

# 1 Identify kinetic term (continuum,first-quantized)

**Prompt:**You will be instructed to describe the kinetic term of Hamiltonian in twisted bilayer transition metal dichalcogenides in the real space in the single-particle form.The degrees of freedom of the system are: valley index ( $\tau$ ) and layer index ( $l$ ).Express the Kinetic Hamiltonian  $H_K$  using  $E_{+K,t}$ ,  $E_{+K,b}$ ,  $E_{-K,t}$ ,  $E_{-K,b}$  which are only on the diagonal terms, and arrange the basis in the order of  $(+K,b)$ ,  $(+K,t)$ ,  $(-K,b)$ ,  $(-K,t)$ .

Use the following conventions for the symbols:-  $\Delta_{b/t}$  represents the intralayer and interlayer moiré potentials -  $G_i$  represents the moiré reciprocal lattice vectors -  $\kappa_+$  and  $\kappa_-$  represent the mBZ corners -  $m^*$  represents the effective mass -  $\Delta_D$  represents the layer-differentiating potential proportional to the out-of-plane electric field.

**Completion:**The kinetic term of the Hamiltonian in twisted bilayer transition metal dichalcogenides in the real space in the single-particle form can be written as:

$$H_K = \begin{pmatrix} E_{+K,b} + \Delta_b + \Delta_D & 0 & 0 & 0 \\ 0 & E_{+K,t} + \Delta_t - \Delta_D & 0 & 0 \\ 0 & 0 & E_{-K,b} + \Delta_b + \Delta_D & 0 \\ 0 & 0 & 0 & E_{-K,t} + \Delta_t - \Delta_D \end{pmatrix}$$

Here, the diagonal terms represent the kinetic energy of the electrons in the different valleys and layers. The  $E_{+K,b}$ ,  $E_{+K,t}$ ,  $E_{-K,b}$ , and  $E_{-K,t}$  terms represent the kinetic energy in the  $+K$  and  $-K$  valleys for the bottom (b) and top (t) layers, respectively. The  $\Delta_b$  and  $\Delta_t$  terms represent the intralayer and interlayer moiré potentials for the bottom and top layers, respectively. The  $\Delta_D$  term represents the layer-differentiating potential proportional to the out-of-plane electric field. The off-diagonal terms are zero, indicating no coupling between different valleys and layers in the kinetic term of the Hamiltonian.

# 2 Define energy dispersion (continuum)

**Prompt:**You will be instructed to construct each term, namely  $E_{+K,t}$ ,  $E_{+K,b}$ ,  $E_{-K,t}$ ,  $E_{-K,b}$ .For all energy dispersions,  $E_{+K,t}$ ,  $E_{+K,b}$ ,  $E_{-K,t}$ ,  $E_{-K,b}$ , it characterizes the parabolic dispersion for holes.In addition, a shift of  $\kappa_+$  and  $\kappa_-$  in the momentum  $k$  for  $-\frac{\hbar^2(k-\kappa_+)^2}{2m^*}$  and  $-\frac{\hbar^2(k-\kappa_-)^2}{2m^*}$ , respectively.You should follow the EXAMPLE below to obtain correct energy dispersion, select the correct EXAMPLE by noticing the type of dispersion.Finally, in the real space, the momentum  $k = -i\partial_r$ . You should keep the form of  $k$  in the Hamiltonian for short notations but should remember  $k$  is an operator.You should recall that

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

.Return the expression for  $E_{+K,t}$ ,  $E_{+K,b}$ ,  $E_{-K,t}$ ,  $E_{-K,b}$  in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian  $H_K$ .

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): $k$  is the momentum,  $\kappa_+$  and  $\kappa_-$  are the mBZ corners,  $m^*$  is the effective mass and is taken as  $0.6m_e$ , where  $m_e$  is the free electron mass.

EXAMPLE 1:A parabolic dispersion for electron is  $E_\alpha = \frac{\hbar^2 k^2}{2m_\alpha}$ , where  $\alpha$  indicates the type of electron.

If there is a further shift of  $q$  in the momentum  $k$ , the dispersion will become  $E_\alpha = \frac{\hbar^2(k-q)^2}{2m_\alpha}$ .

EXAMPLE 2: A cos dispersion is  $E_\alpha = -\cos(ka/2)$ , where  $\alpha$  indicates the type of particle. If there is a further shift of  $q$  in the momentum  $k$ , the dispersion will become  $E_\alpha = -\cos((k-q)a/2)$ . However, there could be more prefactors before cos depending on the geometry of the lattice.

EXAMPLE 3:A dirac dispersion for electron/hole is a 2 by 2 matrix, i.e.,  $h_\theta(k) =$

$-\hbar v_D |k| \begin{pmatrix} 0 & e^{i(\theta_k - \theta)} \\ e^{-i(\theta_k - \theta)} & 0 \end{pmatrix}$ , where  $v_D$  is the Fermi velocity,  $\theta$  is the twist angle, and  $\theta_k$  indicates the azimuth angle of  $k$ . If there is a further shift of  $K_\theta$  in the momentum  $k$ , the dispersion will

become  $h_\theta(k) = -\hbar v_D |k - K_\theta| \begin{pmatrix} 0 & e^{i(\theta_k - K_\theta - \theta)} \\ e^{-i(\theta_k - K_\theta - \theta)} & 0 \end{pmatrix}$ .

**Completion:**Given the parabolic dispersion for holes and the shift in momentum, we should follow EXAMPLE 2 to construct the energy dispersion terms  $E_{+K,t}$ ,  $E_{+K,b}$ ,  $E_{-K,t}$ ,  $E_{-K,b}$ .

The energy dispersion terms are constructed as follows:

$$E_{+K,t} = -\frac{\hbar^2(k-\kappa_+)^2}{2m^*}$$

$$\begin{aligned}
E_{+K,b} &= -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} \\
E_{-K,t} &= -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} \\
E_{-K,b} &= -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*}
\end{aligned}$$

Substituting these into the Kinetic Hamiltonian  $H_K$ , we get:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} & 0 & 0 & 0 \\ 0 & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} & 0 & 0 \\ 0 & 0 & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} & 0 \\ 0 & 0 & 0 & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} \end{pmatrix}$$

Remember that in real space, the momentum  $\mathbf{k} = -i\partial_{\mathbf{r}}$ .

### 3 Identify potential term (continuum)

**Prompt:** You will be instructed to describe the potential term of Hamiltonian  $H_P$  in the real space in the single-particle form. The potential Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian. The diagonal terms are  $\Delta_b(\mathbf{r})$  and  $\Delta_t(\mathbf{r})$ . The off-diagonal terms are the coupling between layer index  $l$  and valley index  $\tau$ ,  $\Delta_T(\mathbf{r})$  and  $\Delta_T^\dagger(\mathbf{r})$ , which should be kept hermitian. All other terms are zero. Express the potential Hamiltonian  $H_P$  using  $\Delta_b(\mathbf{r})$  and  $\Delta_t(\mathbf{r})$  and  $\Delta_T(\mathbf{r})$  and  $\Delta_T^\dagger(\mathbf{r})$ . Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): The intralayer and interlayer moiré potentials are  $\Delta_{b/t} = 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} \pm \phi)$  and  $\Delta_T = w(1 + e^{-i\mathbf{G}_2 \cdot \mathbf{r}} + e^{-i\mathbf{G}_3 \cdot \mathbf{r}})$ , respectively.  $\mathbf{G}_i = \frac{4\pi}{\sqrt{3}a_M}(\cos \frac{i-1}{3}\pi, \sin \frac{i-1}{3}\pi)$  are moiré reciprocal lattice vectors with  $a_M$  being the moiré lattice constant.  $\boldsymbol{\kappa}_+ = 2\mathbf{G}_1/3 - \mathbf{G}_2/3$  and  $\boldsymbol{\kappa}_- = \mathbf{G}_1/3 + \mathbf{G}_2/3$  are the mBZ corners.  $m^*$  is the effective mass and is taken as  $0.6m_e$ , where  $m_e$  is the free electron mass. Layer-differentiating potential proportional to  $\Delta_D$  is included in  $H_K$  to take into account the out-of-plane electric field. For  $K'$  valley, the continuum model Hamiltonian can be deduced by acting time reversal operator on  $H_K$ .

**Completion:** The potential Hamiltonian  $H_P$  in the real space in the single-particle form, given the conventions and the instructions, can be written as:

$$H_P = \begin{pmatrix} \Delta_b(\mathbf{r}) & 0 & 0 & \Delta_T(\mathbf{r}) \\ 0 & \Delta_t(\mathbf{r}) & \Delta_T^\dagger(\mathbf{r}) & 0 \\ 0 & \Delta_T(\mathbf{r}) & \Delta_b(\mathbf{r}) & 0 \\ \Delta_T^\dagger(\mathbf{r}) & 0 & 0 & \Delta_t(\mathbf{r}) \end{pmatrix}$$

Here,  $\Delta_b(\mathbf{r})$  and  $\Delta_t(\mathbf{r})$  are the diagonal terms representing the intralayer moiré potentials for the bottom and top layers, respectively.  $\Delta_T(\mathbf{r})$  and  $\Delta_T^\dagger(\mathbf{r})$  are the off-diagonal terms representing the interlayer moiré potentials, ensuring the hermiticity of the Hamiltonian. All other terms are zero, as per the instructions.

### 4 Define potential term (continuum)

**Prompt:** You will be instructed to construct each term  $H_P$ , namely,  $\Delta_{b/t}$ ,  $\Delta_T$ , and  $\Delta_D$ . The expression for diagonal terms are:  $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r})$  and  $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r})$ . The expression for off-diagonal terms are:  $\Delta_T(\mathbf{r})$  and  $\Delta_T^\dagger(\mathbf{r})$ . You should recall that

$$H_P = \begin{pmatrix} \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) & 0 & 0 \\ \Delta_T^\dagger(\mathbf{r}) & \Delta_t(\mathbf{r}) & 0 & 0 \\ 0 & 0 & \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ 0 & 0 & \Delta_T^\dagger(\mathbf{r}) & \Delta_t(\mathbf{r}) \end{pmatrix}$$

. Return the expressions for  $\Delta_{b/t}$ ,  $\Delta_T$ , and  $\Delta_D$ , and substitute it into the potential Hamiltonian  $H_P$ . Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or have conflicts in the conventions, you should stop and let me know):  $\Delta_{b/t} = 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} \pm \phi)$ ,  $\Delta_T = w(1 + e^{-i\mathbf{G}_2 \cdot \mathbf{r}} + e^{-i\mathbf{G}_3 \cdot \mathbf{r}})$ ,  $\mathbf{G}_i = \frac{4\pi}{\sqrt{3}a_M}(\cos \frac{i-1}{3}\pi, \sin \frac{i-1}{3}\pi)$ ,  $\boldsymbol{\kappa}_+ = 2\mathbf{G}_1/3 - \mathbf{G}_2/3$ ,  $\boldsymbol{\kappa}_- = \mathbf{G}_1/3 + \mathbf{G}_2/3$ ,  $m^* = 0.6m_e$ , and  $\Delta_D$  is the layer-differentiating potential.

**Completion:** The expressions for the terms in the potential Hamiltonian  $H_P$  are given as follows:

1. The intralayer moiré potentials for the bottom and top layers are represented by the diagonal terms  $\Delta_b(\mathbf{r})$  and  $\Delta_t(\mathbf{r})$ , respectively. They are given by:

$$\Delta_b(\mathbf{r}) = 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi)$$

$$\Delta_t(\mathbf{r}) = 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} - \phi)$$

2. The interlayer moiré potentials are represented by the off-diagonal terms  $\Delta_T(\mathbf{r})$  and  $\Delta_T^\dagger(\mathbf{r})$ . They are given by:

$$\Delta_T(\mathbf{r}) = w(1 + e^{-i\mathbf{G}_2 \cdot \mathbf{r}} + e^{-i\mathbf{G}_3 \cdot \mathbf{r}})$$

$$\Delta_T^\dagger(\mathbf{r}) = w^*(1 + e^{i\mathbf{G}_2 \cdot \mathbf{r}} + e^{i\mathbf{G}_3 \cdot \mathbf{r}})$$

3. The layer-differentiating potential  $\Delta_D$  is included in  $H_K$  to take into account the out-of-plane electric field. However, the expression for  $\Delta_D$  is not provided in the question or the background information.

Substituting these expressions into the potential Hamiltonian  $H_P$ , we get:

$$H_P = \begin{pmatrix} 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi) & w(1 + e^{-i\mathbf{G}_2 \cdot \mathbf{r}} + e^{-i\mathbf{G}_3 \cdot \mathbf{r}}) & 0 & 0 \\ w^*(1 + e^{i\mathbf{G}_2 \cdot \mathbf{r}} + e^{i\mathbf{G}_3 \cdot \mathbf{r}}) & 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} - \phi) & 0 & 0 \\ 0 & 0 & 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} + \phi) & w(1 + e^{-i\mathbf{G}_2 \cdot \mathbf{r}} + e^{-i\mathbf{G}_3 \cdot \mathbf{r}}) \\ 0 & 0 & w^*(1 + e^{i\mathbf{G}_2 \cdot \mathbf{r}} + e^{i\mathbf{G}_3 \cdot \mathbf{r}}) & 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} - \phi) \end{pmatrix}$$

Please note that the expression for  $\Delta_D$  is not provided, and hence it is not included in the above Hamiltonian.

## 5 Second-quantization (matrix)

**Prompt:** You will be instructed to construct the second quantized form of the total noninteracting Hamiltonian in the real space. The noninteracting Hamiltonian in the real space  $H_0$  is the sum of Kinetic Hamiltonian  $H_K$  and Potential Hamiltonian  $H_P$ . To construct the second quantized form of a Hamiltonian. You should construct the creation and annihilation operators from the basis explicitly. You should follow the EXAMPLE below to convert a Hamiltonian from the single-particle form to second-quantized form. Finally by "total", it means you need to take a summation over the real space position  $r$ . Return the second quantized form of the total noninteracting Hamiltonian  $\hat{H}_0$ .

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):  $H_0$  is the noninteracting Hamiltonian in the real space.

**EXAMPLE:** For a Hamiltonian  $H$ , where  $H = \begin{pmatrix} H_{a,a} & H_{a,b} \\ H_{b,a} & H_{b,b} \end{pmatrix}$  and the order of basis is (a), (b), we can construct the creation operators  $\psi_a^\dagger$  and  $\psi_b^\dagger$ , and the annihilation operator  $\psi_a$  and  $\psi_b$ . The corresponding second quantized form is  $\hat{H} = \vec{\psi}^\dagger H \vec{\psi}$ , where  $\vec{\psi} = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$  and  $\vec{\psi}^\dagger = (\psi_a^\dagger \quad \psi_b^\dagger)$ .

**Completion:** The noninteracting Hamiltonian in the real space  $H_0$  is the sum of Kinetic Hamiltonian  $H_K$  and Potential Hamiltonian  $H_P$ . The order of basis is  $(+K, b)$ ,  $(+K, t)$ ,  $(-K, b)$ ,  $(-K, t)$ . We can construct the creation operators  $\psi_{+K,b}^\dagger$ ,  $\psi_{+K,t}^\dagger$ ,  $\psi_{-K,b}^\dagger$ , and  $\psi_{-K,t}^\dagger$ , and the annihilation operators  $\psi_{+K,b}$ ,  $\psi_{+K,t}$ ,  $\psi_{-K,b}$ , and  $\psi_{-K,t}$ .

The corresponding second quantized form is  $\hat{H}_0 = \vec{\psi}^\dagger H_0 \vec{\psi}$ , where  $\vec{\psi} = \begin{pmatrix} \psi_{+K,b} \\ \psi_{+K,t} \\ \psi_{-K,b} \\ \psi_{-K,t} \end{pmatrix}$  and  $\vec{\psi}^\dagger =$

$$(\psi_{+K,b}^\dagger \quad \psi_{+K,t}^\dagger \quad \psi_{-K,b}^\dagger \quad \psi_{-K,t}^\dagger).$$

Finally, we need to take a summation over the real space position  $r$ . Therefore, the second quantized form of the total noninteracting Hamiltonian  $\hat{H}_0$  is given by:

$$\hat{H}_0 = \sum_{\mathbf{r}} \vec{\psi}^\dagger(\mathbf{r}) H_0 \vec{\psi}(\mathbf{r})$$

## 6 Second-quantization (summation)

**Prompt:** You will be instructed to expand the second-quantized form Hamiltonian  $\hat{H}_0$  using  $H_0$  and  $\psi_{\tau,l}(r)$ . You should follow the EXAMPLE below to expand the Hamiltonian. You should use any previous knowledge to simplify it. For example, if any term of  $H_0$  is zero, you should remove it from the summation. You should recall that  $\hat{H}_0$  is  $\hat{H}_0 = \sum_{\mathbf{r}} \vec{\psi}^\dagger(\mathbf{r}) H_0 \vec{\psi}(\mathbf{r})$ . Return the expanded form of  $\hat{H}_0$  after simplification.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): None

EXAMPLE: For a  $\hat{H} = \vec{\psi}^\dagger H \vec{\psi}$ , where  $\vec{\psi} = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$  and  $\vec{\psi}^\dagger = (\psi_a^\dagger \ \psi_b^\dagger)$ , we can expand it as  $\hat{H} = \sum_{i,j=\{a,b\}} \psi_i^\dagger H_{i,j} \psi_j$ .

**Completion:** Given the second-quantized form of the Hamiltonian  $\hat{H}_0 = \sum_{\mathbf{r}} \vec{\psi}^\dagger(\mathbf{r}) H_0 \vec{\psi}(\mathbf{r})$ ,

where  $\vec{\psi} = \begin{pmatrix} \psi_{+K,b} \\ \psi_{+K,t} \\ \psi_{-K,b} \\ \psi_{-K,t} \end{pmatrix}$  and  $\vec{\psi}^\dagger = (\psi_{+K,b}^\dagger \ \psi_{+K,t}^\dagger \ \psi_{-K,b}^\dagger \ \psi_{-K,t}^\dagger)$ , we can expand it as  $\hat{H}_0 =$

$$\sum_{\mathbf{r}} \sum_{i,j=\{+K,b;+K,t;-K,b;-K,t\}} \psi_i^\dagger(\mathbf{r}) H_{0i,j} \psi_j(\mathbf{r}).$$

Here,  $H_{0i,j}$  are the matrix elements of the Hamiltonian  $H_0$  in the basis  $(+K, b)$ ,  $(+K, t)$ ,  $(-K, b)$ ,  $(-K, t)$ . The specific form of  $H_{0i,j}$  depends on the explicit form of  $H_0$ , which is not provided in the question. If any of the  $H_{0i,j}$  is zero, it should be removed from the summation.

## 7 Fourier transform noninteracting term to momentum space (continuum)

**Prompt:** You will be instructed to convert the total noninteracting Hamiltonian in the second quantized form from the basis in real space to the basis by momentum space. To do that, you should apply the Fourier transformation to  $\psi_{\tau,l}(r)$  in the real space to the  $\psi_{\tau,l}(k)$  in the momentum space, which is defined as  $\psi_{\tau,l}^\dagger(k) = \frac{1}{\sqrt{A}} \int dr \psi_{\tau,l}^\dagger(r) e^{ik \cdot r}$ , where  $r$  is integrated over the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. Express the total noninteracting Hamiltonian  $\hat{H}_0$  in terms of  $\psi_{\tau,l}(k)$ . 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):  $\psi_{l,\tau}(k)$  : electron annihilation operator at momentum  $k$ , layer  $l$ , and valley  $\tau$ ;  $\psi_{l,\tau}^\dagger(k)$  : electron creation operator at momentum  $k$ , layer  $l$ , and valley  $\tau$ ;  $V$  : area of unit cell in the real space

EXAMPLE: Write a Hamiltonian  $\hat{H}$  in the second quantized form,  $\hat{H} = \int dr \psi(r)^\dagger H(r) \psi(r)$ , where  $r$  is integrated over the entire real space. Define the Fourier transformation  $c^\dagger(k) = \frac{1}{\sqrt{V}} \int \psi^\dagger(r) e^{ik \cdot r} dr$ , where  $r$  is integrated over the entire real space, and  $V$  is the area of the unit cell in the real space. This leads to the inverse Fourier transformation  $\psi^\dagger(r) = \frac{1}{\sqrt{V}} \sum_k c^\dagger(k) e^{-ik \cdot r}$ , where  $k$  is summed over the extended Brillouin zone (i.e., the entire momentum space),  $\Omega$  is the area of Brillouin zone in the momentum space. Thus, substitute  $\psi^\dagger(r)$  and  $\psi(r)$  into  $\hat{H}$ , we get

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

, where we define the Fourier transformation of  $H(r)$  as  $H(k_1, k_2) = \frac{1}{V} \int dr e^{-i(k_1 - k_2) \cdot r} H(r)$ .

**Completion:** Following the example, we first define the Fourier transformation of the creation and annihilation operators as:

$$\psi_{\tau,l}^\dagger(k) = \frac{1}{\sqrt{A}} \int dr \psi_{\tau,l}^\dagger(r) e^{ik \cdot r}$$

$$\psi_{\tau,l}(k) = \frac{1}{\sqrt{A}} \int dr \psi_{\tau,l}(r) e^{-ik \cdot r}$$

This leads to the inverse Fourier transformations:

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

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

Substituting these into the Hamiltonian  $\hat{H}_0$ , we get:

$$\hat{H}_0 = \sum_r \sum_{i,j=\{+K,b;+K,t;-K,b;-K,t\}} \frac{1}{\sqrt{A}} \sum_{k_1} \psi_i^\dagger(k_1) e^{-ik_1 \cdot r} H_{0i,j} \frac{1}{\sqrt{A}} \sum_{k_2} \psi_j(k_2) e^{ik_2 \cdot r}$$

Simplifying, we get:

$$\hat{H}_0 = \sum_{i,j=\{+K,b;+K,t;-K,b;-K,t\}} \sum_{k_1,k_2} \psi_i^\dagger(k_1) H_{0i,j}(k_1,k_2) \psi_j(k_2)$$

where we define the Fourier transformation of  $H_{0i,j}(r)$  as  $H_{0i,j}(k_1,k_2) = \frac{1}{A} \int dr e^{-i(k_1-k_2) \cdot r} H_{0i,j}(r)$ .

## 8 Identify interacting term (momentum space)

**Prompt:** You will be instructed to construct the interaction part of the Hamiltonian  $H_{\text{int}}$  in the momentum space. The interaction Hamiltonian is a product of four parts. The first part is the product of four operators with two creation and two annihilation operators following the normal order, namely, creation operators are before annihilation operators. You should follow the order of 1, 2, 2, 1 for the  $l, \tau$ , and 1, 2, 3, 4 for the  $k$ . The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators. The third part is the interaction form. You should use Coulomb interaction with  $V(q) = V_{ll'}(q) = \frac{e^2}{2\epsilon\epsilon_0|q|} [\tanh(d_{\text{gate}}|q|) + (1 - \delta_{ll'})(e^{-d|q|} - 1)]$ , where  $q$  is the transferred total momentum between a creation operator and an annihilation operator with the same  $l, \tau$ , namely  $q = k_1 - k_4$ . The fourth part is the normalization factor, you should use  $\frac{1}{2A}$  here. Finally, the summation should be running over all  $l, \tau$ , and  $k$ . Return the interaction term  $H_{\text{int}}$  in terms of  $c_{l\tau k+q}^\dagger$ ,  $c_{l'\tau' k'-q}^\dagger$ ,  $c_{l'\tau' k'}$  and  $c_{l\tau k}$  and  $V(q)$  (with  $q$  expressed in terms of  $k$ ).

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):  $A$  is the area of the system,  $l$  and  $l'$  label layers and  $\tau$  and  $\tau'$  label valleys.  $\epsilon$  is the relative dielectric constant,  $\epsilon_0$  is the vacuum permittivity,  $d_{\text{gate}}$  is the distance between the sample and the symmetric metal gate, and  $d$  is the distance between the two monolayers.

**Completion:** The interaction Hamiltonian  $H_{\text{int}}$  in momentum space can be constructed as follows:

$$H_{\text{int}} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{k,k',q} V_{ll'}(q) c_{l\tau k+q}^\dagger c_{l'\tau' k'-q}^\dagger c_{l'\tau' k'} c_{l\tau k}$$

where  $V_{ll'}(q) = \frac{e^2}{2\epsilon\epsilon_0|q|} [\tanh(d_{\text{gate}}|q|) + (1 - \delta_{ll'})(e^{-d|q|} - 1)]$  is the Coulomb interaction, and  $q = k_1 - k_4$  is the transferred total momentum between a creation operator and an annihilation operator with the same  $l, \tau$ . The summation runs over all  $l, \tau$ , and  $k$ . The factor of  $1/2A$  is the normalization factor.

## 9 Wick's theorem expansion

**Prompt:** You will be instructed to perform a Hartree-Fock approximation to expand the interaction term,  $H_{\text{int}}$ . You should use Wick's theorem to expand the four-fermion term in  $H_{\text{int}}$  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  $H_{\text{int}}$  is  $H_{\text{int}} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{k,k',q} V_{ll'}(q) c_{l\tau k+q}^\dagger c_{l'\tau' k'-q}^\dagger c_{l'\tau' k'} c_{l\tau k}$ . Return the expanded interaction term after Hartree-Fock approximation as  $H_{\text{int}}^{MF}$ .

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):  $H_{\text{int}}$  is the interaction term,  $A$  is the area of the system,  $l$  and  $l'$  label layers,  $\tau$  and  $\tau'$  label valleys,  $k, k'$ , and  $q$  are wave vectors,  $V_{ll'}(q)$  is the Coulomb interaction,  $c_{l\tau k+q}^\dagger$  and  $c_{l'\tau' k'-q}^\dagger$  are creation operators, and  $c_{l'\tau' k'}$  and  $c_{l\tau k}$  are annihilation operators.

EXAMPLE 1: For a four-fermion term  $a_1^\dagger a_2^\dagger a_3 a_4$ , using Wick's theorem and preserving only the normal terms. this is expanded as  $a_1^\dagger a_2^\dagger a_3 a_4 = \langle a_1^\dagger a_4 \rangle a_2^\dagger a_3 + \langle a_2^\dagger a_3 \rangle a_1^\dagger a_4 - \langle a_1^\dagger a_4 \rangle \langle a_2^\dagger a_3 \rangle - \langle a_1^\dagger a_3 \rangle a_2^\dagger a_4 - \langle a_2^\dagger a_4 \rangle a_1^\dagger a_3 + \langle a_1^\dagger a_3 \rangle \langle a_2^\dagger a_4 \rangle$ . Be cautious about the order of the index and sign before each term here.

EXAMPLE 2: For a four-fermion term  $a_1^\dagger a_2 a_3^\dagger a_4$ , using Wick's theorem and preserving only the normal terms. this is expanded as  $a_1^\dagger a_2 a_3^\dagger a_4 = \langle a_1^\dagger a_2 \rangle a_3^\dagger a_4 + \langle a_3^\dagger a_4 \rangle a_1^\dagger a_2 - \langle a_1^\dagger a_2 \rangle \langle a_3^\dagger a_4 \rangle - \langle a_1^\dagger a_4 \rangle a_3^\dagger a_2 - \langle a_3^\dagger a_2 \rangle a_1^\dagger a_4 + \langle a_1^\dagger a_4 \rangle \langle a_3^\dagger a_2 \rangle$ . Be cautious about the order of the index and sign before each term here.

**Completion:** The interaction term  $H_{\text{int}}$  is a four-fermion term with the form  $c_{l\tau k+q}^\dagger c_{l'\tau' k'-q}^\dagger c_{l'\tau' k'} c_{l\tau k}$ . This is similar to the form in EXAMPLE 1, so we can use Wick's theorem to expand it into quadratic terms, preserving only the normal terms:

$$H_{\text{int}} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ll'}(\mathbf{q}) \left[ \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} + \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle \right. \\ \left. - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} + \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle \right]$$

The expanded interaction term after Hartree-Fock approximation is then:

$$H_{\text{int}}^{MF} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ll'}(\mathbf{q}) \left[ \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} + \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \right. \\ \left. - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \right]$$

## 10 Drop constant terms

**Prompt:** You will be instructed to extract the quadratic terms in the  $H_{\text{int}}$ . 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  $H_{\text{int}}$ , denoted as  $H_{\text{int}}^{(2)}$ . You should recall that  $H_{\text{int}}$  is

$$H_{\text{int}} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ll'}(\mathbf{q}) \left[ \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} + \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle \right. \\ \left. - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} + \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle \right].$$

Return  $H_{\text{int}}^{(2)}$ .

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):  $H_{\text{int}}$  is the interaction Hamiltonian,  $A$  is the area of the system,  $l$  and  $l'$  label layers,  $\tau$  and  $\tau'$  label valleys,  $\mathbf{k}$ ,  $\mathbf{k}'$ , and  $\mathbf{q}$  are wave vectors,  $V_{ll'}(\mathbf{q})$  is the Coulomb interaction,  $c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger$  and  $c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger$  are creation operators, and  $c_{l'\tau'\mathbf{k}'}$  and  $c_{l\tau\mathbf{k}}$  are annihilation operators.

**Completion:** The quadratic terms in the interaction Hamiltonian  $H_{\text{int}}$  are those that are proportional to  $c^\dagger c$ . These terms do not include those that are solely expectations or products of expectations. Therefore, the quadratic terms in  $H_{\text{int}}$ , denoted as  $H_{\text{int}}^{(2)}$ , are:

$$H_{\text{int}}^{(2)} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ll'}(\mathbf{q}) \left[ \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} + \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \right. \\ \left. - \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \right]$$

This expression includes only the terms that are proportional to  $c^\dagger c$  and excludes terms that are solely expectations or products of expectations.

## 11 Identify momentum transfer in interaction

**Prompt:** You will be instructed to expand interaction term  $V(q)$  in the MF quadratic term  $H_{\text{int}}$ . If you find the  $V(q)$  in  $H_{\text{int}}$  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  $H_{\text{int}}$  is

$$H_{\text{int}}^{MF} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ll'}(\mathbf{q}) \left[ \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} + \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \right. \\ \left. - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \right].$$

Return  $H_{\text{int}}$  with expanded interaction.

**Completion:** The interaction term  $V_{ll'}(\mathbf{q})$  in  $H_{\text{int}}^{MF}$  already contains the momentum  $\mathbf{q}$  which is in the summation sign. Therefore, the interaction term is already expanded and there is no need to replace  $\mathbf{q}$  with another momentum. The expanded interaction term remains as  $V_{ll'}(\mathbf{q})$ . Thus, the mean-field Hamiltonian  $H_{\text{int}}^{MF}$  remains unchanged:

$$H_{\text{int}}^{MF} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ll'}(\mathbf{q}) \left[ \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} + \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \right. \\ \left. - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} \right]$$

## 12 Combine Hartree/Fock terms

**Prompt:** You will be instructed to simplify the quadratic term  $H_{\text{int}}$  through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term. The logic is that the expected value ( $\langle c_{l,\tau,k+q}^\dagger c_{l,\tau,k} \rangle$ ) in the first Hartree term ( $\langle c_{l,\tau,k+q}^\dagger c_{l,\tau,k} \rangle c_{l',\tau',k'-q}^\dagger c_{l',\tau',k'}^\dagger$ ) has the same form as the quadratic operators in the second Hartree term ( $\langle c_{l',\tau',k'-q}^\dagger c_{l',\tau',k'}^\dagger \rangle c_{l,\tau,k+q}^\dagger c_{l,\tau,k}$ ), and vice versa. The same applies to the Fock term. This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree term, you can make the second Hartree term look identical to the first Hartree term, as long as  $V(q) = V(-q)$ , which is naturally satisfied in Coulomb interaction. You should follow the EXAMPLE below to simplify it through relabeling the index. You should perform this trick of "relabeling the index" for both two Hartree terms and two Fock terms to reduce them to one Hartree term, and one Fock term. You should recall that  $H_{\text{int}}$  is

$$H_{\text{int}}^{MF} = \frac{1}{2A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ll'}(\mathbf{q}) \left[ \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}^\dagger + \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}^\dagger \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \right. \\ \left. - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}^\dagger \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} - \langle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}^\dagger \right].$$

Return the simplified  $H_{\text{int}}$  which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term)

**EXAMPLE:** Given a Hamiltonian  $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4) (\langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) + \langle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \rangle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)) \delta_{k_1+k_2,k_3+k_4}$ , where  $V(q) = V(-q)$ . In the second term, we relabel the index to swap the index in expected value and the index in quadratic operators, namely,  $\sigma_1 \leftrightarrow \sigma_2$ ,  $\sigma_3 \leftrightarrow \sigma_4$ ,  $k_1 \leftrightarrow k_2$ ,  $k_3 \leftrightarrow k_4$ . After the replacement, the second term becomes  $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_2 - k_3) \langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$ . Note that the Kronecker dirac function  $\delta_{k_4+k_3,k_2+k_1}$  implies  $k_1 + k_2 = k_3 + k_4$ , i.e.,  $k_2 - k_3 = k_4 - k_1$ . Thus, the second term simplifies to  $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_4 - k_1) \langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$ . Because  $V(q) = V(-q)$ , meaning  $V(k_4 - k_1) = V(k_1 - k_4)$ , the second term further simplifies to  $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4) \langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$ . Note that this form of second term after relabeling is identical to the first term. Finally, we have the simplified Hamiltonian as  $\hat{H} = 2 \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1 - k_4) \langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4) \rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) \delta_{k_4+k_3,k_2+k_1}$ .

**Completion:** To simplify the quadratic term  $\hat{H}_{\text{int}}$ , we can relabel the indices in the second Hartree term and the second Fock term.

For the second Hartree term, we swap the indices as follows:  $l \leftrightarrow l'$ ,  $\tau \leftrightarrow \tau'$ ,  $\mathbf{k} \leftrightarrow \mathbf{k}'$ , and  $\mathbf{q} \rightarrow -\mathbf{q}$ . After the replacement, the second Hartree term becomes:

$$\langle c_{l'\tau'\mathbf{k}'+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}^\dagger \rangle c_{l\tau\mathbf{k}-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}}$$

Since  $V_{ll'}(\mathbf{q}) = V_{ll'}(-\mathbf{q})$  due to the nature of the Coulomb interaction, the second Hartree term simplifies to:

$$V_{ll'}(\mathbf{q}) \langle c_{l'\tau'\mathbf{k}'+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}^\dagger \rangle c_{l\tau\mathbf{k}-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}}$$

which is identical to the first Hartree term.

For the second Fock term, we swap the indices as follows:  $l \leftrightarrow l'$ ,  $\tau \leftrightarrow \tau'$ ,  $\mathbf{k} \leftrightarrow \mathbf{k}'$ , and  $\mathbf{q} \rightarrow -\mathbf{q}$ . After the replacement, the second Fock term becomes:

$$\langle c_{l'\tau'\mathbf{k}'+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}$$

Again, since  $V_{ll'}(\mathbf{q}) = V_{ll'}(-\mathbf{q})$ , the second Fock term simplifies to:

$$V_{ll'}(\mathbf{q}) \langle c_{l'\tau'\mathbf{k}'+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l\tau\mathbf{k}-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}$$

which is identical to the first Fock term.

Therefore, the simplified  $H_{\text{int}}$  reduces from four terms to only two terms:

$$H_{\text{int}}^{MF} = \frac{1}{A} \sum_{l,\tau} \sum_{l',\tau'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ll'}(\mathbf{q}) \left[ \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}^\dagger - \langle c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'}^\dagger \rangle c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l\tau\mathbf{k}} \right]$$