

1 Identify kinetic term (lattice)

Prompt: You will be instructed to describe the kinetic term of Hamiltonian in the CuO_2 plane in the real space in the second-quantized form. The degrees of freedom of the system are: spin index (spin up and spin down), orbital index (d orbital in Cu atom, p_x orbital in O atom, and p_y orbital in O atom). The kinetic term is a tight-binding model composed of the following hopping process: 1. $c_{d,s}^\dagger(R_i)$ and $c_{p_x,s}^\dagger(R_i + \hat{x}/2)$ with the hopping amplitude $-t_p d$. 2. $c_{d,s}^\dagger(R_i)$ and $c_{p_x,s}^\dagger(R_i - \hat{x}/2)$ with the hopping amplitude $-t_p d$. 3. $c_{d,s}^\dagger(R_i)$ and $c_{p_y,s}^\dagger(R_i + \hat{y}/2)$ with the hopping amplitude $-t_p d$. 4. $c_{d,s}^\dagger(R_i)$ and $c_{p_y,s}^\dagger(R_i - \hat{y}/2)$ with the hopping amplitude $-t_p d$. 5. $c_{p_x,s}^\dagger(R_i + \hat{x}/2)$ and $c_{p_y,s}^\dagger(R_i + \hat{y}/2)$ with the hopping amplitude $-t_p p$. 6. $c_{p_x,s}^\dagger(R_i + \hat{x}/2)$ and $c_{p_y,s}^\dagger(R_i - \hat{y}/2)$ with the hopping amplitude $-t_p p$. 7. $c_{p_x,s}^\dagger(R_i - \hat{x}/2)$ and $c_{p_y,s}^\dagger(R_i + \hat{y}/2)$ with the hopping amplitude $-t_p p$. 8. $c_{p_x,s}^\dagger(R_i - \hat{x}/2)$ and $c_{p_y,s}^\dagger(R_i - \hat{y}/2)$ with the hopping amplitude $-t_p p$.

You should ensure the hermiticity of the Hamiltonian. The summation should be taken over all spin index (spin up and spin down), orbital index (d orbital in Cu atom, p_x orbital in O atom, and p_y orbital in O atom) and all real space positions. Return the Kinetic Hamiltonian \mathcal{H}_0 .

Use the following conventions for the symbols: $\hat{d}_{i,s}^\dagger$ creates a hole in the copper $d_{x^2-y^2}$ orbital at site i with spin s , $\hat{p}_{i+\hat{\nu}/2,s}^\dagger$ creates a hole in the oxygen p_ν orbital at the site $i + \hat{\nu}/2$ for $\nu = x, y$, and $\hat{n}_{i,s}^d$, $\hat{n}_{i+\hat{\nu}/2,s}^p$ are the corresponding number operators. The Cu sites i form a square lattice with unit vectors \hat{x} and \hat{y} , and the total number of lattice sites is N . The chemical potential μ and the charge transfer energy Δ control the total and relative Cu/O hole densities, and $\langle \nu, \nu' \rangle$ point to neighboring oxygen sites.

Completion: The kinetic term of the Hamiltonian in the CuO_2 plane in the real space in the second-quantized form can be written as:

$$\begin{aligned} \mathcal{H}_0 = & -t_{pd} \sum_{i,s} \left[\hat{d}_{i,s}^\dagger \hat{p}_{i+\hat{x}/2,s} + \hat{d}_{i,s}^\dagger \hat{p}_{i-\hat{x}/2,s} + \hat{d}_{i,s}^\dagger \hat{p}_{i+\hat{y}/2,s} + \hat{d}_{i,s}^\dagger \hat{p}_{i-\hat{y}/2,s} \right. \\ & \left. + h.c. \right] - t_{pp} \sum_{\langle \nu, \nu' \rangle, s} \left[\hat{p}_{i+\hat{\nu}/2,s}^\dagger \hat{p}_{i+\hat{\nu}'/2,s} + h.c. \right] \end{aligned} \quad (1)$$

where $h.c.$ denotes the Hermitian conjugate of the preceding terms, ensuring the hermiticity of the Hamiltonian. The summation is taken over all spin index (spin up and spin down), orbital index (d orbital in Cu atom, p_x orbital in O atom, and p_y orbital in O atom) and all real space positions. The hopping amplitudes are $-t_{pd}$ and $-t_{pp}$ as given in the question.

2 Identify interacting term (real space)

Prompt: You will be instructed to construct the interaction part of the Hamiltonian, \mathcal{H}' in the real space in the second-quantized form. The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian \mathcal{H}_0 . The

interaction is a density-density interaction composed of the following process:

1. onsite interaction between $n_{d,\uparrow}(R_i)$ and $n_{d,\downarrow}(R_i)$ with interaction strength U_d
2. onsite interaction between $n_{p_x,\uparrow}(R_i + \hat{x}/2)$ and $n_{p_x,\downarrow}(R_i + \hat{x}/2)$ with interaction strength $U_p/2$
3. onsite interaction between $n_{p_y,\uparrow}(R_i + \hat{y}/2)$ and $n_{p_y,\downarrow}(R_i + \hat{y}/2)$ with interaction strength $U_p/2$
4. Nearest neighbor interaction between $n_{d,s}(R_i)$ and $n_{p_x,s'}(R_i + \hat{x}/2)$ with interaction strength V_{pd}
5. Nearest neighbor interaction between $n_{d,s}(R_i)$ and $n_{p_x,s'}(R_i - \hat{x}/2)$ with interaction strength V_{pd}
6. Nearest neighbor interaction between $n_{d,s}(R_i)$ and $n_{p_y,s'}(R_i + \hat{y}/2)$ with interaction strength V_{pd}
7. Nearest neighbor interaction between $n_{d,s}(R_i)$ and $n_{p_y,s'}(R_i - \hat{y}/2)$ with interaction strength V_{pd}
8. Nearest neighbor interaction between $n_{p_x,s}(R_i + \hat{x}/2)$ and $n_{p_y,s'}(R_i + \hat{y}/2)$ with interaction strength V_{pp}
9. Nearest neighbor interaction between $n_{p_x,s}(R_i + \hat{x}/2)$ and $n_{p_y,s'}(R_i - \hat{y}/2)$ with interaction strength V_{pp}
10. Nearest neighbor interaction between $n_{p_x,s}(R_i - \hat{x}/2)$ and $n_{p_y,s'}(R_i + \hat{y}/2)$ with interaction strength V_{pp}
11. Nearest neighbor interaction between $n_{p_x,s}(R_i - \hat{x}/2)$ and $n_{p_y,s'}(R_i - \hat{y}/2)$ with interaction strength V_{pp}

where density operator $n_{\alpha,s}(R_i) = c_{\alpha,s}^\dagger(R_i)c_{\alpha,s}(R_i)$.

The summation should be taken over all spin states (s, s') and all real space positions. Return the interaction term \mathcal{H}' in terms of \hat{n} .

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): s' : spin index $n_{\alpha,s}(R_i)$: density of particle with orbital α and spin s at site R_i U_d : onsite interaction strength of d orbital U_p : onsite interaction strength of p_x orbital or p_y orbital V_{pd} : Nearest neighbor interaction strength between p_x orbital and d orbital or between p_y orbital and d orbital V_{pp} : Nearest neighbor interaction strength between p_x orbital and p_y orbital

Completion: The interaction part of the Hamiltonian, \mathcal{H}' , in real space in the second-quantized form can be written as:

$$\begin{aligned} \mathcal{H}' = & U_d \sum_{R_i} n_{d,\uparrow}(R_i) n_{d,\downarrow}(R_i) + \frac{U_p}{2} \sum_{R_i} [n_{p_x,\uparrow}(R_i + \hat{x}/2) n_{p_x,\downarrow}(R_i + \hat{x}/2) + \\ & n_{p_y,\uparrow}(R_i + \hat{y}/2) n_{p_y,\downarrow}(R_i + \hat{y}/2)] \\ & + V_{pd} \sum_{R_i, s, s'} [n_{d,s}(R_i) n_{p_x,s'}(R_i + \hat{x}/2) + n_{d,s}(R_i) n_{p_x,s'}(R_i - \hat{x}/2) + n_{d,s}(R_i) n_{p_y,s'}(R_i + \hat{y}/2) \\ & + n_{d,s}(R_i) n_{p_y,s'}(R_i - \hat{y}/2)] \\ & + V_{pp} \sum_{R_i, s, s'} [n_{p_x,s}(R_i + \hat{x}/2) n_{p_y,s'}(R_i + \hat{y}/2) + n_{p_x,s}(R_i + \hat{x}/2) n_{p_y,s'}(R_i - \hat{y}/2) \\ & + n_{p_x,s}(R_i - \hat{x}/2) n_{p_y,s'}(R_i + \hat{y}/2) + n_{p_x,s}(R_i - \hat{x}/2) n_{p_y,s'}(R_i - \hat{y}/2)] \end{aligned}$$

where $n_{\alpha,s}(R_i) = c_{\alpha,s}^\dagger(R_i)c_{\alpha,s}(R_i)$ is the density operator. The summation is taken over all spin states (s, s') and all real space positions.

3 Fourier transform noninteracting term to momentum space (lattice)

Prompt: You will be instructed to convert the noninteracting Hamiltonian \mathcal{H}_0 in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to $c_{\alpha,s}^\dagger(R_i)$ in the real space to the $c_{\alpha,s}^\dagger(k)$ in the momentum space, which is defined as

$c_{\alpha,s}^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_{\alpha,s}^\dagger(R_i) e^{ik \cdot R_i}$, where i is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. You should recall that $H_0 = -t_{pd} \sum_{R_i,s} (c_{d,s}^\dagger(R_i) c_{p_x,s}(R_i + \hat{x}/2) + c_{p_x,s}^\dagger(R_i + \hat{x}/2) c_{d,s}(R_i) + c_{d,s}^\dagger(R_i) c_{p_y,s}(R_i - \hat{x}/2) + c_{p_y,s}^\dagger(R_i - \hat{x}/2) c_{d,s}(R_i) + c_{d,s}^\dagger(R_i) c_{p_y,s}(R_i + \hat{y}/2) + c_{p_y,s}^\dagger(R_i + \hat{y}/2) c_{d,s}(R_i) + c_{d,s}^\dagger(R_i) c_{p_x,s}(R_i - \hat{y}/2) + c_{p_x,s}^\dagger(R_i - \hat{y}/2) c_{d,s}(R_i)) - t_{pp} \sum_{R_i,s} (c_{p_x,s}^\dagger(R_i + \hat{x}/2) c_{p_y,s}(R_i + \hat{y}/2) + c_{p_y,s}^\dagger(R_i + \hat{y}/2) c_{p_x,s}(R_i + \hat{x}/2) + c_{p_x,s}^\dagger(R_i + \hat{x}/2) c_{p_y,s}(R_i - \hat{y}/2) + c_{p_y,s}^\dagger(R_i - \hat{y}/2) c_{p_x,s}(R_i + \hat{x}/2) + c_{p_x,s}^\dagger(R_i - \hat{x}/2) c_{p_y,s}(R_i + \hat{y}/2) + c_{p_y,s}^\dagger(R_i + \hat{y}/2) c_{p_x,s}(R_i - \hat{x}/2) + c_{p_x,s}^\dagger(R_i - \hat{x}/2) c_{p_y,s}(R_i - \hat{y}/2) + c_{p_y,s}^\dagger(R_i - \hat{y}/2) c_{p_x,s}(R_i - \hat{x}/2))$ Express the total noninteracting Hamiltonian \mathcal{H}_0 in terms of $c_{\alpha,s}^\dagger(k)$. 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): $c_{\alpha,s}(k)$: electron annihilation operator at momentum k , spin s and orbital α $c_{\alpha,s}^\dagger(k)$: electron creation operator at momentum k , spin s and orbital α N : number of the unit cells in the real space

EXAMPLE: Write a Kinetic Hamiltonian \hat{H} in the second quantized form in the real space, $\hat{H} = \sum_{i,j} t(R_i - R_j) c^\dagger(R_i) c(R_j)$, where i, j are summed over the entire real space. Define the Fourier transformation $c^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c^\dagger(R_i) e^{ik \cdot R_i}$, where i is integrated over the entire real space containing N unit cells, N is the number of unit cells. This leads to the inverse Fourier transformation $c^\dagger(R_i) = \frac{1}{\sqrt{N}} \sum_k c^\dagger(k) e^{-ik \cdot R_i}$, where k is first Brillouin zone. Thus, substitute $c^\dagger(R_i)$ and $c(R_j)$ into \hat{H} , we get

$$\begin{aligned} \hat{H} &= \sum_{i,j} t(R_i - R_j) \frac{1}{\sqrt{N}} \sum_{k_1} c^\dagger(k_1) e^{-ik_1 \cdot R_i} \frac{1}{\sqrt{N}} \sum_{k_2} c(k_2) e^{ik_2 \cdot R_j} \\ &= \frac{1}{N} \sum_{i,j} \sum_{k_1,k_2} c^\dagger(k_1) c(k_2) e^{-ik_1 \cdot R_i} e^{ik_2 \cdot R_j} t(R_i - R_j) \end{aligned} \quad (2)$$

Now make a replacement by defining $n = R_i - R_j$. The Hamiltonian become

$$\hat{H} = \frac{1}{N} \sum_{i,n} \sum_{k_1,k_2} c^\dagger(k_1) c(k_2) t(n) e^{-i(k_1 - k_2) \cdot R_i} e^{-ik_2 \cdot n} \quad (3)$$

Because $\frac{1}{N} \sum_i e^{-i(k_1 - k_2) \cdot R_i} = \delta(k_1, k_2)$, where $\delta(k_1, k_2)$ is the Kronecker delta function. therefore

$$\hat{H} = \sum_{k_1,k_2} \sum_n t(n) e^{-ik_2 \cdot n} c^\dagger(k_1) c(k_2) \delta(k_1, k_2) \quad (4)$$

Using the property of Kronecker delta function and sum over k_2 , we obtain

$$\hat{H} = \sum_{k_1} \sum_n t(n) e^{-ik_1 \cdot n} c^\dagger(k_1) c(k_1) \quad (5)$$

For simplicity, we replace k_1 with k , we obtain

$$\hat{H} = \sum_k \sum_n t(n) e^{-ik \cdot n} c^\dagger(k) c(k) \quad (6)$$

If we define energy dispersion $E(k) = \sum_n t(n) e^{-ik \cdot n}$, where n is the summation of all hopping pairs, the Hamiltonian in the momentum space is

$$\hat{H} = \sum_k E(k) c^\dagger(k) c(k) \quad (7)$$

Completion: To convert the noninteracting Hamiltonian \mathcal{H}_0 from the basis in real space to the basis in momentum space, we apply the Fourier transformation to $c_{\alpha,s}^\dagger(R_i)$ and $c_{\alpha,s}(R_i)$ in the real space.

The Fourier transformations are defined as:

$$c_{\alpha,s}^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_{\alpha,s}^\dagger(R_i) e^{ik \cdot R_i}$$

$$c_{\alpha,s}(k) = \frac{1}{\sqrt{N}} \sum_i c_{\alpha,s}(R_i) e^{-ik \cdot R_i}$$

The inverse Fourier transformations are:

$$c_{\alpha,s}^\dagger(R_i) = \frac{1}{\sqrt{N}} \sum_k c_{\alpha,s}^\dagger(k) e^{-ik \cdot R_i}$$

$$c_{\alpha,s}(R_i) = \frac{1}{\sqrt{N}} \sum_k c_{\alpha,s}(k) e^{ik \cdot R_i}$$

Substituting these into \mathcal{H}_0 , we get:

$$\begin{aligned} \mathcal{H}_0 = & -t_{pd} \sum_{k_1, k_2, s} (c_{d,s}^\dagger(k_1) c_{p_x,s}(k_2) e^{-ik_2 \cdot \hat{x}/2} + c_{p_x,s}^\dagger(k_1) c_{d,s}(k_2) e^{ik_1 \cdot \hat{x}/2} + c_{d,s}^\dagger(k_1) c_{p_y,s}(k_2) e^{-ik_2 \cdot \hat{y}/2} + \\ & c_{p_y,s}^\dagger(k_1) c_{d,s}(k_2) e^{ik_1 \cdot \hat{y}/2}) \\ & -t_{pp} \sum_{k_1, k_2, s} (c_{p_x,s}^\dagger(k_1) c_{p_y,s}(k_2) e^{-ik_2 \cdot \hat{y}/2} e^{ik_1 \cdot \hat{x}/2} + c_{p_y,s}^\dagger(k_1) c_{p_x,s}(k_2) e^{-ik_2 \cdot \hat{x}/2} e^{ik_1 \cdot \hat{y}/2}) \end{aligned}$$

Using the property of Kronecker delta function $\frac{1}{N} \sum_i e^{-i(k_1 - k_2) \cdot R_i} = \delta(k_1, k_2)$, we can simplify the Hamiltonian to:

$$\begin{aligned} \mathcal{H}_0 = & -t_{pd} \sum_{k,s} (c_{d,s}^\dagger(k) c_{p_x,s}(k) e^{-ik \cdot \hat{x}/2} + c_{p_x,s}^\dagger(k) c_{d,s}(k) e^{ik \cdot \hat{x}/2} + c_{d,s}^\dagger(k) c_{p_y,s}(k) e^{-ik \cdot \hat{y}/2} + \\ & c_{p_y,s}^\dagger(k) c_{d,s}(k) e^{ik \cdot \hat{y}/2}) \\ & -t_{pp} \sum_{k,s} (c_{p_x,s}^\dagger(k) c_{p_y,s}(k) e^{-ik \cdot \hat{y}/2} e^{ik \cdot \hat{x}/2} + c_{p_y,s}^\dagger(k) c_{p_x,s}(k) e^{-ik \cdot \hat{x}/2} e^{ik \cdot \hat{y}/2}) \end{aligned}$$

This is the noninteracting Hamiltonian \mathcal{H}_0 in the basis of momentum space.

4 Fourier transform interacting term to momentum space (lattice)

Prompt: You will be instructed to convert the interacting Hamiltonian, \mathcal{H}_{int} , in the second-quantized form the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to $c_{\alpha,s}^\dagger(R_i)$ in the real space to the $c_{\alpha,s}^\dagger(k)$ in the momentum space, which is defined as $c_{\alpha,s}^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_{\alpha,s}^\dagger(R_i) e^{ik \cdot R_i}$, where i is integrated over all sites in the entire real space, and k is defined within the first Brillouin zone. You should follow the EXAMPLE below to apply the Fourier transformation. Note that interaction have no position dependence now You should recall that \mathcal{H}_{int} is $U_d \sum_{R_i} n_{d,\uparrow}(R_i) n_{d,\downarrow}(R_i) + \frac{U_p}{2} \sum_{R_i} [n_{p_x,\uparrow}(R_i + \hat{x}/2) n_{p_x,\downarrow}(R_i + \hat{x}/2) + n_{p_y,\uparrow}(R_i + \hat{y}/2) n_{p_y,\downarrow}(R_i + \hat{y}/2)] + V_{pd} \sum_{R_i, s, s'} [n_{d,s}(R_i) n_{p_x,s'}(R_i + \hat{x}/2) + n_{d,s}(R_i) n_{p_x,s'}(R_i -$

$\hat{x}/2) + n_{d,s}(R_i)n_{p_y,s'}(R_i + \hat{y}/2) + n_{d,s}(R_i)n_{p_y,s'}(R_i - \hat{y}/2)] + V_{pp} \sum_{R_i, s, s'} \sum_{\sigma_x, \sigma_y} n_{p_x, s}(R_i + \sigma_x \hat{x}/2) n_{p_y, s'}(R_i + \sigma_y \hat{y}/2)$, where σ_x and σ_y both take value of ± 1 . Express \mathcal{H}_{int} in terms of $c_{\alpha, s}^\dagger(k)$. Simplify any summation index if possible.

EXAMPLE: Write an interacting Hamiltonian \hat{H}^{int} in the second quantized form in the real space, $\hat{H}^{int} = \sum_{s, s'} \sum_{i, j} U(R_i - R_j) c_s^\dagger(R_i) c_{s'}^\dagger(R_j) c_{s'}(R_j) c_s(R_i)$, where i, j are summed over the entire real space. Define the Fourier transformation $c_s^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_s^\dagger(R_i) e^{ik \cdot R_i}$, where i is integrated over the entire real space containing N unit cells, N is the number of unit cells. This leads to the inverse Fourier transformation $c_s^\dagger(R_i) = \frac{1}{\sqrt{N}} \sum_k c_s^\dagger(k) e^{-ik \cdot R_i}$, where k is summed over the first Brillouin zone. Thus, substitute $c^\dagger(R_i)$ and $c(R_j)$ into \hat{H}^{int} , we get

$$\begin{aligned} \hat{H}^{int} &= \sum_{s, s'} \sum_{i, j} U(R_i - R_j) \frac{1}{\sqrt{N}} \sum_{k_1} c_s^\dagger(k_1) e^{-ik_1 \cdot R_i} \frac{1}{\sqrt{N}} \sum_{k_2} c_{s'}^\dagger(k_2) e^{-ik_2 \cdot R_j} \frac{1}{\sqrt{N}} \sum_{k_3} c_{s'}(k_3) e^{ik_3 \cdot R_j} \frac{1}{\sqrt{N}} \sum_{k_4} c_s(k_4) e^{ik_4 \cdot R_i} \\ &= \sum_{s, s'} \sum_{i, j} \frac{1}{N^2} \sum_{k_1, k_2, k_3, k_4} U(R_i - R_j) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) e^{-i(k_1 - k_4) \cdot R_i} e^{-i(k_2 - k_3) \cdot R_j} \end{aligned} \quad (8)$$

Now make a replacement by defining $n = R_i - R_j$ The Hamiltonian become

$$\begin{aligned} \hat{H}^{int} &= \frac{1}{N^2} \sum_{j, n} \sum_{s, s'} \sum_{k_1, k_2, k_3, k_4} U(n) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) e^{-i(k_1 - k_4) \cdot n} e^{-i(k_1 - k_4 + k_2 - k_3) \cdot r_j} \end{aligned} \quad (9)$$

Because $\frac{1}{N} \sum_i e^{-i(k_1 - k_4 + k_2 - k_3) \cdot R_i} = \sum_G \delta(k_1 - k_4 + k_2 - k_3, G)$, where $\delta(\dots)$ is the Kronecker delta function, and G is the all reciprocal lattices in the momentum space. Therefore,

$$\begin{aligned} \hat{H}^{int} &= \frac{1}{N} \sum_{s, s'} \sum_{k_1, k_2, k_3, k_4} \sum_n U(n) e^{-i(k_1 - k_4) \cdot n} c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(k_1 - k_4 + k_2 - k_3, G) \end{aligned} \quad (10)$$

If we define interaction in the momentum space $U(k) = \sum_n U(n) e^{-ik \cdot n}$, where n is the summation of all hopping pairs, the interacting Hamiltonian in the momentum space is

$$\begin{aligned} \hat{H}^{int} &= \frac{1}{N} \sum_{s, s'} \sum_{k_1, k_2, k_3, k_4} U(k_1 - k_4) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(k_1 - k_4 + k_2 - k_3, G) \end{aligned} \quad (11)$$

Completion: To convert the interacting Hamiltonian \mathcal{H}_{int} from real space to momentum space, we first apply the Fourier transformation to the creation

and annihilation operators in the real space. The Fourier transformation of the creation operator $c_{\alpha,s}^\dagger(R_i)$ and the annihilation operator $c_{\alpha,s}(R_i)$ are given by:

$$c_{\alpha,s}^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_{\alpha,s}^\dagger(R_i) e^{ik \cdot R_i}$$

$$c_{\alpha,s}(k) = \frac{1}{\sqrt{N}} \sum_i c_{\alpha,s}(R_i) e^{-ik \cdot R_i}$$

Substituting these into \mathcal{H}_{int} , we get:

$$\begin{aligned} \mathcal{H}_{\text{int}} = & U_d \sum_{k_1, k_2} c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_1) c_{d,\downarrow}^\dagger(k_2) c_{d,\downarrow}(k_2) + \frac{U_p}{2} \sum_{k_1, k_2} [c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_1) c_{p_x,\downarrow}^\dagger(k_2) c_{p_x,\downarrow}(k_2) + \\ & c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_1) c_{p_y,\downarrow}^\dagger(k_2) c_{p_y,\downarrow}(k_2)] + V_{pd} \sum_{k_1, k_2, k_3, k_4} [c_{d,s}^\dagger(k_1) c_{d,s}(k_1) c_{p_x,s'}^\dagger(k_2) c_{p_x,s'}(k_2) + \\ & c_{d,s}^\dagger(k_1) c_{d,s}(k_1) c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_3) + c_{d,s}^\dagger(k_1) c_{d,s}(k_1) c_{p_y,s'}^\dagger(k_2) c_{p_y,s'}(k_2) + c_{d,s}^\dagger(k_1) c_{d,s}(k_1) c_{p_y,s'}^\dagger(k_4) c_{p_y,s'}(k_4)] + \\ & V_{pp} \sum_{k_1, k_2, k_3, k_4} c_{p_x,s}^\dagger(k_1) c_{p_x,s}(k_1) c_{p_y,s'}^\dagger(k_2) c_{p_y,s'}(k_2) \end{aligned}$$

The summation indices k_1, k_2, k_3, k_4 are defined within the first Brillouin zone. The interaction terms are now expressed in terms of the creation and annihilation operators in the momentum space. The interaction strengths U_d, U_p, V_{pd}, V_{pp} are constants and do not depend on the position or momentum.

5 Wick's theorem expansion

Prompt: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, \hat{H}^{int} . You should use Wick's theorem to expand the four-fermion term in \hat{H}^{int} 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} is $\frac{U_d}{N} \sum_{k_1, k_2, k_3, k_4} c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_2) c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) + \frac{U_p}{2N} \sum_{k_1, k_2, k_3, k_4} \{c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) + c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_2) c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\downarrow}(k_4) \sum_G \delta(k_1 - k_2 + k_3 - k_4, G)\} + 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1, k_2, k_3, k_4} [c_{d,s}^\dagger(k_1) c_{d,s}(k_2) c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \cos(\frac{k_3 - k_4}{2} \cdot \hat{x}) + c_{d,s}^\dagger(k_1) c_{d,s}(k_2) c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \cos(\frac{k_3 - k_4}{2} \cdot \hat{y})] + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x, \sigma_y} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_2 - k_1 + k_4 - k_3, G) e^{-i(k_1 - k_2) \cdot \sigma_x \hat{x} / 2 - i(k_3 - k_4) \cdot \sigma_y \hat{y} / 2} c_{p_x,s}^\dagger(k_1) c_{p_x,s}(k_2) c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4)$. turn the expanded interaction term after Hartree-Fock approximation as $\hat{H}^{int, HF}$.

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): $\langle c_{\alpha,s}^\dagger(k_1) c_{\alpha',s'}(k_2) \rangle$: expectation of $c_{\alpha,s}^\dagger(k_1) c_{\alpha',s'}(k_2)$ over the many-body ground states

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 $a_1^\dagger a_2^\dagger a_3 a_4 = \langle a_1^\dagger a_4 \rangle a_2^\dagger a_3 + \langle a_2^\dagger a_3 \rangle a_1^\dagger a_4 - \langle a_1^\dagger a_3 \rangle a_2^\dagger a_4 - \langle a_2^\dagger a_4 \rangle a_1^\dagger a_3 + \langle a_1^\dagger a_3 \rangle \langle a_2^\dagger a_4 \rangle$. 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{H}^{int} can be expanded using the Hartree-Fock approximation and Wick's theorem as follows:

$$\begin{aligned} \hat{H}^{int,HF} = & \frac{U_d}{N} \sum_{k_1, k_2, k_3, k_4} \left[\langle c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_2) \rangle c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) + \langle c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) \rangle c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_2) - \langle c_{d,\uparrow}^\dagger(k_1) c_{d,\downarrow}^\dagger(k_3) \rangle c_{d,\uparrow}(k_2) c_{d,\downarrow}(k_4) \right. \\ & + \frac{U_p}{2N} \sum_{k_1, k_2, k_3, k_4} \left[\langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) \rangle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) + \langle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) \rangle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) - \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\downarrow}^\dagger(k_3) \rangle c_{p_x,\uparrow}(k_2) c_{p_x,\downarrow}(k_4) \right. \\ & + \frac{U_p}{2N} \sum_{k_1, k_2, k_3, k_4} \left[\langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_2) \rangle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\downarrow}(k_4) + \langle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\downarrow}(k_4) \rangle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_2) - \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\downarrow}^\dagger(k_3) \rangle c_{p_y,\uparrow}(k_2) c_{p_y,\downarrow}(k_4) \right. \\ & + 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1, k_2, k_3, k_4} \left[\langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) \right. \\ & \left. \left. + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x, \sigma_y} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_2 - k_1 + k_4 - k_3, G) e^{-i(k_1 - k_2) \cdot \sigma_x \hat{x}/2 - i(k_3 - k_4) \cdot \sigma_y \hat{y}/2} \left[\langle c_{p_x,s}^\dagger(k_1) c_{p_x,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \right. \right. \right. \end{aligned}$$

Here, the order of the indices and the signs before each term have been carefully considered according to the examples provided.

6 Drop constant terms

Prompt: You will be instructed to extract the quadratic terms in the \mathcal{H}_{MF} . The quadratic terms mean terms that are proportional to $c^\dagger c$, which excludes terms that are solely expectations or products of expectations. You should only preserve the quadratic terms in \mathcal{H}_{MF} , denoted as $\hat{H}^{int,HF}$. You should recall that \mathcal{H}_{MF} is

$$\begin{aligned} & \frac{U_d}{N} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left[\langle c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_2) \rangle c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) + \right. \\ & \langle c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) \rangle c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_2) - \langle c_{d,\uparrow}^\dagger(k_1) c_{d,\downarrow}^\dagger(k_3) \rangle \langle c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) \rangle - \langle c_{d,\uparrow}^\dagger(k_1) c_{d,\downarrow}^\dagger(k_4) \rangle \langle c_{d,\downarrow}^\dagger(k_3) c_{d,\uparrow}(k_2) \rangle - \\ & \langle c_{d,\downarrow}^\dagger(k_3) c_{d,\uparrow}(k_2) \rangle \langle c_{d,\uparrow}^\dagger(k_1) c_{d,\downarrow}(k_4) \rangle + \langle c_{d,\uparrow}^\dagger(k_1) c_{d,\downarrow}(k_4) \rangle \langle c_{d,\downarrow}^\dagger(k_3) c_{d,\uparrow}(k_2) \rangle \left. \right] + \frac{U_p}{2N} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_1 - \\ & k_2 + k_3 - k_4, G) \left\{ \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) \rangle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) + \langle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) \rangle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) - \right. \\ & \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) \rangle \langle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) \rangle - \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\downarrow}^\dagger(k_4) \rangle \langle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\uparrow}(k_2) \rangle - \\ & \langle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\uparrow}(k_2) \rangle \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\downarrow}(k_4) \rangle + \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\downarrow}(k_4) \rangle \langle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\uparrow}(k_2) \rangle + \\ & \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_2) \rangle \langle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\downarrow}(k_4) \rangle + \langle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\downarrow}(k_4) \rangle \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_2) \rangle - \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_2) \rangle \langle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\downarrow}(k_4) \rangle - \\ & \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\downarrow}(k_4) \rangle \langle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\uparrow}(k_2) \rangle - \langle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\uparrow}(k_2) \rangle \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\downarrow}(k_4) \rangle + \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\downarrow}(k_4) \rangle \langle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\uparrow}(k_2) \rangle \left. \right\} \\ & + 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left[\langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \right. \\ & \langle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \rangle \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) - \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle \langle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) - \\ & \langle c_{d,s}^\dagger(k_1) c_{p_x,s'}^\dagger(k_4) \rangle \langle c_{p_x,s'}^\dagger(k_3) c_{d,s}(k_2) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) - \langle c_{p_x,s'}^\dagger(k_3) c_{d,s}(k_2) \rangle \langle c_{d,s}^\dagger(k_1) c_{p_x,s'}^\dagger(k_4) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \\ & \langle c_{d,s}^\dagger(k_1) c_{p_x,s'}^\dagger(k_4) \rangle \langle c_{p_x,s'}^\dagger(k_3) c_{d,s}(k_2) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle \langle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\ & \langle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \rangle \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) - \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle \langle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) - \\ & \langle c_{d,s}^\dagger(k_1) c_{p_y,s'}^\dagger(k_4) \rangle \langle c_{p_y,s'}^\dagger(k_3) c_{d,s}(k_2) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) - \langle c_{p_y,s'}^\dagger(k_3) c_{d,s}(k_2) \rangle \langle c_{d,s}^\dagger(k_1) c_{p_y,s'}^\dagger(k_4) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\ & \langle c_{d,s}^\dagger(k_1) c_{p_y,s'}^\dagger(k_4) \rangle \langle c_{p_y,s'}^\dagger(k_3) c_{d,s}(k_2) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) \left. \right] + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x, \sigma_y} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_2 - \end{aligned}$$

$$k_1+k_4-k_3, G)e^{-i(k_1-k_2)\cdot\sigma_x\hat{x}/2-i(k_3-k_4)\cdot\sigma_y\hat{y}/2}\times\left[\langle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2)\rangle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4)+\right. \\ \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4)\rangle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2)-\langle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2)\rangle\langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4)\rangle- \\ \left.\langle c_{p_x,s}^\dagger(k_1)c_{p_y,s'}(k_4)\rangle c_{p_y,s'}^\dagger(k_3)c_{p_x,s}(k_2)-\langle c_{p_y,s'}^\dagger(k_3)c_{p_x,s}(k_2)\rangle c_{p_x,s}^\dagger(k_1)c_{p_y,s'}(k_4)+\right. \\ \left.\langle c_{p_x,s}^\dagger(k_1)c_{p_y,s'}(k_4)\rangle\langle c_{p_y,s'}^\dagger(k_3)c_{p_x,s}(k_2)\rangle\right].\text{Return } \hat{H}^{int,HF}.$$

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): $\hat{H}^{int,HF,2}$: the quadratic terms in $\hat{H}^{int,HF}$

Completion: The quadratic terms in $\hat{H}^{int,HF}$, denoted as $\hat{H}^{int,HF,2}$, are those terms that are proportional to $c^\dagger c$ and exclude terms that are solely expectations or products of expectations. From the given \mathcal{H}_{MF} , we can extract the quadratic terms as follows:

$$\begin{aligned} \hat{H}^{int,HF,2} = & \frac{U_d}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) [\langle c_{d,\uparrow}^\dagger(k_1)c_{d,\uparrow}(k_2)\rangle c_{d,\downarrow}^\dagger(k_3)c_{d,\downarrow}(k_4) + \\ & \langle c_{d,\downarrow}^\dagger(k_3)c_{d,\downarrow}(k_4)\rangle c_{d,\uparrow}^\dagger(k_1)c_{d,\uparrow}(k_2) - \langle c_{d,\uparrow}^\dagger(k_1)c_{d,\downarrow}(k_4)\rangle\langle c_{d,\downarrow}^\dagger(k_3)c_{d,\uparrow}(k_2) - \langle c_{d,\downarrow}^\dagger(k_3)c_{d,\uparrow}(k_2)\rangle c_{d,\uparrow}^\dagger(k_1)c_{d,\downarrow}(k_4)] \\ & + \frac{U_p}{2N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) \left\{ \langle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_2)\rangle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\downarrow}(k_4) + \right. \\ & \langle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\downarrow}(k_4)\rangle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_2) - \langle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\downarrow}(k_4)\rangle\langle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\uparrow}(k_2) - \langle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\uparrow}(k_2)\rangle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\downarrow}(k_4) \\ & \langle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\uparrow}(k_2)\rangle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\downarrow}(k_4) + \langle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\downarrow}(k_4)\rangle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\uparrow}(k_2) - \langle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\downarrow}(k_4)\rangle\langle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\uparrow}(k_2) - \\ & \left. \langle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\uparrow}(k_2)\rangle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\downarrow}(k_4) \right\} \\ & + 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) \left[\langle c_{d,s}^\dagger(k_1)c_{d,s}(k_2)\rangle c_{p_x,s'}^\dagger(k_3)c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \right. \\ & \langle c_{p_x,s'}^\dagger(k_3)c_{p_x,s'}(k_4)\rangle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) - \langle c_{d,s}^\dagger(k_1)c_{p_x,s'}(k_4)\rangle\langle c_{p_x,s'}^\dagger(k_3)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) - \\ & \langle c_{p_x,s'}^\dagger(k_3)c_{d,s}(k_2)\rangle c_{d,s}^\dagger(k_1)c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \langle c_{d,s}^\dagger(k_1)c_{d,s}(k_2)\rangle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\ & \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4)\rangle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) - \langle c_{d,s}^\dagger(k_1)c_{p_y,s'}(k_4)\rangle\langle c_{p_y,s'}^\dagger(k_3)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) - \\ & \left. \langle c_{p_y,s'}^\dagger(k_3)c_{d,s}(k_2)\rangle c_{d,s}^\dagger(k_1)c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) \right] \\ & + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x,\sigma_y} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_2-k_1+k_4-k_3, G) e^{-i(k_1-k_2)\cdot\sigma_x\hat{x}/2-i(k_3-k_4)\cdot\sigma_y\hat{y}/2} \times \\ & \left[\langle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2)\rangle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) + \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4)\rangle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2) - \right. \\ & \left. \langle c_{p_x,s}^\dagger(k_1)c_{p_y,s'}(k_4)\rangle c_{p_y,s'}^\dagger(k_3)c_{p_x,s}(k_2) - \langle c_{p_y,s'}^\dagger(k_3)c_{p_x,s}(k_2)\rangle c_{p_x,s}^\dagger(k_1)c_{p_y,s'}(k_4) \right] \end{aligned}$$

This is the final form of $\hat{H}^{int,HF,2}$, which contains only the quadratic terms in $\hat{H}^{int,HF}$.

7 Keep Hartree term

Prompt: You will be instructed to keep only the Hartree term in $\hat{H}^{int,HF,2}$. Here,

Hartree term only means that only the expected value in the form $\langle c_{\alpha_1,s_1}^\dagger(k_1)c_{\alpha_1,s_1}(k_2)\rangle$

(Note that the two indices are the same) should be the preserved. All other expected value terms should be dropped. You should recall that $\hat{H}^{int,HF,2}$

$$\text{is } \frac{U_d}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) [\langle c_{d,\uparrow}^\dagger(k_1)c_{d,\uparrow}(k_2)\rangle c_{d,\downarrow}^\dagger(k_3)c_{d,\downarrow}(k_4) + \\ \langle c_{d,\downarrow}^\dagger(k_3)c_{d,\downarrow}(k_4)\rangle c_{d,\uparrow}^\dagger(k_1)c_{d,\uparrow}(k_2) - \langle c_{d,\uparrow}^\dagger(k_1)c_{d,\downarrow}(k_4)\rangle\langle c_{d,\downarrow}^\dagger(k_3)c_{d,\uparrow}(k_2) - \langle c_{d,\downarrow}^\dagger(k_3)c_{d,\uparrow}(k_2)\rangle c_{d,\uparrow}^\dagger(k_1)c_{d,\downarrow}(k_4) -$$

$$\begin{aligned}
& \langle c_{d,\downarrow}^\dagger(k_3)c_{d,\uparrow}(k_2) \rangle c_{d,\uparrow}^\dagger(k_1)c_{d,\downarrow}(k_4) + \langle c_{d,\uparrow}^\dagger(k_1)c_{d,\downarrow}(k_4) \rangle \langle c_{d,\downarrow}^\dagger(k_3)c_{d,\uparrow}(k_2) \rangle + \frac{U_p}{2N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1 - \\
& k_2 + k_3 - k_4, G) \left\{ \langle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_2) \rangle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\downarrow}(k_4) + \langle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\downarrow}(k_4) \rangle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_2) - \right. \\
& \langle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_2) \rangle \langle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\downarrow}(k_4) \rangle - \langle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\downarrow}(k_4) \rangle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\uparrow}(k_2) - \\
& \langle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\downarrow}(k_4) \rangle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_2) + \langle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\downarrow}(k_4) \rangle \langle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\uparrow}(k_2) \rangle + \\
& \langle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\uparrow}(k_2) \rangle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\downarrow}(k_4) + \langle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\downarrow}(k_4) \rangle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\uparrow}(k_2) - \langle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\uparrow}(k_2) \rangle \langle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\downarrow}(k_4) \rangle \\
& \langle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\downarrow}(k_4) \rangle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\uparrow}(k_2) - \langle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\uparrow}(k_2) \rangle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\downarrow}(k_4) + \langle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\downarrow}(k_4) \rangle \langle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\uparrow}(k_2) \rangle \\
& 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left[\langle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3)c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \right. \\
& \langle c_{p_x,s'}^\dagger(k_3)c_{p_x,s'}(k_4) \rangle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) - \langle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \rangle \langle c_{p_x,s'}^\dagger(k_3)c_{p_x,s'}(k_4) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) - \\
& \langle c_{d,s}^\dagger(k_1)c_{p_x,s'}(k_4) \rangle c_{p_x,s'}^\dagger(k_3)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) - \langle c_{p_x,s'}^\dagger(k_3)c_{d,s}(k_2) \rangle c_{d,s}^\dagger(k_1)c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \\
& \langle c_{d,s}^\dagger(k_1)c_{p_x,s'}(k_4) \rangle \langle c_{p_x,s'}^\dagger(k_3)c_{d,s}(k_2) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \langle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\
& \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \rangle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) - \langle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \rangle \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) - \\
& \langle c_{d,s}^\dagger(k_1)c_{p_y,s'}(k_4) \rangle c_{p_y,s'}^\dagger(k_3)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) - \langle c_{p_y,s'}^\dagger(k_3)c_{d,s}(k_2) \rangle c_{d,s}^\dagger(k_1)c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\
& \langle c_{d,s}^\dagger(k_1)c_{p_y,s'}(k_4) \rangle \langle c_{p_y,s'}^\dagger(k_3)c_{d,s}(k_2) \rangle \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) \Big] + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x,\sigma_y} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_2 - \\
& k_1 + k_4 - k_3, G) e^{-i(k_1-k_2) \cdot \sigma_x \hat{x} / 2 - i(k_3-k_4) \cdot \sigma_y \hat{y} / 2} \times \left[\langle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) + \right. \\
& \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \rangle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2) - \langle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2) \rangle \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \rangle - \\
& \langle c_{p_x,s}^\dagger(k_1)c_{p_y,s'}(k_4) \rangle c_{p_y,s'}^\dagger(k_3)c_{p_x,s}(k_2) - \langle c_{p_y,s'}^\dagger(k_3)c_{p_x,s}(k_2) \rangle c_{p_x,s}^\dagger(k_1)c_{p_y,s'}(k_4) + \\
& \left. \langle c_{p_x,s}^\dagger(k_1)c_{p_y,s'}(k_4) \rangle \langle c_{p_y,s'}^\dagger(k_3)c_{p_x,s}(k_2) \rangle \right] \text{Return the simplified Hamiltonian with} \\
& \hat{H}^{int,Hartree}.
\end{aligned}$$

Completion: The Hartree term in $\hat{H}^{int,HF,2}$ only preserves the expected value in the form $\langle c_{\alpha_1,s_1}^\dagger(k_1)c_{\alpha_1,s_1}(k_2) \rangle$. Therefore, we only keep the terms in the Hamiltonian that match this form and drop all other terms. The simplified Hamiltonian with $\hat{H}^{int,Hartree}$ is then:

$$\begin{aligned}
\hat{H}^{int,Hartree} &= \frac{U_d}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) [\langle c_{d,\uparrow}^\dagger(k_1)c_{d,\uparrow}(k_2) \rangle c_{d,\downarrow}^\dagger(k_3)c_{d,\downarrow}(k_4) + \\
& \langle c_{d,\downarrow}^\dagger(k_3)c_{d,\downarrow}(k_4) \rangle c_{d,\uparrow}^\dagger(k_1)c_{d,\uparrow}(k_2)] + \frac{U_p}{2N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left\{ \langle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_2) \rangle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\downarrow}(k_4) \right. \\
& \langle c_{p_x,\downarrow}^\dagger(k_3)c_{p_x,\downarrow}(k_4) \rangle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_2) + \langle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\uparrow}(k_2) \rangle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\downarrow}(k_4) + \langle c_{p_y,\downarrow}^\dagger(k_3)c_{p_y,\downarrow}(k_4) \rangle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\uparrow}(k_2) \\
& 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left[\langle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3)c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \right. \\
& \langle c_{p_x,s'}^\dagger(k_3)c_{p_x,s'}(k_4) \rangle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \langle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\
& \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \rangle c_{d,s}^\dagger(k_1)c_{d,s}(k_2) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) \Big] + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x,\sigma_y} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_2 - \\
& k_1 + k_4 - k_3, G) e^{-i(k_1-k_2) \cdot \sigma_x \hat{x} / 2 - i(k_3-k_4) \cdot \sigma_y \hat{y} / 2} \times \left[\langle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) + \right. \\
& \left. \langle c_{p_y,s'}^\dagger(k_3)c_{p_y,s'}(k_4) \rangle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_2) \right]
\end{aligned}$$

8 Relabel the index

Prompt: You will be instructed to simplify the quadratic term $\hat{H}^{int,Hartree}$ through relabeling the index. The logic is that the expected value ($\langle c_{\alpha_1,s_1}^\dagger(k_1)c_{\alpha_1,s_1}(k_2) \rangle$)

in the first Hartree term ($\langle c_{\alpha_1, s_1}^\dagger(k_1) c_{\alpha_1, s_1}(k_2) \rangle c_{\alpha_2, s_2}^\dagger(k_3) c_{\alpha_2, s_2}(k_4)$) has the same form as the quadratic operators in the second Hartree term ($\langle c_{\alpha_2, s_2}^\dagger(k_3) c_{\alpha_2, s_2}(k_4) \rangle c_{\alpha_1, s_1}^\dagger(k_1) c_{\alpha_1, s_1}(k_2)$), and vice versa. The same applies to the Fock term. Namely, a replacement of $k_1 \leftrightarrow k_3$ and $k_2 \leftrightarrow k_4$ is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes spin index. This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree or Fock term, you can make the second Hartree or Fock term look identical to the first Hartree or Fock 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 recall that $\hat{H}^{int, Hartree}$ is $\frac{U_d}{N} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left[\langle c_{d, \uparrow}^\dagger(k_1) c_{d, \uparrow}(k_2) \rangle c_{d, \downarrow}^\dagger(k_3) c_{d, \downarrow}(k_4) + \langle c_{d, \downarrow}^\dagger(k_3) c_{d, \downarrow}(k_4) \rangle c_{d, \uparrow}^\dagger(k_1) c_{d, \uparrow}(k_2) \right] + \frac{U_p}{2N} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left\{ \langle c_{p, \uparrow}^\dagger(k_1) c_{p, \uparrow}(k_2) \rangle c_{p, \downarrow}^\dagger(k_3) c_{p, \downarrow}(k_4) + \langle c_{p, \downarrow}^\dagger(k_3) c_{p, \downarrow}(k_4) \rangle c_{p, \uparrow}^\dagger(k_1) c_{p, \uparrow}(k_2) + \langle c_{p, \uparrow}^\dagger(k_1) c_{p, \uparrow}(k_2) \rangle c_{p, \downarrow}^\dagger(k_3) c_{p, \downarrow}(k_4) + \langle c_{p, \downarrow}^\dagger(k_3) c_{p, \downarrow}(k_4) \rangle c_{p, \uparrow}^\dagger(k_1) c_{p, \uparrow}(k_2) \right\} + 2V_{pd} \sum_{s, s'} \frac{1}{N} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left[\langle c_{d, s}^\dagger(k_1) c_{d, s}(k_2) \rangle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \cos\left(\frac{k_3 - k_4}{2} \cdot \hat{x}\right) + \langle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \rangle c_{d, s}^\dagger(k_1) c_{d, s}(k_2) \cos\left(\frac{k_3 - k_4}{2} \cdot \hat{x}\right) + \langle c_{d, s}^\dagger(k_1) c_{d, s}(k_2) \rangle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \cos\left(\frac{k_3 - k_4}{2} \cdot \hat{y}\right) + \langle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \rangle c_{d, s}^\dagger(k_1) c_{d, s}(k_2) \cos\left(\frac{k_3 - k_4}{2} \cdot \hat{y}\right) \right] + 2V_{pd} \sum_{s, s'} \frac{1}{N} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_1 - k_2 + k_3 - k_4, G) \left[\langle c_{d, s}^\dagger(k_1) c_{d, s}(k_2) \rangle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \cos\left(\frac{k_3 - k_4}{2} \cdot \hat{x}\right) + \langle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \rangle c_{d, s}^\dagger(k_1) c_{d, s}(k_2) \cos\left(\frac{k_3 - k_4}{2} \cdot \hat{x}\right) + \langle c_{d, s}^\dagger(k_1) c_{d, s}(k_2) \rangle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \cos\left(\frac{k_3 - k_4}{2} \cdot \hat{y}\right) + \langle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \rangle c_{d, s}^\dagger(k_1) c_{d, s}(k_2) \cos\left(\frac{k_3 - k_4}{2} \cdot \hat{y}\right) \right] + \frac{V_{pp}}{N} \sum_{s, s'} \sum_{\sigma_x, \sigma_y} \sum_{k_1, k_2, k_3, k_4} \sum_G \delta(k_2 - k_1 + k_4 - k_3, G) e^{-i(k_1 - k_2) \cdot \sigma_x \hat{x} / 2 - i(k_3 - k_4) \cdot \sigma_y \hat{y} / 2} \times \left[\langle c_{p, s}^\dagger(k_1) c_{p, s}(k_2) \rangle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) + \langle c_{p, s'}^\dagger(k_3) c_{p, s'}(k_4) \rangle c_{p, s}^\dagger(k_1) c_{p, s}(k_2) \right]$

Return the simplified $\hat{H}^{int, Hartree}$.

EXAMPLE: Given a Hamiltonian $\hat{H} = \sum_{k_1, k_2, k_3, k_4, \sigma_1, \sigma_2, \sigma_3, \sigma_4} V(k_1 - k_4) (\langle c_{d, \sigma_1}^\dagger(k_1) c_{d, \sigma_4}(k_4) \rangle c_{p, \sigma_2}^\dagger(k_2) c_{p, \sigma_3}(k_3) + \langle c_{p, \sigma_2}^\dagger(k_2) c_{d, \sigma_3}(k_3) \rangle c_{d, \sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)) \delta_{k_1 + k_2, k_3 + k_4}$, 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, $\sigma_1 \leftrightarrow \sigma_2$, $\sigma_3 \leftrightarrow \sigma_4$, $k_1 \leftrightarrow k_2$, $k_3 \leftrightarrow k_4$. Important: d and p cannot be swapped because they are not indices in the summation. After the replacement, the second term becomes $\sum_{k_1, k_2, k_3, k_4, \sigma_1, \sigma_2, \sigma_3, \sigma_4} V(k_2 - k_3) \langle c_{p, \sigma_1}^\dagger(k_1) c_{p, \sigma_4}(k_4) \rangle c_{d, \sigma_2}^\dagger(k_2) c_{d, \sigma_3}(k_3) \delta_{k_4 + k_3, k_2 + k_1}$. Note that the Kronecker delta 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 $\sum_{k_1, k_2, k_3, k_4, \sigma_1, \sigma_2, \sigma_3, \sigma_4} V(k_4 - k_1) \langle c_{p, \sigma_1}^\dagger(k_1) c_{p, \sigma_4}(k_4) \rangle c_{d, \sigma_2}^\dagger(k_2) c_{d, \sigma_3}(k_3) \delta_{k_4 + k_3, k_2 + k_1}$. Because $V(q) = V(-q)$, meaning $V(k_4 - k_1) = V(k_1 - k_4)$, the second term further simplifies to $\sum_{k_1, k_2, k_3, k_4, \sigma_1, \sigma_2, \sigma_3, \sigma_4} V(k_1 - k_4) \langle c_{p, \sigma_1}^\dagger(k_1) c_{p, \sigma_4}(k_4) \rangle c_{d, \sigma_2}^\dagger(k_2) c_{d, \sigma_3}(k_3) \delta_{k_4 + k_3, k_2 + k_1}$. Finally, we have the simplified Hamiltonian as $\hat{H} = \sum_{k_1, k_2, k_3, k_4, \sigma_1, \sigma_2, \sigma_3, \sigma_4} V(k_1 - k_4) (\langle c_{d, \sigma_1}^\dagger(k_1) c_{d, \sigma_4}(k_4) \rangle c_{p, \sigma_2}^\dagger(k_2) c_{p, \sigma_3}(k_3) + \langle c_{p, \sigma_1}^\dagger(k_1) c_{p, \sigma_4}(k_4) \rangle c_{d, \sigma_2}^\dagger(k_2) c_{d, \sigma_3}(k_3)) \delta_{k_4 + k_3, k_2 + k_1}$.

Completion: Following the example, we can simplify $\hat{H}^{int, Hartree}$ by relabeling the indices in the second Hartree term of each interaction. The relabeling swaps the indices in the expectation value and the quadratic operators, namely, $k_1 \leftrightarrow k_3$, $k_2 \leftrightarrow k_4$.

After the replacement, the simplified $\hat{H}^{int,Hartree}$ is:

$$\begin{aligned}
\hat{H}^{int,Hartree} = & \frac{U_d}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) \left[\langle c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_2) \rangle c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) + \right. \\
& \langle c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_2) \rangle c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) \Big] \\
& + \frac{U_p}{2N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) \left\{ \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) \rangle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) + \right. \\
& \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) \rangle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) + \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_2) \rangle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\downarrow}(k_4) + \\
& + 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) \left[\langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \right. \\
& \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\
& \left. \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) \right] \\
& + 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) \left[\langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \right. \\
& \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\
& \left. \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) \right] \\
& + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x,\sigma_y} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_2-k_1+k_4-k_3, G) e^{-i(k_1-k_2) \cdot \sigma_x \hat{x}/2 - i(k_3-k_4) \cdot \sigma_y \hat{y}/2} \times \\
& \left[\langle c_{p_x,s}^\dagger(k_1) c_{p_x,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) + \langle c_{p_x,s}^\dagger(k_1) c_{p_x,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \right]
\end{aligned}$$

This is the simplified $\hat{H}^{int,Hartree}$ after relabeling the indices.

9 Identify order parameters in Hartree term

Prompt: You will be instructed to simplify the Hartree term, $\hat{H}^{int,Hartree}$, by reducing the momentum inside the expected value $\langle c_{\alpha_i,s_i}^\dagger(k_i) c_{\alpha_j,s_j}(k_j) \rangle$. The expected value $\langle c_{\alpha_i,s_i}^\dagger(k_i) c_{\alpha_j,s_j}(k_j) \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c_{\alpha_i,s_i}^\dagger(k_i) c_{\alpha_j,s_j}(k_j) \rangle = \langle c_{\alpha_i,s_i}^\dagger(k_i) c_{\alpha_j,s_j}(k_j) \rangle \delta_{k_i,k_j}$. You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i . Once you reduce one momentum inside the expected value $\langle \dots \rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term. You should recall that $\hat{H}^{int,Hartree}$ is $\frac{U_d}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) -$

$$\begin{aligned}
& k_4, G) \left[\langle c_{d,\uparrow}^\dagger(k_1) c_{d,\uparrow}(k_2) \rangle c_{d,\downarrow}^\dagger(k_3) c_{d,\downarrow}(k_4) + \langle c_{d,\downarrow}^\dagger(k_1) c_{d,\downarrow}(k_2) \rangle c_{d,\uparrow}^\dagger(k_3) c_{d,\uparrow}(k_4) \right] + \frac{U_p}{2N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1 - \\
& k_2+k_3-k_4, G) \left\{ \langle c_{p_x,\uparrow}^\dagger(k_1) c_{p_x,\uparrow}(k_2) \rangle c_{p_x,\downarrow}^\dagger(k_3) c_{p_x,\downarrow}(k_4) + \langle c_{p_x,\downarrow}^\dagger(k_1) c_{p_x,\downarrow}(k_2) \rangle c_{p_x,\uparrow}^\dagger(k_3) c_{p_x,\uparrow}(k_4) + \right. \\
& \langle c_{p_y,\uparrow}^\dagger(k_1) c_{p_y,\uparrow}(k_2) \rangle c_{p_y,\downarrow}^\dagger(k_3) c_{p_y,\downarrow}(k_4) + \langle c_{p_y,\downarrow}^\dagger(k_1) c_{p_y,\downarrow}(k_2) \rangle c_{p_y,\uparrow}^\dagger(k_3) c_{p_y,\uparrow}(k_4) \Big\} + \\
& 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_1-k_2+k_3-k_4, G) \left[\langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_x,s'}^\dagger(k_3) c_{p_x,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{x}\right) + \right. \\
& \langle c_{p_x,s}^\dagger(k_1) c_{p_x,s}(k_2) \rangle c_{d,s'}^\dagger(k_3) c_{d,s'}(k_4) \cos\left(\frac{k_1-k_2}{2} \cdot \hat{x}\right) + \langle c_{d,s}^\dagger(k_1) c_{d,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) \cos\left(\frac{k_3-k_4}{2} \cdot \hat{y}\right) + \\
& \left. \langle c_{p_y,s}^\dagger(k_1) c_{p_y,s}(k_2) \rangle c_{d,s'}^\dagger(k_3) c_{d,s'}(k_4) \cos\left(\frac{k_1-k_2}{2} \cdot \hat{y}\right) \right] + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x,\sigma_y} \sum_{k_1,k_2,k_3,k_4} \sum_G \delta(k_2 - \\
& k_1+k_4-k_3, G) e^{-i(k_1-k_2) \cdot \sigma_x \hat{x}/2 - i(k_3-k_4) \cdot \sigma_y \hat{y}/2} \times \left[\langle c_{p_x,s}^\dagger(k_1) c_{p_x,s}(k_2) \rangle c_{p_y,s'}^\dagger(k_3) c_{p_y,s'}(k_4) + \right.
\end{aligned}$$

$\langle c_{p_y,s}^\dagger(k_1)c_{p_y,s}(k_2)\rangle c_{p_x,s'}^\dagger(k_3)c_{p_x,s'}(k_4)\rangle$. Return the final simplified Hartree term $\hat{H}^{int,Hartree}$.

EXAMPLE: Given a Hamiltonian where the Hartree term $\hat{H}^{Hartree} = \sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4) \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4) \rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \sum_G \delta_{k_1+k_2-k_3-k_4,G}$, where k_i is the momentum inside first Brillouin zone, G is the reciprocal lattice vectors, and s_i is a certain index for the degree of freedom other than momentum. Inside the expected value, we realize $\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4) \rangle$ is nonzero only when $k_1 = k_4$, i.e., $\langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4) \rangle = \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4) \rangle \delta_{k_1,k_4}$. Thus, the Hartree term becomes $\sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4) \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_4) \rangle \delta_{k_1,k_4} c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \sum_G \delta_{k_1+k_2-k_3-k_4,G}$. Use the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4 , we have $\sum_{k_1,k_2,k_3,s_1,s_2} V(k_1 - k_1) \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1) \rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \sum_G \delta_{k_1+k_2-k_3-k_1,G} = \sum_{k_1,k_2,k_3,s_1,s_2} V(0) \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1) \rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \sum_G \delta_{k_2-k_3,G}$. Because k_i is momentum inside first Brillouin zone, and the difference between k_2 and k_3 cannot exceed the first shell of reciprocal lattice vector, which means G can only take the value of the origin point in the reciprocal lattice, therefore, $\sum_G \delta_{k_2-k_3,G} = \delta_{k_2-k_3,0}$. Thus, the Hartree term simplifies to $\sum_{k_1,k_2,k_3,s_1,s_2} V(0) \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1) \rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_3) \delta_{k_2-k_3,0} = \sum_{k_1,k_2,s_1,s_2} V(0) \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1) \rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_2)$. Therefore, the final simplified Hartree term after reducing one momentum is $\hat{H}^{Hartree} = \sum_{k_1,k_2,s_1,s_2} V(0) \langle c_{s_1}^\dagger(k_1)c_{s_1}(k_1) \rangle c_{s_2}^\dagger(k_2)c_{s_2}(k_2)$.

Completion: Following the example, we can simplify the Hartree term $\hat{H}^{int,Hartree}$ by reducing the momentum inside the expected value $\langle c_{\alpha_i,s_i}^\dagger(k_i)c_{\alpha_j,s_j}(k_j) \rangle$ and using the total momentum conservation to reduce another momentum in the quadratic term.

The simplified Hartree term $\hat{H}^{int,Hartree}$ is:

$$\begin{aligned} & \frac{U_d}{N} \sum_{k_1,k_2} \left[\langle c_{d,\uparrow}^\dagger(k_1)c_{d,\uparrow}(k_1) \rangle c_{d,\downarrow}^\dagger(k_2)c_{d,\downarrow}(k_2) + \langle c_{d,\downarrow}^\dagger(k_1)c_{d,\downarrow}(k_1) \rangle c_{d,\uparrow}^\dagger(k_2)c_{d,\uparrow}(k_2) \right] \\ & + \frac{U_p}{2N} \sum_{k_1,k_2} \left\{ \langle c_{p_x,\uparrow}^\dagger(k_1)c_{p_x,\uparrow}(k_1) \rangle c_{p_x,\downarrow}^\dagger(k_2)c_{p_x,\downarrow}(k_2) + \langle c_{p_x,\downarrow}^\dagger(k_1)c_{p_x,\downarrow}(k_1) \rangle c_{p_x,\uparrow}^\dagger(k_2)c_{p_x,\uparrow}(k_2) + \right. \\ & \left. \langle c_{p_y,\uparrow}^\dagger(k_1)c_{p_y,\uparrow}(k_1) \rangle c_{p_y,\downarrow}^\dagger(k_2)c_{p_y,\downarrow}(k_2) + \langle c_{p_y,\downarrow}^\dagger(k_1)c_{p_y,\downarrow}(k_1) \rangle c_{p_y,\uparrow}^\dagger(k_2)c_{p_y,\uparrow}(k_2) \right\} \\ & + 2V_{pd} \sum_{s,s'} \frac{1}{N} \sum_{k_1,k_2} \left[\langle c_{d,s}^\dagger(k_1)c_{d,s}(k_1) \rangle c_{p_x,s'}^\dagger(k_2)c_{p_x,s'}(k_2) \cos\left(\frac{k_2-k_1}{2} \cdot \hat{x}\right) + \langle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_1) \rangle c_{d,s'}^\dagger(k_2)c_{d,s'}(k_2) \cos\left(\frac{k_2-k_1}{2} \cdot \hat{y}\right) \right. \\ & \left. + \langle c_{p_y,s}^\dagger(k_1)c_{p_y,s}(k_1) \rangle c_{d,s'}^\dagger(k_2)c_{d,s'}(k_2) \cos\left(\frac{k_2-k_1}{2} \cdot \hat{y}\right) \right] \\ & + \frac{V_{pp}}{N} \sum_{s,s'} \sum_{\sigma_x,\sigma_y} \sum_{k_1,k_2} \left[\langle c_{p_x,s}^\dagger(k_1)c_{p_x,s}(k_1) \rangle c_{p_y,s'}^\dagger(k_2)c_{p_y,s'}(k_2) + \langle c_{p_y,s}^\dagger(k_1)c_{p_y,s}(k_1) \rangle c_{p_x,s'}^\dagger(k_2)c_{p_x,s'}(k_2) \right]. \end{aligned}$$

This is the final simplified Hartree term $\hat{H}^{int,Hartree}$ after reducing one momentum inside the expected value and another momentum in the quadratic term.