

The kinetic Hamiltonian H_T for the AB-stacked MoTe₂/WSe₂ system with the considered degrees of freedom can be expressed in a matrix form as follows:

$$H_T = \begin{pmatrix} E_{+K,b} & 0 & 0 & 0 \\ 0 & E_{+K,t} & 0 & 0 \\ 0 & 0 & E_{-K,b} & 0 \\ 0 & 0 & 0 & E_{-K,t} \end{pmatrix}$$

In this matrix:

- The diagonal elements represent the energy levels for each state.
- $E_{+K,b}$ and $E_{+K,t}$ are the energy levels at the +K valley for the bottom and top layers, respectively.
- $E_{-K,b}$ and $E_{-K,t}$ are the energy levels at the -K valley for the bottom and top layers, respectively.
- The off-diagonal elements are all zero, indicating no direct coupling between these states in the kinetic term of the Hamiltonian.

Since the system describes holes with a parabolic dispersion, the dispersion relation is the inverse of that for electrons. Therefore, for a hole, the energy dispersion is $E_\alpha = -\frac{\hbar^2 k^2}{2m_\alpha}$ (negative sign because we are dealing with holes).

Considering the shifts in momentum for top layer terms, the expressions for each energy term will be:

- $E_{+K,b} = -\frac{\hbar^2 k^2}{2m_b}$
- $E_{+K,t} = -\frac{\hbar^2 (k+\kappa)^2}{2m_t}$
- $E_{-K,b} = -\frac{\hbar^2 k^2}{2m_b}$
- $E_{-K,t} = -\frac{\hbar^2 (k-\kappa)^2}{2m_t}$

Substituting these into the kinetic Hamiltonian H_T , we get:

$$H_T = \begin{pmatrix} -\frac{\hbar^2 k^2}{2m_b} & 0 & 0 & 0 \\ 0 & -\frac{\hbar^2 (k+\kappa)^2}{2m_t} & 0 & 0 \\ 0 & 0 & -\frac{\hbar^2 k^2}{2m_b} & 0 \\ 0 & 0 & 0 & -\frac{\hbar^2 (k-\kappa)^2}{2m_t} \end{pmatrix}$$

Here, k remains as an operator, and the energy terms account for the parabolic dispersion of holes with the given mass parameters and momentum shifts.

The potential Hamiltonian H_V in the real space for the AB-stacked MoTe₂/WSe₂ system, considering the specified degrees of freedom and the hermitian nature of the off-diagonal terms, can be expressed as:

$$H_V = \begin{pmatrix} \Delta_b(r) & \Delta_{T,\tau}(\mathbf{r}) & 0 & 0 \\ \Delta_{T,\tau}^\dagger(\mathbf{r}) & \Delta_t(r) & 0 & 0 \\ 0 & 0 & \Delta_b(r) & \Delta_{T,\tau}(\mathbf{r}) \\ 0 & 0 & \Delta_{T,\tau}^\dagger(\mathbf{r}) & \Delta_t(r) \end{pmatrix}$$

In this matrix:

- $\Delta_b(r)$ and $\Delta_t(r)$ are the potential terms for the bottom and top layers respectively, which appear on the diagonal.
- $\Delta_{T,\tau}(\mathbf{r})$ and its hermitian conjugate $\Delta_{T,\tau}^\dagger(\mathbf{r})$ are the off-diagonal terms that represent the coupling between the opposite layers.
- The zero terms represent no direct potential coupling between other combinations of degrees of freedom.

The expressions for $\Delta_t(r)$, $\Delta_b(r)$, $\Delta_{T,\tau}(\mathbf{r})$ and $\Delta_{T,\tau}^\dagger(\mathbf{r})$ are as follows:

- $\Delta_t(r) = V_0 \sum_{i=1}^3 \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi_t)$

- $\Delta_b(r) = V_0 \sum_{i=1}^3 \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi_b)$
- $\Delta_{T,+K}(\mathbf{r}) = T_0 \sum_{i=1}^3 e^{i\mathbf{G}_i \cdot \mathbf{r}}$
- $\Delta_{T,-K}(\mathbf{r}) = T_0 \sum_{i=1}^3 e^{-i\mathbf{G}_i \cdot \mathbf{r}}$

Substituting these into the potential Hamiltonian H_V , we get:

$$H_V = \begin{pmatrix} V_0 \sum_{i=1}^3 \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi_b) & T_0 \sum_{i=1}^3 e^{i\mathbf{G}_i \cdot \mathbf{r}} & 0 & 0 \\ T_0 \sum_{i=1}^3 e^{-i\mathbf{G}_i \cdot \mathbf{r}} & V_0 \sum_{i=1}^3 \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi_t) & 0 & 0 \\ 0 & 0 & V_0 \sum_{i=1}^3 \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi_b) & T_0 \sum_{i=1}^3 e^{-i\mathbf{G}_i \cdot \mathbf{r}} \\ 0 & 0 & T_0 \sum_{i=1}^3 e^{i\mathbf{G}_i \cdot \mathbf{r}} & V_0 \sum_{i=1}^3 \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi_t) \end{pmatrix}$$

Here, ϕ_t and ϕ_b are the phase shifts for the top and bottom layers respectively, and \mathbf{G}_i are the reciprocal lattice vectors of the moiré pattern. The potential terms represent intralayer potentials and interlayer tunneling, consistent with the AB-stacked MoTe₂/WSe₂ system described.

First, let's express the kinetic and potential Hamiltonians in the single-particle form:

- Kinetic Hamiltonian H_T :

$$H_T = \begin{pmatrix} E_{+K,b} & 0 & 0 & 0 \\ 0 & E_{+K,t} & 0 & 0 \\ 0 & 0 & E_{-K,b} & 0 \\ 0 & 0 & 0 & E_{-K,t} \end{pmatrix}$$

- Potential Hamiltonian H_V :

$$H_V = \begin{pmatrix} \Delta_b(r) & \Delta_{T,+K}(\mathbf{r}) & 0 & 0 \\ \Delta_{T,+K}^\dagger(\mathbf{r}) & \Delta_t(r) & 0 & 0 \\ 0 & 0 & \Delta_b(r) & \Delta_{T,-K}(\mathbf{r}) \\ 0 & 0 & \Delta_{T,-K}^\dagger(\mathbf{r}) & \Delta_t(r) \end{pmatrix}$$

Now, to construct the second quantized form, let's define the creation (ψ^\dagger) and annihilation (ψ) operators for each of the basis states: (+K,bottom), (+K,top), (-K,bottom), and (-K,top). The basis order corresponds to the order of terms in the Hamiltonians.

The second quantized form of the total noninteracting Hamiltonian \hat{H}^0 is given by:

$$\hat{H}^0 = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) (H_T + H_V) \Psi(\mathbf{r})$$

where $\Psi(\mathbf{r})$ is the column vector of annihilation operators and $\Psi^\dagger(\mathbf{r})$ is the row vector of creation operators, defined as:

$$\begin{aligned} \Psi(\mathbf{r}) &= \begin{pmatrix} \psi_{+K,b}(\mathbf{r}) \\ \psi_{+K,t}(\mathbf{r}) \\ \psi_{-K,b}(\mathbf{r}) \\ \psi_{-K,t}(\mathbf{r}) \end{pmatrix}, \quad \Psi^\dagger(\mathbf{r}) \\ &= \left(\psi_{+K,b}^\dagger(\mathbf{r}) \quad \psi_{+K,t}^\dagger(\mathbf{r}) \quad \psi_{-K,b}^\dagger(\mathbf{r}) \quad \psi_{-K,t}^\dagger(\mathbf{r}) \right) \end{aligned}$$

The creation and annihilation operators correspond to different layers and valleys as indicated by their subscripts. The spin index of these fermion operators is both layer and valley dependent as per the conventions provided. The integration over \mathbf{r} takes the sum over all space, accounting for the real space position in the Hamiltonian.

First, let's define the Fourier transformation for the creation and annihilation operators:

$$c_{\tau,l}^\dagger(k) = \frac{1}{\sqrt{V}} \int d\mathbf{r} \psi_{\tau,l}^\dagger(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}$$

$$c_{\tau,l}(k) = \frac{1}{\sqrt{V}} \int d\mathbf{r} \psi_{\tau,l}(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}$$

where V is the volume of the system.

The inverse Fourier transformation is then:

$$\psi_{\tau,l}^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k c_{\tau,l}^\dagger(k) e^{-i\mathbf{k} \cdot \mathbf{r}}$$

$$\psi_{\tau,l}(r) = \frac{1}{\sqrt{V}} \sum_k c_{\tau,l}(k) e^{ik \cdot r}$$

Substituting these into \hat{H}^0 , we get:

$$\begin{aligned} \hat{H}^0 &= \int dr \frac{1}{\sqrt{V}} \sum_{k_1} c_{\tau,l}^\dagger(k_1) e^{-ik_1 \cdot r} H(r) \frac{1}{\sqrt{V}} \sum_{k_2} c_{\tau,l}(k_2) e^{ik_2 \cdot r} \\ &= \sum_{k_1, k_2} c_{\tau,l}^\dagger(k_1) \frac{1}{V} \int dr e^{-i(k_1 - k_2) \cdot r} H(r) c_{\tau,l}(k_2) \\ &= \sum_{k_1, k_2} c_{\tau,l}^\dagger(k_1) H_\tau(k_1, k_2) c_{\tau,l}(k_2) \end{aligned}$$

where $H_\tau(k_1, k_2)$ is the Fourier transform of the Hamiltonian $H(r)$ and is defined as:

$$H_\tau(k_1, k_2) = \frac{1}{V} \int dr e^{-i(k_1 - k_2) \cdot r} H(r)$$

This represents the total noninteracting Hamiltonian \hat{H}^0 in the momentum space, with k_1 and k_2 being the momentum indices summed over the extended Brillouin zone. The Hamiltonian matrix elements are nonzero only when $\mathbf{k}_\alpha - \mathbf{k}_\beta$ equals a linear combination of moiré reciprocal lattice vectors (including the zero vector), according to Bloch's theorem.

Given the definition of the hole operator $b_{\mathbf{k},l,\tau} = c_{\mathbf{k},l,\tau}^\dagger$ and the particle-hole transformation, the transformed Hamiltonian can be written as:

$$\hat{H}_{\text{hole}}^0 = \sum_{\tau, \mathbf{k}_\alpha, \mathbf{k}_\beta} b_{\mathbf{k}_\alpha, l_\alpha, \tau} h_{\mathbf{k}_\alpha, l_\alpha, \mathbf{k}_\beta, l_\beta}^{(\tau)} b_{\mathbf{k}_\beta, l_\beta, \tau}^\dagger$$

This expression represents the total noninteracting Hamiltonian \hat{H}^0 in terms of the hole operators $b_{\mathbf{k},l,\tau}$ and $b_{\mathbf{k},l,\tau}^\dagger$. The Hamiltonian matrix elements $h_{\mathbf{k}_\alpha, l_\alpha, \mathbf{k}_\beta, l_\beta}^{(\tau)}$ remain unchanged, as they depend on the system's physical properties, which are independent of the chosen particle or hole representation. The transformation effectively switches the roles of filled and empty states in the system, which is a common technique in studying systems where the particle-like excitations are holes rather than electrons.

Starting from the given Hamiltonian in the hole basis:

$$\hat{H}^0 = \sum_{\tau, \mathbf{k}_\alpha, \mathbf{k}_\beta} b_{\mathbf{k}_\alpha, l_\alpha, \tau} h_{\mathbf{k}_\alpha, l_\alpha, \mathbf{k}_\beta, l_\beta}^{(\tau)} b_{\mathbf{k}_\beta, l_\beta, \tau}^\dagger$$

We apply the fermionic anticommutation relations:

$$[b_{\mathbf{k}_\alpha, l_\alpha, \tau}, b_{\mathbf{k}_\beta, l_\beta, \tau}^\dagger]_+ = \delta_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \delta_{l_\alpha, l_\beta} \delta_{\tau, \tau}$$

which implies:

$$b_{\mathbf{k}_\alpha, l_\alpha, \tau} b_{\mathbf{k}_\beta, l_\beta, \tau}^\dagger = \delta_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \delta_{l_\alpha, l_\beta} \delta_{\tau, \tau} - b_{\mathbf{k}_\beta, l_\beta, \tau}^\dagger b_{\mathbf{k}_\alpha, l_\alpha, \tau}$$

Substituting this into \hat{H}^0 :

$$\hat{H}^0 = \sum_{\tau, \mathbf{k}_\alpha, \mathbf{k}_\beta} (\delta_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \delta_{l_\alpha, l_\beta} \delta_{\tau, \tau} - b_{\mathbf{k}_\beta, l_\beta, \tau}^\dagger b_{\mathbf{k}_\alpha, l_\alpha, \tau}) h_{\mathbf{k}_\alpha, l_\alpha, \mathbf{k}_\beta, l_\beta}^{(\tau)}$$

Simplifying and reordering the indices:

$$\hat{H}^0 = \sum_{\tau, \mathbf{k}_\alpha, \mathbf{k}_\beta} \delta_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \delta_{l_\alpha, l_\beta} \delta_{\tau, \tau} h_{\mathbf{k}_\alpha, l_\alpha, \mathbf{k}_\beta, l_\beta}^{(\tau)} - \sum_{\tau, \mathbf{k}_\alpha, \mathbf{k}_\beta} b_{\mathbf{k}_\beta, l_\beta, \tau}^\dagger h_{\mathbf{k}_\alpha, l_\alpha, \mathbf{k}_\beta, l_\beta}^{(\tau)} b_{\mathbf{k}_\alpha, l_\alpha, \tau}$$

Using the fact that $h_{\mathbf{k}_\alpha, l_\alpha, \mathbf{k}_\beta, l_\beta}^{(\tau)}$ is Hermitian, and relabeling the indices:

$$\hat{H}^0 = \sum_{\tau, \mathbf{k}} h_{\mathbf{k}l, \mathbf{k}l}^{(\tau)} - \sum_{\tau, \mathbf{k}_\alpha, \mathbf{k}_\beta} b_{\mathbf{k}_\alpha, l_\alpha, \tau}^\dagger [h_{\mathbf{k}_\beta, l_\beta, \mathbf{k}_\alpha, l_\alpha}^{(\tau)}]^* b_{\mathbf{k}_\beta, l_\beta, \tau}$$

This is the Hamiltonian \hat{H}^0 in the normal order of $b_{\mathbf{k},l,\tau}$ operators, with \mathbf{k}_α always appearing before \mathbf{k}_β in the indices, and the Hamiltonian matrix elements $h_{\mathbf{k}_\alpha, l_\alpha, \mathbf{k}_\beta, l_\beta}^{(\tau)}$ transposed and conjugated accordingly.

The interaction Hamiltonian \hat{H}_{int} in momentum space is given by:

$$\hat{H}_{\text{int}} = \frac{1}{2A} \sum_{\substack{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta \\ l_\alpha, l_\beta \\ \tau_\alpha, \tau_\beta}} V(\mathbf{q}) \delta(\mathbf{k}_\alpha + \mathbf{k}_\beta - \mathbf{k}_\gamma - \mathbf{k}_\delta) b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha}$$

where

$$V(\mathbf{q}) = \frac{e^2}{2\epsilon_0\epsilon_r|\mathbf{q}|} \frac{\tanh(|\mathbf{q}|d)}{|\mathbf{q}|d}$$

and

$$\mathbf{q} = \mathbf{k}_\alpha - \mathbf{k}_\delta$$

In this Hamiltonian:

- $b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger$ and $b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger$ are creation operators.
- $b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta}$ and $b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha}$ are annihilation operators.
- $V(\mathbf{q})$ is the dual-gated screened Coulomb interaction potential.
- The delta function $\delta(\mathbf{k}_\alpha + \mathbf{k}_\beta - \mathbf{k}_\gamma - \mathbf{k}_\delta)$ enforces momentum conservation.
- The normalization factor is $\frac{1}{2A}$, where A is the area of the system.

This Hamiltonian describes the interaction between particles (holes in this case) in the AB-stacked MoTe₂/WSe₂ system, taking into account the screening effect due to the dual-gated setup and momentum conservation.

Using Wick's theorem and preserving only the normal terms, the interaction term \hat{H}_{int} can be expanded. The order of the product is $1^\dagger, 2^\dagger, 3, 4$, so following Example 1:

$$\begin{aligned} \hat{H}_{\text{int}} = & \frac{1}{2A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} \left(\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right. \\ & + \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \\ & - \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle \\ & \left. - \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} - \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right) \\ & + \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\gamma + \mathbf{k}_\delta} \end{aligned}$$

This expansion of \hat{H}_{int} yields \hat{H}^{HF} , the Hartree-Fock Hamiltonian, where each term is the product of a creation operator and an annihilation operator (normal terms), and expectation values represent average occupations in the system. The terms involve sums over all possible combinations of momenta, layers, and spins, and include the interaction potential $V(\mathbf{k}_\alpha - \mathbf{k}_\delta)$, ensuring momentum conservation.

From the Hartree-Fock Hamiltonian \hat{H}^{HF} , the quadratic terms can be extracted as $\hat{H}_{\text{int}}^{\text{HF}}$:

$$\begin{aligned} \hat{H}_{\text{int}}^{\text{HF}} = & \frac{1}{2A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} \left(\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right. \\ & + \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \\ & - \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \\ & \left. - \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right) V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\gamma + \mathbf{k}_\delta} \end{aligned}$$

This expression for $\hat{H}_{\text{int}}^{\text{HF}}$ includes only the quadratic terms from the Hartree-Fock Hamiltonian. Each term involves a product of a creation operator and an annihilation operator, weighted by the expectation values of the corresponding operator pairs. The interaction potential $V(\mathbf{k}_\alpha - \mathbf{k}_\delta)$ is included, and momentum conservation is enforced by the delta function $\delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\gamma + \mathbf{k}_\delta}$. This Hamiltonian represents the effective interaction between particles (holes) in the system after applying the Hartree-Fock approximation.

Starting with the Hartree-Fock interaction Hamiltonian $\hat{H}_{\text{int}}^{\text{HF}}$ and using the relabeling trick as described, we can simplify it:

Original $\hat{H}_{\text{int}}^{\text{HF}}$:

$$\begin{aligned} \hat{H}_{\text{int}}^{\text{HF}} = \frac{1}{2A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} & \left(\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right. \\ & + \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \\ & \left. - \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} - \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right) \\ & V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\gamma + \mathbf{k}_\delta} \end{aligned}$$

Relabeling the indices in the second and fourth terms:

- Swap $\mathbf{k}_\alpha \leftrightarrow \mathbf{k}_\beta$ and $\mathbf{k}_\gamma \leftrightarrow \mathbf{k}_\delta$ in the second term.
- Swap $\mathbf{k}_\alpha \leftrightarrow \mathbf{k}_\beta$ and $\mathbf{k}_\gamma \leftrightarrow \mathbf{k}_\delta$ in the fourth term.

After relabeling, these terms become identical to the first and third terms respectively, due to $V(\mathbf{k}_\alpha - \mathbf{k}_\delta) = V(-(\mathbf{k}_\alpha - \mathbf{k}_\delta)) = V(\mathbf{k}_\delta - \mathbf{k}_\alpha)$, and the delta function enforcing momentum conservation. Thus, the simplified $\hat{H}_{\text{int}}^{\text{HF}}$ reduces to:

$$\begin{aligned} \hat{H}_{\text{int}}^{\text{HF}} = \frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} & \left(\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right. \\ & \left. - \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \right) \\ & V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\gamma + \mathbf{k}_\delta} \end{aligned}$$

This simplified Hamiltonian consists of just two terms, one Hartree and one Fock term, thus reducing the complexity of $\hat{H}_{\text{int}}^{\text{HF}}$ in the Hartree-Fock approximation.

Starting with the Hartree term in $\hat{H}_{\text{int}}^{\text{HF}}$:

$$\hat{H}_{\text{int}}^{\text{HF}} = \frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\gamma + \mathbf{k}_\delta}$$

By using the property that the expectation value is nonzero only when $\mathbf{k}_\alpha = \mathbf{k}_\delta$:

$$\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle = \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha} \rangle \delta_{\mathbf{k}_\alpha, \mathbf{k}_\delta}$$

The Hartree term becomes:

$$\hat{H}_{\text{Hartree}} = \frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma} \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} V(0) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\gamma + \mathbf{k}_\alpha}$$

Simplifying further using momentum conservation:

$$\hat{H}_{\text{Hartree}} = \frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha} \rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\beta, l_\beta, \tau_\beta} V(0)$$

This is the final simplified Hartree term, H_{Hartree} , reduced to two momenta in the summation with the interaction potential $V(0)$ representing the static screened Coulomb interaction at zero momentum transfer.

Starting with the Fock term in $\hat{H}_{\text{int}}^{\text{HF}}$:

$$\hat{H}_{\text{int}}^{\text{HF}} = -\frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\gamma + \mathbf{k}_\delta}$$

By using the property that the expectation value is nonzero only when $k_\alpha = k_\gamma$:

$$\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle = \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle \delta_{\mathbf{k}_\alpha, \mathbf{k}_\gamma}$$

The Fock term becomes:

$$\hat{H}_{\text{Fock}} = -\frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\delta} \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\beta, \tau_\beta} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\alpha + \mathbf{k}_\delta}$$

Simplifying further using momentum conservation:

$$\hat{H}_{\text{Fock}} = -\frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\beta, \tau_\beta} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\beta, l_\alpha, \tau_\alpha} \rangle V(\mathbf{k}_\alpha - \mathbf{k}_\beta)$$

This is the final simplified Fock term, H_{Fock} , reduced to two momenta in the summation with the interaction potential $V(\mathbf{k}_\alpha - \mathbf{k}_\beta)$ representing the screened Coulomb interaction between the relevant momentum states.

Starting with the given Hartree term H_{Hartree} and Fock term H_{Fock} :

Hartree term H_{Hartree} :

$$H_{\text{Hartree}} = \frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\beta, l_\beta, \tau_\beta} \rangle V(0)$$

Fock term H_{Fock} :

$$H_{\text{Fock}} = -\frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\beta, \tau_\beta} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\beta, l_\alpha, \tau_\alpha} \rangle V(\mathbf{k}_\alpha - \mathbf{k}_\beta)$$

Since the quadratic operators in the Fock term already match those in the Hartree term, there is no need for additional relabeling. The final combined sum of the Hartree and Fock terms is:

$$\begin{aligned} H_{\text{combined}} &= H_{\text{Hartree}} + H_{\text{Fock}} \\ &= \frac{1}{A} \sum_{\substack{\tau_\alpha, \tau_\beta \\ l_\alpha, l_\beta}} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta} \left(\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\beta, l_\beta, \tau_\beta} \rangle V(0) \right. \\ &\quad \left. - \langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\alpha, l_\beta, \tau_\beta} \rangle \langle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\beta, l_\alpha, \tau_\alpha} \rangle V(\mathbf{k}_\alpha - \mathbf{k}_\beta) \right) \end{aligned}$$

This expression represents the final combined sum of the Hartree and Fock terms, simplified and ready to be used in further calculations.