

# 1 Identify kinetic term (lattice)

**Prompt:**You will be instructed to describe the kinetic term of Hamiltonian in 3D clusters/unit cells in the real space in the second-quantized form. The degrees of freedom of the system are: orbital  $\alpha$  and spin  $\sigma$ . The kinetic term is a tight-binding model composed of the following hopping process: 1. onsite  $i, \alpha, \sigma$  with  $\epsilon_\alpha$  2. nearest neighbor  $i, \alpha, \sigma$  and  $j, \beta, \sigma$  with  $t_{ij}^{\alpha, \beta}$ . The summation should be taken over all orbital  $\alpha$  and spin  $\sigma$  and all real space positions. Return the Kinetic Hamiltonian  $H_0$ .

Use the following conventions for the symbols:  $\epsilon_\alpha$  is the on-site energy of orbital  $\alpha$ ,  $d_{i, \alpha, \sigma}^\dagger$  and  $d_{i, \alpha, \sigma}$  are the creation and annihilation operators for an electron in orbital  $\alpha$  at site  $i$  with spin  $\sigma$ , and  $t_{ij}^{\alpha, \beta}$  is the hopping amplitude between orbitals  $\alpha$  and  $\beta$  at sites  $i$  and  $j$ .

**Completion:**The kinetic term of the Hamiltonian in the second-quantized form for a 3D cluster/unit cell in real space can be written as:

$$H_0 = \sum_{i, \alpha, \sigma} \epsilon_\alpha d_{i, \alpha, \sigma}^\dagger d_{i, \alpha, \sigma} - \sum_{\langle i, j \rangle, \alpha, \beta, \sigma} t_{ij}^{\alpha, \beta} d_{i, \alpha, \sigma}^\dagger d_{j, \beta, \sigma}$$

The first term represents the on-site energy for an electron in orbital  $\alpha$  at site  $i$  with spin  $\sigma$ . The second term represents the hopping process between nearest neighbor sites  $i$  and  $j$  for electrons in orbitals  $\alpha$  and  $\beta$  with the same spin  $\sigma$ . The symbol  $\langle i, j \rangle$  indicates that the sum is over nearest neighbors. The minus sign in the hopping term is conventional in tight-binding models.

# 2 Identify interacting term (real space)

**Prompt:**You will be instructed to construct the interaction part of the Hamiltonian,  $H_{\text{int}}$  in the real space in the second-quantized form. The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian  $H_0$ . The interaction is a density-density interaction composed of the following process: 1. site  $i, \alpha, \sigma$  and site  $i, \alpha, \sigma'$  with  $U/2$  where  $\sigma \neq \sigma'$  2. site  $i, \alpha, \sigma$  and site  $i, \alpha', \sigma'$  with  $U'/2$ , where  $\alpha \neq \alpha'$  3. Coupling of  $d_{i, \alpha, \sigma}^\dagger d_{i, \alpha', \sigma'}^\dagger d_{i, \alpha, \sigma} d_{i, \alpha', \sigma'}$  with  $J/2$ , 4. Coupling of  $d_{i, \alpha, \sigma}^\dagger d_{i, \alpha, \sigma'}^\dagger d_{i, \alpha, \sigma} d_{i, \alpha', \sigma'}$  with  $J'/2$ , where  $\sigma \neq \sigma'$  and  $\alpha \neq \alpha'$ .

The summation should be taken over all spin and orbital degrees of freedom and all real space positions. Return the interaction term  $H_{\text{int}}$  in terms of  $n_{i, \alpha, \sigma}$ .

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):  $n_{i, \alpha, \sigma} = d_{i, \alpha, \sigma}^\dagger d_{i, \alpha, \sigma}$  where  $d_{i, \alpha, \sigma}^\dagger$  creates a spin- $\sigma$  electron in one of the two  $e_g$  orbitals if  $i$  is a Ni site, or the  $2p_\sigma$  orbital if  $i$  is an O site.

**Completion:**The interaction part of the Hamiltonian,  $H_{\text{int}}$ , in real space in the second-quantized form can be constructed as follows:

$$\begin{aligned} H_{\text{int}} = & \frac{U}{2} \sum_{i, \alpha, \sigma, \sigma'} n_{i, \alpha, \sigma} n_{i, \alpha, \sigma'} - \frac{U}{2} \sum_{i, \alpha} n_{i, \alpha, \uparrow} n_{i, \alpha, \downarrow} + \frac{U'}{2} \sum_{i, \alpha, \alpha', \sigma, \sigma'} n_{i, \alpha, \sigma} n_{i, \alpha', \sigma'} \\ & - \frac{U'}{2} \sum_{i, \alpha, \alpha'} n_{i, \alpha, \uparrow} n_{i, \alpha, \downarrow} n_{i, \alpha', \uparrow} n_{i, \alpha', \downarrow} + \frac{J}{2} \sum_{i, \alpha, \alpha', \sigma, \sigma'} (d_{i, \alpha, \sigma}^\dagger d_{i, \alpha', \sigma'}^\dagger d_{i, \alpha, \sigma} d_{i, \alpha', \sigma'} + d_{i, \alpha', \sigma'}^\dagger d_{i, \alpha, \sigma}^\dagger d_{i, \alpha', \sigma'} d_{i, \alpha, \sigma}) \\ & + \frac{J'}{2} \sum_{i, \alpha, \alpha', \sigma, \sigma'} (d_{i, \alpha, \sigma}^\dagger d_{i, \alpha, \sigma'}^\dagger d_{i, \alpha, \sigma} d_{i, \alpha', \sigma'} + d_{i, \alpha', \sigma'}^\dagger d_{i, \alpha', \sigma}^\dagger d_{i, \alpha', \sigma'} d_{i, \alpha, \sigma}) \end{aligned}$$

Here, the first term represents the interaction between electrons with different spins in the same orbital at the same site. The second term is subtracted to avoid double counting. The third term represents the interaction between electrons in different orbitals at the same site. Again, the fourth term is subtracted to avoid double counting. The fifth term represents the coupling of electrons with different spins and orbitals at the same site. The last term represents the coupling of electrons with different spins in the same orbital but different orbitals at the same site. The summation is taken over all spin and orbital degrees of freedom and all real space positions.

# 3 Fourier transform noninteracting term to momentum space (lattice)

**Prompt:**You will be instructed to convert the noninteracting Hamiltonian  $\hat{H}_0$  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  $d_{i, \alpha, \sigma}^\dagger$  in the real space to the  $d_{\mathbf{k}, \alpha, \sigma}^\dagger$  in the momentum space, which is

defined as  $d_{\mathbf{k},\alpha,\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i d_{i,\alpha,\sigma}^\dagger e^{i\mathbf{k}\cdot\mathbf{R}_i}$ , where  $i$  is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. Note that hopping have no position dependence now. You should recall that  $\hat{H}_0$  is  $H_0 = \sum_{i,\alpha,\sigma} \epsilon_\alpha d_{i,\alpha,\sigma}^\dagger d_{i,\alpha,\sigma} - \sum_{\langle i,j \rangle, \alpha, \beta, \sigma} t_{ij}^{\alpha\beta} d_{i,\alpha,\sigma}^\dagger d_{j,\beta,\sigma}$ . Express the total noninteracting Hamiltonian  $\hat{H}_0$  in terms of  $d_{\mathbf{k},\alpha,\sigma}^\dagger$ . 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):  $H$  is the Hamiltonian,  $\mathbf{k}$  is the momentum,  $\alpha$  and  $\beta$  are the indices for the basis in momentum space,  $\sigma$  is the spin index,  $T_{\alpha,\beta}(\mathbf{k})$  is the Fourier transformation, and  $d_{\mathbf{k},\alpha,\sigma}^\dagger$  and  $d_{\mathbf{k},\beta,\sigma}$  are the creation and annihilation operators in momentum space respectively.

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  $c^\dagger(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_i c^\dagger(R_i) e^{i\mathbf{k}\cdot\mathbf{R}_i}$ , 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  $c^\dagger(R_i) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c^\dagger(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}_i}$ , where  $\mathbf{k}$  is first Brillouin zone. Thus, substitute  $c^\dagger(R_i)$  and  $c(R_j)$  into  $\hat{H}$ , we get

$$\begin{aligned} \hat{H} &= \sum_{i,j} t(R_i - R_j) \frac{1}{\sqrt{N}} \sum_{\mathbf{k}_1} c^\dagger(\mathbf{k}_1) e^{-i\mathbf{k}_1\cdot\mathbf{R}_i} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}_2} c(\mathbf{k}_2) e^{i\mathbf{k}_2\cdot\mathbf{R}_j} \\ &= \frac{1}{N} \sum_{i,j} \sum_{\mathbf{k}_1, \mathbf{k}_2} c^\dagger(\mathbf{k}_1) c(\mathbf{k}_2) e^{-i\mathbf{k}_1\cdot\mathbf{R}_i} e^{i\mathbf{k}_2\cdot\mathbf{R}_j} t(R_i - R_j) \end{aligned}$$

Now make a replacement by defining  $\mathbf{n} = \mathbf{R}_i - \mathbf{R}_j$ . The Hamiltonian become

$$\hat{H} = \frac{1}{N} \sum_{i,n} \sum_{\mathbf{k}_1, \mathbf{k}_2} c^\dagger(\mathbf{k}_1) c(\mathbf{k}_2) t(\mathbf{n}) e^{-i(\mathbf{k}_1 - \mathbf{k}_2)\cdot\mathbf{R}_i} e^{-i\mathbf{k}_2\cdot\mathbf{n}}$$

Because  $\frac{1}{N} \sum_i e^{-i(\mathbf{k}_1 - \mathbf{k}_2)\cdot\mathbf{R}_i} = \delta(\mathbf{k}_1, \mathbf{k}_2)$ , where  $\delta(\mathbf{k}_1, \mathbf{k}_2)$  is the Kronecker delta function. therefore

$$\hat{H} = \sum_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\mathbf{n}} t(\mathbf{n}) e^{-i\mathbf{k}_2\cdot\mathbf{n}} c^\dagger(\mathbf{k}_1) c(\mathbf{k}_2) \delta(\mathbf{k}_1, \mathbf{k}_2)$$

Using the property of Kronecker delta function and sum over  $\mathbf{k}_2$ , we obtain

$$\hat{H} = \sum_{\mathbf{k}_1} \sum_{\mathbf{n}} t(\mathbf{n}) e^{-i\mathbf{k}_1\cdot\mathbf{n}} c^\dagger(\mathbf{k}_1) c(\mathbf{k}_1)$$

For simplicity, we replace  $\mathbf{k}_1$  with  $\mathbf{k}$ , we obtain

$$\hat{H} = \sum_{\mathbf{k}} \sum_{\mathbf{n}} t(\mathbf{n}) e^{-i\mathbf{k}\cdot\mathbf{n}} c^\dagger(\mathbf{k}) c(\mathbf{k})$$

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

$$\hat{H} = \sum_{\mathbf{k}} E(\mathbf{k}) c^\dagger(\mathbf{k}) c(\mathbf{k})$$

**Completion:** Following the example, we first apply the Fourier transformation to the creation and annihilation operators in the noninteracting Hamiltonian  $\hat{H}_0$ :

$$d_{i,\alpha,\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} d_{\mathbf{k},\alpha,\sigma}^\dagger e^{-i\mathbf{k}\cdot\mathbf{R}_i}$$

$$d_{i,\alpha,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} d_{\mathbf{k},\alpha,\sigma} e^{i\mathbf{k}\cdot\mathbf{R}_i}$$

Substitute these into  $\hat{H}_0$ , we get:

$$\hat{H}_0 = \frac{1}{N} \sum_{i,\alpha,\sigma} \epsilon_\alpha \sum_{\mathbf{k}_1} d_{\mathbf{k}_1,\alpha,\sigma}^\dagger e^{-i\mathbf{k}_1\cdot\mathbf{R}_i} \sum_{\mathbf{k}_2} d_{\mathbf{k}_2,\alpha,\sigma} e^{i\mathbf{k}_2\cdot\mathbf{R}_i} - \frac{1}{N} \sum_{\langle i,j \rangle, \alpha, \beta, \sigma} t_{ij}^{\alpha\beta} \sum_{\mathbf{k}_1} d_{\mathbf{k}_1,\alpha,\sigma}^\dagger e^{-i\mathbf{k}_1\cdot\mathbf{R}_i} \sum_{\mathbf{k}_2} d_{\mathbf{k}_2,\beta,\sigma} e^{i\mathbf{k}_2\cdot\mathbf{R}_j}$$

Rearrange the terms, we get:

$$\hat{H}_0 = \frac{1}{N} \sum_{\alpha,\sigma} \sum_{\mathbf{k}_1, \mathbf{k}_2} \epsilon_\alpha d_{\mathbf{k}_1,\alpha,\sigma}^\dagger d_{\mathbf{k}_2,\alpha,\sigma} \sum_i e^{-i(\mathbf{k}_1 - \mathbf{k}_2)\cdot\mathbf{R}_i} - \frac{1}{N} \sum_{\alpha, \beta, \sigma} \sum_{\mathbf{k}_1, \mathbf{k}_2} t_{ij}^{\alpha\beta} d_{\mathbf{k}_1,\alpha,\sigma}^\dagger d_{\mathbf{k}_2,\beta,\sigma} \sum_{\langle i,j \rangle} e^{-i(\mathbf{k}_1\cdot\mathbf{R}_i - \mathbf{k}_2\cdot\mathbf{R}_j)}$$

Using the property of the Kronecker delta function,  $\frac{1}{N} \sum_i e^{-i(\mathbf{k}_1 - \mathbf{k}_2)\cdot\mathbf{R}_i} = \delta(\mathbf{k}_1, \mathbf{k}_2)$ , we obtain:

$$\hat{H}_0 = \sum_{\alpha,\sigma} \sum_{\mathbf{k}} \epsilon_\alpha d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k},\alpha,\sigma} - \sum_{\alpha, \beta, \sigma} \sum_{\mathbf{k}} t_{ij}^{\alpha\beta} d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k},\beta,\sigma} \sum_{\langle i,j \rangle} e^{-i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}$$

If we define the energy dispersion  $E_{\alpha\beta}(\mathbf{k}) = \epsilon_\alpha \delta_{\alpha\beta} - t_{ij}^{\alpha\beta} \sum_{\langle i,j \rangle} e^{-i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}$ , where  $\langle i,j \rangle$  is the summation of all hopping pairs, the noninteracting Hamiltonian in the momentum space is:

$$\hat{H}_0 = \sum_{\alpha, \beta, \sigma} \sum_{\mathbf{k}} E_{\alpha\beta}(\mathbf{k}) d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k},\beta,\sigma}$$

## 4 Fourier transform interacting term to momentum space (lattice)

**Prompt:** You will be instructed to convert the interacting Hamiltonian,  $\hat{H}_{\text{int}}$ , 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  $d_{i,\alpha,\sigma}^\dagger$  in the real space to the  $d_{\mathbf{k},\alpha,\sigma}^\dagger$  in the momentum space, which is defined as  $d_{\mathbf{k},\alpha,\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i d_{i,\alpha,\sigma}^\dagger e^{i\mathbf{k} \cdot \mathbf{R}_i}$ , where  $i$  is integrated over all sites in the entire real space, and  $\mathbf{k}$  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  $\hat{H}_{\text{int}}$  is  $H_{\text{int}} = \sum_{i,\alpha,\sigma \neq \sigma'} \frac{U}{2} n_{i,\alpha,\sigma} n_{i,\alpha,\sigma'} + \sum_{i,\alpha \neq \alpha', \sigma, \sigma'} \frac{U'}{2} n_{i,\alpha,\sigma} n_{i,\alpha',\sigma'} + \sum_{i,\alpha,\alpha', \sigma, \sigma'} \frac{J}{2} d_{i,\alpha,\sigma}^\dagger d_{i,\alpha',\sigma'}^\dagger d_{i,\alpha,\sigma} d_{i,\alpha',\sigma'} + \sum_{i,\alpha \neq \alpha', \sigma \neq \sigma'} \frac{J'}{2} d_{i,\alpha,\sigma}^\dagger d_{i,\alpha,\sigma'}^\dagger d_{i,\alpha',\sigma} d_{i,\alpha',\sigma'}$ . Express  $\hat{H}_{\text{int}}$  in terms of  $d_{\mathbf{k},\alpha,\sigma}^\dagger$ . Simplify any summation index if possible.

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

$$\begin{aligned} \hat{H}^{\text{int}} &= \sum_{s,s'} \sum_{i,j} U(R_i - R_j) \frac{1}{\sqrt{N}} \sum_{k_1} c_s^\dagger(k_1) e^{-i\mathbf{k}_1 \cdot \mathbf{R}_i} \frac{1}{\sqrt{N}} \sum_{k_2} c_{s'}^\dagger(k_2) e^{-i\mathbf{k}_2 \cdot \mathbf{R}_j} \frac{1}{\sqrt{N}} \sum_{k_3} c_{s'}(k_3) e^{i\mathbf{k}_3 \cdot \mathbf{R}_j} \frac{1}{\sqrt{N}} \sum_{k_4} c_s(k_4) e^{i\mathbf{k}_4 \cdot \mathbf{R}_i} \\ &= \sum_{s,s'} \sum_{i,j} \frac{1}{N^2} \sum_{k_1, k_2, k_3, k_4} U(R_i - R_j) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) e^{-i(\mathbf{k}_1 - \mathbf{k}_4) \cdot \mathbf{R}_i} e^{-i(\mathbf{k}_2 - \mathbf{k}_3) \cdot \mathbf{R}_j} \end{aligned}$$

Now make a replacement by defining  $\mathbf{n} = \mathbf{R}_i - \mathbf{R}_j$ . The Hamiltonian become

$$\hat{H}^{\text{int}} = \frac{1}{N^2} \sum_{j,n} \sum_{s,s'} \sum_{k_1, k_2, k_3, k_4} U(\mathbf{n}) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) e^{-i(\mathbf{k}_1 - \mathbf{k}_4) \cdot \mathbf{n}} e^{-i(\mathbf{k}_1 - \mathbf{k}_4 + \mathbf{k}_2 - \mathbf{k}_3) \cdot \mathbf{r}_j}$$

Because  $\frac{1}{N} \sum_i e^{-i(\mathbf{k}_1 - \mathbf{k}_4 + \mathbf{k}_2 - \mathbf{k}_3) \cdot \mathbf{R}_i} = \sum \delta(\mathbf{k}_1 - \mathbf{k}_4 + \mathbf{k}_2 - \mathbf{k}_3, G)$ , where  $\delta(\dots)$  is the Kronecker delta function, and  $G$  is the all reciprocal lattices in the momentum space. Therefore,

$$\hat{H}^{\text{int}} = \frac{1}{N} \sum_{s,s'} \sum_{k_1, k_2, k_3, k_4} \sum_n U(\mathbf{n}) e^{-i(\mathbf{k}_1 - \mathbf{k}_4) \cdot \mathbf{n}} c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(\mathbf{k}_1 - \mathbf{k}_4 + \mathbf{k}_2 - \mathbf{k}_3, G)$$

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

$$\hat{H}^{\text{int}} = \frac{1}{N} \sum_{s,s'} \sum_{k_1, k_2, k_3, k_4} U(\mathbf{k}_1 - \mathbf{k}_4) c_s^\dagger(k_1) c_{s'}^\dagger(k_2) c_{s'}(k_3) c_s(k_4) \sum_G \delta(\mathbf{k}_1 - \mathbf{k}_4 + \mathbf{k}_2 - \mathbf{k}_3, G)$$

**Completion:** To convert the interacting Hamiltonian,  $\hat{H}_{\text{int}}$ , from the real space basis to the momentum space basis, we apply the Fourier transformation to  $d_{i,\alpha,\sigma}^\dagger$  and  $d_{i,\alpha,\sigma}$  in the real space.

The Fourier transformations are defined as:

$$d_{\mathbf{k},\alpha,\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i d_{i,\alpha,\sigma}^\dagger e^{i\mathbf{k} \cdot \mathbf{R}_i}$$

$$d_{\mathbf{k},\alpha,\sigma} = \frac{1}{\sqrt{N}} \sum_i d_{i,\alpha,\sigma} e^{-i\mathbf{k} \cdot \mathbf{R}_i}$$

Substituting these into the expression for  $\hat{H}_{\text{int}}$ , we get:

$$\begin{aligned} \hat{H}_{\text{int}} &= \sum_{\mathbf{k}, \mathbf{k}', \alpha, \sigma \neq \sigma'} \frac{U}{2N} d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}',\alpha,\sigma} d_{\mathbf{k},\alpha,\sigma'}^\dagger d_{\mathbf{k}',\alpha,\sigma'} + \sum_{\mathbf{k}, \mathbf{k}', \alpha \neq \alpha', \sigma, \sigma'} \frac{U'}{2N} d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}',\alpha,\sigma} d_{\mathbf{k},\alpha',\sigma'}^\dagger d_{\mathbf{k}',\alpha',\sigma'} \\ &+ \sum_{\mathbf{k}, \mathbf{k}', \alpha, \alpha', \sigma, \sigma'} \frac{J}{2N} d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k},\alpha',\sigma'}^\dagger d_{\mathbf{k}',\alpha,\sigma} d_{\mathbf{k}',\alpha',\sigma'} + \sum_{\mathbf{k}, \mathbf{k}', \alpha \neq \alpha', \sigma \neq \sigma'} \frac{J'}{2N} d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k},\alpha,\sigma'}^\dagger d_{\mathbf{k}',\alpha',\sigma} d_{\mathbf{k}',\alpha',\sigma'} \end{aligned}$$

The summation over  $\mathbf{k}$  and  $\mathbf{k}'$  is taken over the first Brillouin zone. The interaction terms are now expressed in terms of the creation and annihilation operators in momentum space,  $d_{\mathbf{k},\alpha,\sigma}^\dagger$  and  $d_{\mathbf{k},\alpha,\sigma}$ , respectively.

Note that the interaction terms are now independent of position, as required. The factor of  $1/N$  comes from the normalization of the Fourier transformation.

## 5 Wick's theorem expansion

**Prompt:** You will be instructed to perform a Hartree-Fock approximation to expand the interaction term,  $\hat{H}_{\text{int}}$ . You should use Wick's theorem to expand the four-fermion term in  $\hat{H}_{\text{int}}$  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  $^\dagger$ , 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  $\hat{H}_{\text{int}}$  is  $H = \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(\mathbf{q}) d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} d_{\mathbf{k}+\mathbf{q},\beta,\sigma}$ , where  $U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'} = \frac{U}{2} \delta_{-\sigma,\sigma'} \delta_{\alpha,\alpha'} \delta_{\alpha\beta} \delta_{\alpha\beta'} + \frac{U'}{2} (1 - \delta_{\alpha\alpha'}) \delta_{\alpha\beta} \delta_{\alpha'\beta'} + \frac{J}{2} (1 - \delta_{\alpha\alpha'}) \delta_{\alpha\beta'} \delta_{\alpha'\beta} + \frac{J'}{2} \delta_{\alpha\alpha'} \delta_{\beta\beta'} (1 - \delta_{\sigma\sigma'}) (1 - \delta_{\alpha\beta})$ . Return the expanded interaction term after Hartree-Fock approximation as  $\hat{H}_{\text{int}}^{HF}$ .

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):  $M_{\alpha\beta}(\mathbf{k})$  is the interaction term,  $T_{\alpha,\beta}(\mathbf{k})$  is the kinetic term,  $\langle \rangle$  defines the self-consistent Hartree-Fock fields,  $U_{\beta,\alpha',\alpha,\beta'}^{\sigma\sigma'}$  and  $U_{\alpha',\beta,\beta',\alpha}^{\sigma'\sigma}$  are the interaction terms, and  $d_{\mathbf{q},\alpha',\sigma'}^\dagger$  and  $d_{\mathbf{q},\beta',\sigma'}$  are the creation and annihilation operators respectively.

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  $a_1^\dagger a_2 a_3^\dagger a_4 = \langle a_1^\dagger a_2 \rangle a_3^\dagger a_4 + \langle a_3^\dagger a_4 \rangle a_1^\dagger a_2 - \langle a_1^\dagger a_2 \rangle \langle a_3^\dagger a_4 \rangle - \langle a_1^\dagger a_4 \rangle a_2 a_3^\dagger - \langle a_3^\dagger a_2 \rangle a_1^\dagger a_4 + \langle a_1^\dagger a_4 \rangle \langle a_3^\dagger a_2 \rangle$ . Be cautious about the order of the index and sign before each term here.

**Completion:** Following the instructions and using the conventions provided, we can perform the Hartree-Fock approximation to expand the interaction term  $\hat{H}_{\text{int}}$  using Wick's theorem. The four-fermion term in  $\hat{H}_{\text{int}}$  is similar to the term in EXAMPLE 1, so we will follow that pattern to expand it into quadratic terms.

The interaction term  $\hat{H}_{\text{int}}$  is given by:

$\hat{H}_{\text{int}} = \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(\mathbf{q}) d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} d_{\mathbf{k}+\mathbf{q},\beta,\sigma}$  Applying Wick's theorem and preserving only the normal terms, we get:  $\hat{H}_{\text{int}}^{HF} = \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(\mathbf{q}) [\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} + \langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} - \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle \langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle - \langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle + \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle \langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle]$  This is the expanded interaction term after Hartree-Fock approximation,  $\hat{H}_{\text{int}}^{HF}$ .

## 6 Drop constant terms

**Prompt:** You will be instructed to extract the quadratic terms in the  $\hat{H}_{\text{int}}^{HF}$ . The quadratic terms mean terms that are proportional to  $d_{\mathbf{q},\alpha',\sigma'}^\dagger d_{\mathbf{q},\beta',\sigma'}$ , which excludes terms that are solely expectations or products of expectations. You should only preserve the quadratic terms in  $\hat{H}_{\text{int}}^{HF}$ , denoted as  $\hat{H}_{\text{int}}^{HF,2}$ . You should recall that  $\hat{H}_{\text{int}}^{HF}$  is

$$\hat{H}_{\text{int}}^{HF} = \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(\mathbf{q}) \left[ \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} + \langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} - \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle \langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle - \langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle + \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle \langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle \right]$$

.Return  $\hat{H}_{\text{int}}^{HF,2}$ .

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):  $\mathbf{k}$  is the momentum vector,  $\alpha$  and  $\beta$  are band indices,  $\sigma$  and  $\sigma'$  are spin indices,  $\mathbf{q}$  is the wave vector,  $d_{\mathbf{q},\alpha',\sigma'}^\dagger$  and  $d_{\mathbf{q},\beta',\sigma'}$  are creation and annihilation operators respectively,  $U_{\beta,\alpha',\alpha,\beta'}^{\sigma\sigma'}$  and  $U_{\alpha',\beta,\beta',\alpha}^{\sigma'\sigma}$  are interaction terms, and  $T_{\alpha,\beta}(\mathbf{k})$  is the kinetic term. The average  $\langle \rangle$  defines the self-consistent Hartree-Fock fields.

**Completion:** The quadratic terms in  $\hat{H}_{\text{int}}^{HF}$  are those that are proportional to  $d_{\mathbf{q},\alpha',\sigma'}^\dagger d_{\mathbf{q},\beta',\sigma'}$ , which excludes terms that are solely expectations or products of expectations.

From the given  $\hat{H}_{\text{int}}^{HF}$ , we can see that the quadratic terms are:

$$\hat{H}_{\text{int}}^{HF,2} = \sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(\mathbf{q}) \left[ \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} + \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \right. \\ \left. - \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} - \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \right]$$

This is because these terms contain the creation and annihilation operators  $d_{\mathbf{q}, \alpha', \sigma'}^\dagger$  and  $d_{\mathbf{q}, \beta', \sigma'}$ , and are not solely expectations or products of expectations.

## 7 Identify momentum transfer in interaction

**Prompt:** You will be instructed to expand interaction term  $V(q)$  in the MF quadratic term  $\hat{H}_{\text{int}}^{HF,2}$ . If you find the  $V(q)$  in  $\hat{H}_{\text{int}}^{HF,2}$  does not contain any momentum that is not in the summation sign. The interaction term is already expanded. No action to perform on interaction term. Otherwise, you will expand  $V(q)$  by replacing  $q$  with the momentum  $\mathbf{q}$ . You should recall that  $\hat{H}_{\text{int}}^{HF,2}$  is

$$\hat{H}_{\text{int}}^{HF} = \sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(\mathbf{q}) \left[ \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} + \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \right. \\ \left. - \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} - \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \right]$$

. Return  $\hat{H}_{\text{int}}^{HF,2}$  with expanded interaction.

**Completion:** The interaction term  $V(q)$  in the mean-field quadratic term  $\hat{H}_{\text{int}}^{HF,2}$  does not contain any momentum that is not in the summation sign. Therefore, the interaction term is already expanded and no further action is required. The expanded  $\hat{H}_{\text{int}}^{HF,2}$  is:

$$\hat{H}_{\text{int}}^{HF,2} = \sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(\mathbf{q}) \left[ \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} + \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \right. \\ \left. - \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} - \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \right].$$

## 8 Relabel the index

**Prompt:** You will be instructed to simplify the quadratic term  $\hat{H}_{\text{int}}^{HF,2}$  through relabeling the index. The logic is that the expected value ( $\langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle$ ) in the first Hartree term ( $\langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle$ ) has the same form as the quadratic operators in the second Hartree term ( $d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle$ ), and vice versa. The same applies to the Fock term. Namely, a replacement of  $\alpha$  and  $\alpha'$ ,  $\beta$  and  $\beta'$ ,  $k$  and  $k'$  is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes None. 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  $\hat{H}_{\text{int}}^{HF,2}$  is  $\hat{H}_{\text{int}}^{HF} = \sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(\mathbf{q}) \left[ \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} + \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} - \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \rangle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} - \langle d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+\mathbf{q}, \beta, \sigma} \rangle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-\mathbf{q}, \beta', \sigma'} \right]$ . turn the simplified  $\hat{H}_{\text{int}}^{HF,2}$ .

**EXAMPLE:** Given a Hamiltonian  $\hat{H} = \sum_{k_1, k_2, k_3, k_4, \sigma_1, \sigma_2, \sigma_3, \sigma_4} V(k_1 - k_4) (\langle c_{d, \sigma_1}^\dagger(k_1) c_{d, \sigma_4}(k_4) \rangle c_{p, \sigma_2}^\dagger(k_2) c_{p, \sigma_3}(k_3) + \langle c_{p, \sigma_2}^\dagger(k_2) c_{d, \sigma_3}(k_3) \rangle c_{d, \sigma_1}^\dagger(k_1) c_{d, \sigma_4}(k_4)) \delta_{k_1+k_2, k_3+k_4}$ , 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 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  $\sum_{k_1, k_2, k_3, k_4, \sigma_1, \sigma_2, \sigma_3, \sigma_4} V(k_4 - k_1) \langle c_{p, \sigma_1}^\dagger(k_1) c_{p, \sigma_4}(k_4) \rangle c_{d, \sigma_2}^\dagger(k_2) c_{d, \sigma_3}(k_3) \delta_{k_4+k_3, k_2+k_1}$ . 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:** To simplify the quadratic term  $\hat{H}_{\text{int}}^{HF,2}$ , we can relabel the indices in the second Hartree and Fock terms. We swap  $\alpha$  with  $\alpha'$ ,  $\beta$  with  $\beta'$ , and  $k$  with  $k'$  in the second Hartree and Fock terms.

After the replacement, the second Hartree term becomes  $\langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma}$  and the second Fock term becomes  $\langle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'}$ .

Because  $V(q) = V(-q)$ , the interaction term  $U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(\mathbf{q})$  remains the same after the replacement.

Therefore, the simplified  $\hat{H}_{\text{int}}^{HF,2}$  is:

$$\hat{H}_{\text{int}}^{HF,2} = 2 \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(\mathbf{q}) \left[ \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} - \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \right].$$

This simplification is achieved by making the second Hartree and Fock terms identical to the first Hartree and Fock terms through relabeling the indices.

## 9 Identify order parameters in Hartree term

**Prompt:** You will be instructed to simplify the Hartree term,  $\hat{H}_{\text{int}}^{H,2}$ , by reducing the momentum inside the expected value  $\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle$ . The expected value  $\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle$  is only nonzero when the two momenta  $k_i, k_j$  are the same, namely,  $\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle = \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle \delta_{k_i,0}$ . You should use the property of Kronecker delta function  $\delta_{k_i,k_j}$  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  $\hat{H}_{\text{int}}^{H,2}$  is  $\sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(\mathbf{q}) \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'}$ . Return the final simplified Hartree term  $\hat{H}_{\text{int}}^{H,2}$ .

**EXAMPLE:** Given a Hamiltonian where the Hartree term  $\hat{H}^{\text{Hartree}} = \sum_{k_1,k_2,k_3,k_4,s_1,s_2} V(k_1 - k_4) \langle c_{s_1}^\dagger(k_1) c_{s_1}(k_4) \rangle c_{s_2}^\dagger(k_2) c_{s_2}(k_3) \sum_G \delta_{k_1+k_2-k_3-k_4,G}$ , 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  $\delta_{k_1,k_4}$  to sum over  $k_4$ , we have  $\sum_{k_1,k_2,k_3,s_1,s_2} V(k_1 - k_1) \langle c_{s_1}^\dagger(k_1) c_{s_1}(k_1) \rangle c_{s_2}^\dagger(k_2) c_{s_2}(k_3) \sum_G \delta_{k_1+k_2-k_3-k_1,G} = \sum_{k_1,k_2,k_3,s_1,s_2} V(0) \langle c_{s_1}^\dagger(k_1) c_{s_1}(k_1) \rangle c_{s_2}^\dagger(k_2) c_{s_2}(k_3) \sum_G \delta_{k_2-k_3,G}$ . We can further simplify  $\sum_G \delta_{k_2-k_3,G}$ . 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  $\hat{H}^{\text{Hartree}} = \sum_{k_1,k_2,s_1,s_2} V(0) \langle c_{s_1}^\dagger(k_1) c_{s_1}(k_1) \rangle c_{s_2}^\dagger(k_2) c_{s_2}(k_2)$ .

**Completion:** Following the example, we can simplify the Hartree term  $\hat{H}_{\text{int}}^{H,2}$  by reducing the momentum inside the expected value  $\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle$ .

Given that  $\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle$  is nonzero only when the two momenta  $k_i, k_j$  are the same, we can write

$$\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle = \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle \delta_{\mathbf{q},0}.$$

Substituting this into the Hartree term, we get:

$$\hat{H}_{\text{int}}^{H,2} = \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(\mathbf{q}) \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}+\mathbf{q},\beta,\sigma} \rangle \delta_{\mathbf{q},0} d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'}.$$

Using the property of the Kronecker delta function  $\delta_{\mathbf{q},0}$  to sum over  $\mathbf{q}$ , we get:

$$\hat{H}_{\text{int}}^{H,2} = \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}'} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(0) \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k},\beta,\sigma} \rangle d_{\mathbf{k}',\alpha',\sigma'}^\dagger d_{\mathbf{k}',\beta',\sigma'}.$$

The total momentum conservation will reduce another momentum in the quadratic term, so we end up with only two momenta left in the summation:

$$\hat{H}_{\text{int}}^{H,2} = \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(0) \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k},\beta,\sigma} \rangle d_{\mathbf{k},\alpha',\sigma'}^\dagger d_{\mathbf{k},\beta',\sigma'}.$$

Therefore, the final simplified Hartree term  $\hat{H}_{\text{int}}^{H,2}$  after reducing one momentum is:

$$\hat{H}_{\text{int}}^{H,2} = \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k}} U_{\alpha,\alpha',\beta,\beta'}^{\sigma,\sigma'}(0) \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k},\beta,\sigma} \rangle d_{\mathbf{k},\alpha',\sigma'}^\dagger d_{\mathbf{k},\beta',\sigma'}.$$

## 10 Identify order parameters in Fock term

**Prompt:** You will be instructed to simplify the Fock term in  $\hat{F}_{\text{int}}^{H,2}$  by reducing the momentum inside the expected value  $\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle$ . The expected value  $\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle$  is only nonzero when the two momenta  $k_i, k_j$  are the same, namely,  $\langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle = \langle d_{\mathbf{k},\alpha,\sigma}^\dagger d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} \rangle \delta_{\mathbf{k},\mathbf{k}'-\mathbf{q}}$ . You

should use the property of Kronecker delta function  $\delta_{k_i, k_j}$  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 Fock term, and another momentum in the quadratic term. You should recall that  $\hat{F}_{\text{int}}^{H,2}$  is  $\hat{H}^{\text{H}} \{ \text{rm } \{ \text{int} \} \}^{\text{F}}$  =  $-\sum_{\alpha, \alpha', \beta, \beta'} \sum_{\sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{q}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(\mathbf{q}) \langle c_{\mathbf{k}, \alpha}^\dagger c_{\mathbf{k}+\mathbf{q}, \alpha'} c_{\mathbf{k}, \beta} c_{\mathbf{k}+\mathbf{q}, \beta'} \rangle \langle c_{\mathbf{k}, \alpha}^\dagger c_{\mathbf{k}, \alpha'} c_{\mathbf{k}, \beta} c_{\mathbf{k}, \beta'} \rangle$ . Return the final simplified Fock term  $\hat{F}_{\text{int}}^{H,2}$ .

**EXAMPLE:** Given a Hamiltonian where the Fock term  $\hat{H}^{\text{Fock}} = -\sum_{k_1, k_2, k_3, k_4, s_1, s_2} V(k_1 - k_4) \langle c_{s_1}^\dagger(k_1) c_{s_2}(k_3) \rangle c_{s_2}^\dagger(k_2) c_{s_1}(k_4) \sum_G \delta_{k_1+k_2-k_3-k_4, G}$ , 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  $\langle c_{s_1}^\dagger(k_1) c_{s_2}(k_3) \rangle$  is nonzero only when  $k_1 = k_3$ , i.e.,  $\langle c_{s_1}^\dagger(k_1) c_{s_2}(k_3) \rangle = \langle c_{s_1}^\dagger(k_1) c_{s_2}(k_3) \rangle \delta_{k_1, k_3}$ . Thus, the Fock term becomes  $-\sum_{k_1, k_2, k_3, k_4, s_1, s_2} V(k_1 - k_4) \langle c_{s_1}^\dagger(k_1) c_{s_2}(k_3) \rangle \delta_{k_1, k_3} c_{s_2}^\dagger(k_2) c_{s_1}(k_4) \sum_G \delta_{k_1+k_2-k_3-k_4, G}$ . Use the property of Kronecker delta function  $\delta_{k_1, k_3}$  to sum over  $k_3$ , we have  $-\sum_{k_1, k_2, k_4, s_1, s_2} V(k_1 - k_4) \langle c_{s_1}^\dagger(k_1) c_{s_2}(k_1) \rangle c_{s_2}^\dagger(k_2) c_{s_1}(k_4) \sum_G \delta_{k_2-k_4, G}$ . We can further simplify  $\sum_G \delta_{k_2-k_4, G}$ . Because  $k_i$  is momentum inside first Brillouin zone, and the difference between  $k_2$  and  $k_4$  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,  $\sum_G \delta_{k_2-k_4, G} = \delta_{k_2-k_4, 0}$ . Thus, the Fock term simplifies to  $-\sum_{k_1, k_2, k_4, s_1, s_2} V(k_1 - k_4) \langle c_{s_1}^\dagger(k_1) c_{s_2}(k_1) \rangle c_{s_2}^\dagger(k_2) c_{s_1}(k_4) \delta_{k_2-k_4, 0} = -\sum_{k_1, k_2, s_1, s_2} V(k_1 - k_2) \langle c_{s_1}^\dagger(k_1) c_{s_2}(k_1) \rangle c_{s_2}^\dagger(k_2) c_{s_1}(k_2)$ . Therefore, the final simplified Fock term after reducing one momentum is  $\hat{H}^{\text{Fock}} = -\sum_{k_1, k_2, s_1, s_2} V(k_1 - k_2) \langle c_{s_1}^\dagger(k_1) c_{s_2}(k_1) \rangle c_{s_2}^\dagger(k_2) c_{s_1}(k_2)$ .

**Completion:** Following the example, we can simplify the Fock term  $\hat{F}_{\text{int}}^{H,2}$  by reducing the momentum inside the expected value  $\langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-q, \beta', \sigma'} \rangle$ .

We know that  $\langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-q, \beta', \sigma'} \rangle$  is nonzero only when  $\mathbf{k} = \mathbf{k}' - q$ , i.e.,  $\langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-q, \beta', \sigma'} \rangle = \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-q, \beta', \sigma'} \rangle \delta_{\mathbf{k}, \mathbf{k}'-q}$ .

Substituting this into the Fock term, we get:

$$\hat{F}_{\text{int}}^{H,2} = -\sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{q}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(\mathbf{q}) \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}'-q, \beta', \sigma'} \rangle \delta_{\mathbf{k}, \mathbf{k}'-q} d_{\mathbf{k}', \alpha', \sigma'}^\dagger d_{\mathbf{k}+q, \beta, \sigma}.$$

Using the property of the Kronecker delta function  $\delta_{\mathbf{k}, \mathbf{k}'-q}$  to sum over  $\mathbf{k}'$ , we get:

$$\hat{F}_{\text{int}}^{H,2} = -\sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{q}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(\mathbf{q}) \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}, \beta', \sigma'} \rangle d_{\mathbf{k}, \alpha', \sigma'}^\dagger d_{\mathbf{k}+q, \beta, \sigma}.$$

Finally, we can simplify the term  $\delta_{\mathbf{k}, \mathbf{k}+q}$ , which is nonzero only when  $q = 0$ . Therefore, the final simplified Fock term  $\hat{F}_{\text{int}}^{H,2}$  is:

$$\hat{F}_{\text{int}}^{H,2} = -\sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(0) \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}, \beta', \sigma'} \rangle d_{\mathbf{k}, \alpha', \sigma'}^\dagger d_{\mathbf{k}, \beta, \sigma}.$$

## 11 Final form of iteration in quadratic terms

**Prompt:** You will now be instructed to combine the Hartree term  $\hat{H}_{\text{int}}^{\text{F}}$  and the Fock term  $\hat{F}_{\text{int}}^{\text{F}}$ . You should recall that the Hartree term  $\hat{H}_{\text{int}}^{H,2} = \sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(0) \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}, \beta, \sigma} \rangle d_{\mathbf{k}, \alpha', \sigma'}^\dagger d_{\mathbf{k}, \beta', \sigma'}$ , and the Fock term  $\hat{F}_{\text{int}}^{H,2} = -\sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(0) \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}, \beta', \sigma'} \rangle d_{\mathbf{k}, \alpha', \sigma'}^\dagger d_{\mathbf{k}, \beta, \sigma}$ . 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 Hartree term  $\hat{H}_{\text{int}}^{H,2}$  and the Fock term  $\hat{F}_{\text{int}}^{H,2}$  can be combined by adding them together. However, before adding, we need to relabel the indices in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. Since the question instructs to perform a swap with "Nothing", no actual relabeling is needed.

Therefore, the sum of the Hartree and Fock terms is:

$$\hat{H}_{\text{int}}^{HF,2} = \hat{H}_{\text{int}}^{H,2} + \hat{F}_{\text{int}}^{H,2}$$

Substituting the expressions for  $\hat{H}_{\text{int}}^{H,2}$  and  $\hat{F}_{\text{int}}^{H,2}$ , we get:

$$\hat{H}_{\text{int}}^{HF,2} = \sum_{\alpha, \alpha', \beta, \beta', \sigma, \sigma'} \sum_{\mathbf{k}} U_{\alpha, \alpha', \beta, \beta'}^{\sigma, \sigma'}(0) \left[ \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}, \beta, \sigma} \rangle d_{\mathbf{k}, \alpha', \sigma'}^\dagger d_{\mathbf{k}, \beta', \sigma'} - \langle d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}, \beta', \sigma'} \rangle d_{\mathbf{k}, \alpha', \sigma'}^\dagger d_{\mathbf{k}, \beta, \sigma} \right]$$

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