1}(k_1) H^0_{\tau,l_1,\tau,l_2}(k_1,k_2) b^\dagger_{\tau,l_2}(k_2)$ 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):$b_{\boldsymbol{k},l,\tau} = c^\dagger_{\boldsymbol{k},l,\tau}$
EXAMPLE:For $\hat{H}^0 = \sum_{i,j} b_i H_{i,j} b^\dagger_j$, where b_i satisfies fermion statistics (anticommuting to its self-adjoint operator).This gives '$[b_i, b^\dagger_j]_+ = \delta_{i,j}$', which means $b_i b^\dagger_j = \delta_{i,j} - b^\dagger_j b_i$.Substitute it into $\hat{H}^0$, we have $\hat{H}^0 = \sum_{i,j} (\delta_{i,j} - b^\dagger_j b_i) H_{i,j} = \sum_{i,j} \delta_{i,j} H_{i,j} - \sum_{i,j} b^\dagger_j b_i H_{i,j} = \sum_i H_{i,i} - \sum_{i,j} b^\dagger_j b_i H_{i,j}$.The first term is simply $\sum_i H_{i,i}$ by summing over the index j due to $\delta_{i,j}$. The second term is $-\sum_{i,j} b^\dagger_j b_i H_{i,j}$.Relabeling the index of i and j by swapping them to make it consistent with the original order of index (namely, i appears before j in the index of b and H), it becomes $-\sum_{i,j} b^\dagger_i H_{j,i} b_j$. Finally, to fix the order of the index in H such that i appears before j, we notice that '$H_{j,i} = (H_{i,j})^*$', where '*' means complex conjugate, because the Hamiltonian is Hermitian.Thus, we end up in $\hat{H}^0 = \sum_{i,j} b_i H_{i,j} b^\dagger_j = \sum_i H_{i,i} - \sum_{i,j} b^\dagger_i (H_{i,j})^* b_j$
Completion: The Hamiltonian $\hat{\mathcal{H}}_0$ in the hole basis is given by:

$$\hat{\mathcal{H}}_0 = \sum_{\tau,l_1,l_2,k_1,k_2} b_{\tau,l_1}(k_1) H^0_{\tau,l_1,\tau,l_2}(k_1,k_2) b^\dagger_{\tau,l_2}(k_2)$$

We can use the canonical commutation relation for fermions, $[b_{\tau,l_1}(k_1), b^\dagger_{\tau,l_2}(k_2)]_+ = \delta_{k_1,k_2}\delta_{l_1,l_2}$, to reorder the hole operators to the normal order. This gives us:

$$b_{\tau,l_1}(k_1) b^\dagger_{\tau,l_2}(k_2) = \delta_{k_1,k_2}\delta_{l_1,l_2} - b^\dagger_{\tau,l_2}(k_2) b_{\tau,l_1}(k_1)$$

Substituting this into $\hat{\mathcal{H}}_0$, we get:

$$\hat{\mathcal{H}}_0 = \sum_{\tau,l_1,l_2,k_1,k_2} (\delta_{k_1,k_2}\delta_{l_1,l_2} - b^\dagger_{\tau,l_2}(k_2) b_{\tau,l_1}(k_1)) H^0_{\tau,l_1,\tau,l_2}(k_1,k_2)$$

This simplifies to:

$$\hat{\mathcal{H}}_0 = \sum_{\tau,l,k} H^0_{\tau,l,\tau,l}(k,k) - \sum_{\tau,l_1,l_2,k_1,k_2} b^\dagger_{\tau,l_2}(k_2) H^0_{\tau,l_1,\tau,l_2}(k_1,k_2) b_{\tau,l_1}(k_1)$$

Relabeling the indices to make k_1 appear before k_2 and l_1 appear before l_2 in the indices of b and H^0, we get:

$$\hat{\mathcal{H}}_0 = \sum_{\tau,l,k} H^0_{\tau,l,\tau,l}(k,k) - \sum_{\tau,l_1,l_2,k_1,k_2} b^\dagger_{\tau,l_1}(k_1) H^0_{\tau,l_2,\tau,l_1}(k_2,k_1) b_{\tau,l_2}(k_2)$$

Finally, using the fact that $H^0_{\tau,l_2,\tau,l_1}(k_2,k_1) = [H^0_{\tau,l_1,\tau,l_2}(k_1,k_2)]^*$ because the Hamiltonian is Hermitian, we get:

$$\hat{\mathcal{H}}_0 = \sum_{\tau,l,k} H^0_{\tau,l,\tau,l}(k,k) - \sum_{\tau,l_1,l_2,k_1,k_2} b^\dagger_{\tau,l_1}(k_1) [H^0_{\tau,l_1,\tau,l_2}(k_1,k_2)]^* b_{\tau,l_2}(k_2)$$

This is the final form of the Hamiltonian $\hat{\mathcal{H}}_0$ in the normal order of $b_{\boldsymbol{k},l,\tau}$ and with $\boldsymbol{k}_\alpha$ always appearing before $\boldsymbol{k}_\beta$ in the index of $b_{\boldsymbol{k},l,\tau}$ and $[H^0_{\tau,l_1,\tau,l_2}(k_1,k_2)]^*$.

10 Identify interacting term (momentum space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian $\hat{\mathcal{H}}_{\text{int}}$ 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 the valley index and layer 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.The third part is the interaction form. You should use dual-gate screened Coulomb with $V(q) = 2\pi e^2 \tanh(|\boldsymbol{k}|d)/(\epsilon|\boldsymbol{k}|)$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same the valley index and layer index, namely $q = k_1 - k_4$.The fourth part is the normalization factor, you should use $\frac{1}{2A}$ here. Finally, the summation should be running over all the valley index and layer index, and momentum Return the interaction term $\hat{\mathcal{H}}_{\text{int}}$ in terms of $b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}$, $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}$, $b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$, $b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$ 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):$\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta$ are the momenta, l_α, l_β are the indices of operators, τ_α, τ_β are the spin indices, $V(\boldsymbol{k})$ is the dual-gate screened Coulomb interaction, d is the sample-to-gate distance, and ϵ is the dielectric constant.
Completion: The interaction part of the Hamiltonian $\hat{\mathcal{H}}_{\text{int}}$ in the momentum space can be constructed as follows:

$$\hat{\mathcal{H}}_{\text{int}} = \frac{1}{2A} \sum_{\tau_\alpha,\tau_\beta} \sum_{l_\alpha,l_\beta} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta} b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$$

Here, $V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) = 2\pi e^2 \tanh(|\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta|d)/(\epsilon|\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta|)$ is the dual-gate screened Coulomb interaction, $\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$ is the Kronecker delta function ensuring total momentum conservation, and A is the normalization factor. The summations run over all valley indices τ_α, τ_β, layer indices l_α, l_β, and momenta $\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta$. The operators $b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}$, $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}$, $b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$, and $b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$ are the creation and annihilation operators for holes.

11 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$.You should use Wick's theorem to expand the four-fermion term in $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$ 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 $\hat{H}^{int} = \frac{1}{2V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4} b^\dagger_{l_1,\tau_1}(k_1)b^\dagger_{l_2,\tau_2}(k_2)b_{l_2,\tau_2}(k_3)b_{l_1,\tau_1}(k_4)V(|k_1-k_4|)\delta_{k_1+k_2,k_3+k_4}$.Return the expanded interaction term after Hartree-Fock approximation as $\hat{\mathcal{H}}^{\text{HF}}$.
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):$\hat{\mathcal{H}}^{\text{HF}}$ is the Hartree-Fock Hamiltonian, $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$ is the interaction term in the Hartree-Fock Hamiltonian, $\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta$ are the momentum vectors, l_α, l_β are the orbital quantum numbers, τ_α, τ_β are the spin quantum numbers, $V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta)$ is the interaction potential, $b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}$ and $b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$ are the creation and annihilation operators, and $\langle ... \rangle$ denotes the expectation value.
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: The interaction term $\hat{\mathcal{H}}\text{int}^{\text{HF}}$ can be expanded using Wick's theorem as follows:

$$\begin{aligned}
\hat{\mathcal{H}}\text{int}^{\text{HF}} &= \frac{1}{2V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4} b^\dagger_{l_1,\tau_1}(k_1)b^\dagger_{l_2,\tau_2}(k_2)b_{l_2,\tau_2}(k_3)b_{l_1,\tau_1}(k_4)V(|k_1-k_4|)\delta_{k_1+k_2,k_3+k_4} \\
&= \frac{1}{2V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4} \Big[\langle b^\dagger_{l_1,\tau_1}(k_1)b_{l_1,\tau_1}(k_4)\rangle b^\dagger_{l_2,\tau_2}(k_2)b_{l_2,\tau_2}(k_3) \\
&+ \langle b^\dagger_{l_2,\tau_2}(k_2)b_{l_2,\tau_2}(k_3)\rangle b^\dagger_{l_1,\tau_1}(k_1)b_{l_1,\tau_1}(k_4) \\
&- \langle b^\dagger_{l_1,\tau_1}(k_1)b_{l_1,\tau_1}(k_4)\rangle\langle b^\dagger_{l_2,\tau_2}(k_2)b_{l_2,\tau_2}(k_3)\rangle \\
&- \langle b^\dagger_{l_1,\tau_1}(k_1)b_{l_2,\tau_2}(k_3)\rangle b^\dagger_{l_2,\tau_2}(k_2)b_{l_1,\tau_1}(k_4) \\
&- \langle b^\dagger_{l_2,\tau_2}(k_2)b_{l_1,\tau_1}(k_4)\rangle b^\dagger_{l_1,\tau_1}(k_1)b_{l_2,\tau_2}(k_3) + \langle b^\dagger_{l_1,\tau_1}(k_1)b_{l_2,\tau_2}(k_3)\rangle\langle b^\dagger_{l_2,\tau_2}(k_2)b_{l_1,\tau_1}(k_4)\rangle\Big] V(|k_1-k_4|)\delta_{k_1+k_2,k_3+k_4}
\end{aligned}$$

The Hartree-Fock Hamiltonian is then given by the sum of the non-interacting Hamiltonian $\hat{\mathcal{H}}0$ and the expanded interaction term $\hat{\mathcal{H}}\text{int}^{\text{HF}}$:

$$\hat{\mathcal{H}}^{\text{HF}} = \hat{\mathcal{H}}0 + \hat{\mathcal{H}}\text{int}^{\text{HF}}$$

12 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the Hartree-Fock term symbol, denoted as $\hat{\mathcal{H}}^{\text{HF}}$.The quadratic terms mean terms that are proportional to $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$ and $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in Hartree-Fock term symbol, denoted as $\hat{\mathcal{H}}^{\text{HF}}$, denoted as $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$.You should recall that

$$\begin{aligned}
\hat{H}^{int,HF} = \frac{1}{2V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4} &\Big[\langle b^\dagger_{l_1,\tau_1}(k_1)b_{l_1,\tau_1}(k_4)\rangle b^\dagger_{l_2,\tau_2}(k_2)b_{l_2,\tau_2}(k_3) + \langle b^\dagger_{l_2,\tau_2}(k_2)b_{l_2,\tau_2}(k_3)\rangle b^\dagger_{l_1,\tau_1}(k_1)b_{l_1,\tau_1}(k_4) \\
&- \langle b^\dagger_{l_1,\tau_1}(k_1)b_{l_1,\tau_1}(k_4)\rangle\langle b^\dagger_{l_2,\tau_2}(k_2)b_{l_2,\tau_2}(k_3)\rangle - \langle b^\dagger_{l_1,\tau_1}(k_1)b_{l_2,\tau_2}(k_3)\rangle b^\dagger_{l_2,\tau_2}(k_2)b_{l_1,\tau_1}(k_4) \\
&- \langle b^\dagger_{l_2,\tau_2}(k_2)b_{l_1,\tau_1}(k_4)\rangle b^\dagger_{l_1,\tau_1}(k_1)b_{l_2,\tau_2}(k_3) + \langle b^\dagger_{l_1,\tau_1}(k_1)b_{l_2,\tau_2}(k_3)\rangle\langle b^\dagger_{l_2,\tau_2}(k_2)b_{l_1,\tau_1}(k_4)\rangle\Big] V(|k_1-k_4|)\delta_{k_1+k_2,k_3+k_4}.
\end{aligned}$$

Return $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$.
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):$\hat{\mathcal{H}}^{\text{HF}}$ is the Hartree-Fock term symbol, $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$ is the Hartree-Fock second quantized symbol, and $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$ and $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$ are the bilinear operators.
Completion: The quadratic terms in the Hartree-Fock term symbol $\hat{\mathcal{H}}^{\text{HF}}$ are given by:

$$\hat{\mathcal{H}}_{\text{int}}^{\text{HF}} = \frac{1}{2V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4} \Big[\langle b_{l_1,\tau_1}^\dagger(k_1) b_{l_1,\tau_1}(k_4) \rangle b_{l_2,\tau_2}^\dagger(k_2) b_{l_2,\tau_2}(k_3) + \langle b_{l_2,\tau_2}^\dagger(k_2) b_{l_2,\tau_2}(k_3) \rangle b_{l_1,\tau_1}^\dagger(k_1) b_{l_1,\tau_1}(k_4)$$
$$- \langle b_{l_1,\tau_1}^\dagger(k_1) b_{l_2,\tau_2}(k_3) \rangle b_{l_2,\tau_2}^\dagger(k_2) b_{l_1,\tau_1}(k_4) - \langle b_{l_2,\tau_2}^\dagger(k_2) b_{l_1,\tau_1}(k_4) \rangle b_{l_1,\tau_1}^\dagger(k_1) b_{l_2,\tau_2}(k_3) \Big] V(|k_1-k_4|) \delta_{k_1+k_2,k_3+k_4}$$

This expression includes all the quadratic terms in the Hartree-Fock Hamiltonian. The terms that are solely expectations or products of expectations have been excluded.

13 Combine Hartree/Fock terms

Prompt: You will be instructed to simplify the quadratic term $\hat{\mathcal{H}}^{\text{HF}}$ through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.The logic is that the expected value ($\langle b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}^\dagger b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \rangle$ and $\langle b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}^\dagger b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle$) in the first Hartree term (‘$\langle b_{\tau_1,l_1}^\dagger(k_1) b_{\tau_1,l_1}(k_4) \rangle b_{\tau_2,l_2}^\dagger(k_2) b_{\tau_2,l_2}(k_3)$‘) has the same form as the quadratic operators in the second Hartree term (‘$\langle b_{\tau_2,l_2}^\dagger(k_2) b_{\tau_2,l_2}(k_3) \rangle b_{\tau_1,l_1}^\dagger(k_1) b_{\tau_1,l_1}(k_4)$‘), 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

$$\hat{H}^{int,HF,2} = \frac{1}{2V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4} \Big[\langle b_{l_1,\tau_1}^\dagger(k_1) b_{l_1,\tau_1}(k_4) \rangle b_{l_2,\tau_2}^\dagger(k_2) b_{l_2,\tau_2}(k_3) + \langle b_{l_2,\tau_2}^\dagger(k_2) b_{l_2,\tau_2}(k_3) \rangle b_{l_1,\tau_1}^\dagger(k_1) b_{l_1,\tau_1}(k_4)$$
$$- \langle b_{l_1,\tau_1}^\dagger(k_1) b_{l_2,\tau_2}(k_3) \rangle b_{l_2,\tau_2}^\dagger(k_2) b_{l_1,\tau_1}(k_4) - \langle b_{l_2,\tau_2}^\dagger(k_2) b_{l_1,\tau_1}(k_4) \rangle b_{l_1,\tau_1}^\dagger(k_1) b_{l_2,\tau_2}(k_3) \Big] V(|k_1-k_4|) \delta_{k_1+k_2,k_3+k_4}.$$

Return the simplified $\hat{\mathcal{H}}^{\text{HF}}$ 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 $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4) (\langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) + \langle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \rangle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)) \delta_{k_1+k_2,k_3+k_4}$, where $V(q) = V(-q)$.In the second term, we relabel the index to swap the index in expected value and the index in quadratic operators, namely, $\sigma_1 \leftrightarrow \sigma_2$, $\sigma_3 \leftrightarrow \sigma_4$, $k_1 \leftrightarrow k_2$, $k_3 \leftrightarrow k_4$. After the replacement, the second term becomes $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_2 - k_3) \langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$.Note that the Kronecker dirac function $\delta_{k_4+k_3,k_2+k_1}$ implies $k_1 + k_2 = k_3 + k_4$, i.e., $k_2 - k_3 = k_4 - k_1$. Thus, the second term simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_4 - k_1) \langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$. Because $V(q) = V(-q)$, meaning $V(k_4 - k_1) = V(k_1 - k_4)$, the second term further simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4) \langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$. Note that this form of second term after relabeling is identical to the first term.Finally, we have the simplified Hamiltonian as $\hat{H} = 2 \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4) \langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$.
Completion: Following the example, we can simplify the Hartree-Fock Hamiltonian $\hat{\mathcal{H}}^{\text{HF}}$ by relabeling the indices.
For the Hartree terms, we relabel the indices in the second term as follows: $l_1 \leftrightarrow l_2$, $\tau_1 \leftrightarrow \tau_2$, $k_1 \leftrightarrow k_2$, and $k_3 \leftrightarrow k_4$. After the replacement, the second Hartree term becomes $\langle b_{l_1,\tau_1}^\dagger(k_1) b_{l_1,\tau_1}(k_4) \rangle b_{l_2,\tau_2}^\dagger(k_2) b_{l_2,\tau_2}(k_3)$.
For the Fock terms, we relabel the indices in the second term as follows: $l_1 \leftrightarrow l_2$, $\tau_1 \leftrightarrow \tau_2$, $k_1 \leftrightarrow k_2$, and $k_3 \leftrightarrow k_4$. After the replacement, the second Fock term becomes $\langle b_{l_1,\tau_1}^\dagger(k_1) b_{l_2,\tau_2}(k_3) \rangle b_{l_2,\tau_2}^\dagger(k_2) b_{l_1,\tau_1}(k_4)$.
Since the interaction potential $V(q)$ satisfies $V(q) = V(-q)$, the simplified Hartree-Fock Hamiltonian $\hat{\mathcal{H}}^{\text{HF}}$ is given by:

$$\hat{\mathcal{H}}^{\text{HF}} = \frac{1}{2V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4} \Big[2\langle b_{l_1,\tau_1}^\dagger(k_1) b_{l_1,\tau_1}(k_4) \rangle b_{l_2,\tau_2}^\dagger(k_2) b_{l_2,\tau_2}(k_3)$$
$$- 2\langle b_{l_1,\tau_1}^\dagger(k_1) b_{l_2,\tau_2}(k_3) \rangle b_{l_2,\tau_2}^\dagger(k_2) b_{l_1,\tau_1}(k_4) \Big] V(|k_1-k_4|) \delta_{k_1+k_2,k_3+k_4}$$

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

14 Identify order parameters in Hartree term (extended BZ)

Prompt: You will be instructed to simplify the Hartree term in H_{Hartree} by reducing the momentum inside the expected value $\langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_1,\tau_1,q_4}(k_4) \rangle$.The expected value $\langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_1,\tau_1,q_4}(k_4) \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_1,\tau_1,q_4}(k_4) \rangle = \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_1,\tau_1,q_4}(k_4) \rangle \delta_{k_1,k_4}$.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 H_{Hartree} is $\hat{\mathcal{H}}^{\text{HF}} = \frac{1}{V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4,q_1,q_2,q_3,q_4}\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_1,\tau_1,q_4}(k_4)\rangle b_{l_2,\tau_2,q_2}^{\dagger}(k_2)b_{l_2,\tau_2,q_3}(k_3)V(|k_1+q_1-k_4-q_4|)\delta_{k_1+k_2+q_1+q_2,k_3+k_4+q_3+q_4}$..Return the final simplified Hartree term H_{Hartree}.
EXAMPLE:Given a Hamiltonian where the Hartree term $\hat{H}^{Hartree} = \sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4}V(k_1-k_4+b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_4)\rangle c_{b_2}^{\dagger}(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, where k_i is the momentum inside first Brilloun zone and b_i is the reciprocal lattice.Inside the expected value, we realize $\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_4)\rangle$ is nonzero only when $k_1=k_4$, i.e., $\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_4)\rangle = \langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_4)\rangle\delta_{k_1,k_4}$.Thus, the Hartree term becomes $\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4}V(k_1-k_4+b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_4)\rangle\delta_{k_1,k_4}c_{b_2}^{\dagger}(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.Use the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4}V(k_1-k_1+b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_1)\rangle c_{b_2}^{\dagger}(k_2)c_{b_3}(k_3)\delta_{k_1+k_2+b_1+b_2,k_3+k_1+b_3+b_4} = \sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4}V(b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_1)\rangle c_{b_2}^{\dagger}(k_2)c_{b_3}(k_3)\delta_{k_2+b_1+b_2,k_3+b_3+b_4}$.Because k_i is momentum inside first Brilloun zone while b_i is the reciprocal lattice. It is only when $k_2=k_3$ that $\delta_{k_2+b_1+b_2,k_3+b_3+b_4}$ is nonzero, i.e., $\delta_{k_2+b_1+b_2,k_3+b_3+b_4}=\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_3}$. Therefore, the Hartree term simplifies to $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4}V(b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_1)\rangle c_{b_2}^{\dagger}(k_2)c_{b_3}(k_3)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_3} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4}V(b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_1)\rangle c_{b_2}^{\dagger}(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Hartree term after reducing two momenta is $\hat{H}^{Hartree} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4}V(b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_4}(k_1)\rangle c_{b_2}^{\dagger}(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}$
Completion: The Hartree term H_{Hartree} can be simplified by reducing the momentum inside the expected value $\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_1,\tau_1,q_4}(k_4)\rangle$ and the total momentum conservation.
Given that $\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_1,\tau_1,q_4}(k_4)\rangle$ is nonzero only when $k_1=k_4$, we can use the Kronecker delta function δ_{k_1,k_4} to reduce one momentum k_1 but not b_1.
The Hartree term then becomes:
$\hat{\mathcal{H}}^{\text{HF}} = \frac{1}{V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4,q_1,q_2,q_3,q_4}\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_1,\tau_1,q_4}(k_4)\rangle\delta_{k_1,k_4}b_{l_2,\tau_2,q_2}^{\dagger}(k_2)b_{l_2,\tau_2,q_3}(k_3)V(|k_1+q_1-k_4-q_4|)\delta_{k_1+k_2+q_1+q_2,k_3+k_4+q_3+q_4}$.
Using the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have:
$\hat{\mathcal{H}}^{\text{HF}} = \frac{1}{V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,q_1,q_2,q_3,q_4}\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_1,\tau_1,q_4}(k_1)\rangle b_{l_2,\tau_2,q_2}^{\dagger}(k_2)b_{l_2,\tau_2,q_3}(k_3)V(|k_1+q_1-k_1-q_4|)\delta_{k_1+k_2+q_1+q_2,k_3+k_1+q_3+q_4}$.
The total momentum conservation will reduce another momentum in the quadratic term. Therefore, we end up with only two momenta left in the summation:
$\hat{\mathcal{H}}^{\text{HF}} = \frac{1}{V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,q_1,q_2,q_3,q_4}\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_1,\tau_1,q_4}(k_1)\rangle b_{l_2,\tau_2,q_2}^{\dagger}(k_2)b_{l_2,\tau_2,q_3}(k_2)V(|q_1-q_4|)\delta_{k_1+q_1+q_2,k_2+q_3+q_4}$.
Finally, the simplified Hartree term H_{Hartree} is:
$H_{\text{Hartree}} = \frac{1}{V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,q_1,q_2,q_3,q_4}\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_1,\tau_1,q_4}(k_1)\rangle b_{l_2,\tau_2,q_2}^{\dagger}(k_2)b_{l_2,\tau_2,q_3}(k_2)V(|q_1-q_4|)\delta_{k_1+q_1+q_2,k_2+q_3+q_4}$.

15 Identify order parameters in Fock term (extended BZ)

Prompt: You will be instructed to simplify the Fock term in H_{Fock} by reducing the momentum inside the expected value $\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_2,\tau_2,q_3}(k_3)\rangle$.The expected value $\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_2,\tau_2,q_3}(k_3)\rangle$ is only nonzero when the two momenta k_i,k_j are the same, namely, $\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_2,\tau_2,q_3}(k_3)\rangle = \langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_2,\tau_2,q_3}(k_3)\rangle\delta_{k_1,k_3}$.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 H_{Fock} is $\hat{\mathcal{H}}^{\text{HF}} = -\frac{1}{V}\sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4,q_1,q_2,q_3,q_4}\langle b_{l_1,\tau_1,q_1}^{\dagger}(k_1)b_{l_2,\tau_2,q_3}(k_3)\rangle b_{l_2,\tau_2,q_2}^{\dagger}(k_2)b_{l_1,\tau_1,q_4}(k_4)V(|k_1+q_1-k_4-q_4|)\delta_{k_1+k_2+q_1+q_2,k_3+k_4+q_3+q_4}$.Return the final simplified Fock term H_{Fock}.
EXAMPLE:Given a Hamiltonian where the Fock term $\hat{H}^{Fock} = -\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4}V(k_1-k_4+b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_3}(k_3)\rangle c_{b_2}^{\dagger}(k_2)c_{b_4}(k_4)\delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, 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 Brilloun zone while b_i is the reciprocal lattice. It is only when $k_2=k_4$ that $\delta_{k_2+b_1+b_2,k_4+b_3+b_4}$ is nonzero, i.e., $\delta_{k_2+b_1+b_2,k_4+b_3+b_4}=\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4}$.Therefore, the Fock term simplifies to $-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4}V(k_1-k_4+b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_3}(k_1)\rangle c_{b_2}^{\dagger}(k_2)c_{b_4}(k_4)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4} = -\sum_{k_1,k_2,b_1,b_2,b_3,b_4}V(k_1-k_2+b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_3}(k_1)\rangle c_{b_2}^{\dagger}(k_2)c_{b_4}(k_2)\delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Fock term after reducing two momenta is $\hat{H}^{Fock} = -\sum_{k_1,k_2,b_1,b_2,b_3,b_4}V(k_1-k_2+b_1-b_4)\langle c_{b_1}^{\dagger}(k_1)c_{b_3}(k_1)\rangle c_{b_2}^{\dagger}(k_2)c_{b_4}(k_2)\delta_{b_1+b_2,b_3+b_4}$

Completion: Following the example, we first note that the expected value $\langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_3)\rangle$ is nonzero only when $k_1 = k_3$. Therefore, we can write $\langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_3)\rangle = \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_3)\rangle \delta_{k_1,k_3}$.
Substituting this into the Fock term, we get:
$\hat{\mathcal{H}}^{\rm HF} = -\frac{1}{V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_3,k_4,q_1,q_2,q_3,q_4} \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_3)\rangle \delta_{k_1,k_3} b_{l_2,\tau_2,q_2}^\dagger(k_2) b_{l_1,\tau_1,q_4}(k_4) V(|k_1+q_1-k_4-q_4|)\delta_{k_1+k_2+q_1+q_2,k_3+k_4+q_3+q_4}$.
Using the property of the Kronecker delta function δ_{k_1,k_3} to sum over k_3, we get:
$\hat{\mathcal{H}}^{\rm HF} = -\frac{1}{V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_4,q_1,q_2,q_3,q_4} \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_1)\rangle b_{l_2,\tau_2,q_2}^\dagger(k_2) b_{l_1,\tau_1,q_4}(k_4) V(|k_1+q_1-k_4-q_4|)\delta_{k_1+k_2+q_1+q_2,k_1+k_4+q_3+q_4}$.
Simplifying the delta function, we get:
$\hat{\mathcal{H}}^{\rm HF} = -\frac{1}{V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,k_4,q_1,q_2,q_3,q_4} \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_1)\rangle b_{l_2,\tau_2,q_2}^\dagger(k_2) b_{l_1,\tau_1,q_4}(k_4) V(|k_1+q_1-k_4-q_4|)\delta_{k_2+q_1+q_2,k_4+q_3+q_4}$.
Finally, using the property of the Kronecker delta function $\delta_{k_2+q_1+q_2,k_4+q_3+q_4}$ to sum over k_4, we get the final simplified Fock term:
$H_{\rm Fock} = -\frac{1}{V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,q_1,q_2,q_3,q_4} \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_1)\rangle b_{l_2,\tau_2,q_2}^\dagger(k_2) b_{l_1,\tau_1,q_4}(k_2) V(|k_1+q_1-k_2-q_4|)\delta_{q_1+q_2,q_3+q_4}$.

16 Final form of iteration in quadratic terms

Prompt: You will now be instructed to combine the Hartree term $H_{\rm Hartree}$ and the Fock term $H_{\rm Fock}$.You should recall that the Hartree term $H_{\rm Hartree} = \frac{1}{V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,q_1,q_2,q_3,q_4} \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_1,\tau_1,q_4}(k_1)\rangle b_{l_2,\tau_2,q_2}^\dagger(k_2) b_{l_2,\tau_2,q_3}(k_2) V(|q_1-q_4|)\delta_{q_1+q_2,q_3+q_4}$,and the Fock term $H_{\rm Fock} = -\frac{1}{V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,q_1,q_2,q_3,q_4} \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_1)\rangle b_{l_2,\tau_2,q_2}^\dagger(k_2) b_{l_1,\tau_1,q_4}(k_2) V(|k_1+q_1-k_2-q_4|)\delta_{q_1+q_2,q_3+q_4}$.You should perform the same trick of relabeling the index in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. The relabeling should be done with a swap : Nothing. You should add them, relabel the index in Fock term, and simply their sum. Return the final sum of Hartree and Fock term.
Completion: The sum of the Hartree and Fock terms, after relabeling the index in the Fock term, is given by:
$H_{\rm HF} = H_{\rm Hartree} + H_{\rm Fock}$
$= \frac{1}{V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,q_1,q_2,q_3,q_4} \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_1,\tau_1,q_4}(k_1)\rangle b_{l_2,\tau_2,q_2}^\dagger(k_2) b_{l_2,\tau_2,q_3}(k_2) V(|q_1-q_4|)\delta_{q_1+q_2,q_3+q_4}$
$-\frac{1}{V} \sum_{\tau_1,\tau_2,l_1,l_2,k_1,k_2,q_1,q_2,q_3,q_4} \langle b_{l_1,\tau_1,q_1}^\dagger(k_1) b_{l_2,\tau_2,q_3}(k_1)\rangle b_{l_2,\tau_2,q_2}^\dagger(k_2) b_{l_1,\tau_1,q_4}(k_2) V(|k_1+q_1-k_2-q_4|)\delta_{q_1+q_2,q_3+q_4}$
This is the final sum of the Hartree and Fock terms.