

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

## Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

{..} means a placeholder which you need to fill by extracting information from the excerpt.

{A|B} means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to describe the kinetic term of Hamiltonian in {system} in the {real|momen-  
tum} space in the {single-particle|second-quantized} form.

The degrees of freedom of the system are: {degrees\_of\_freedom}.

Express the Kinetic Hamiltonian {kinetic\_symbol} using {variable} which are only on the diagonal terms, and arrange the basis in the order of {order}. [Note that the sublattice degrees of freedom is suppressed for now and will be stated later]

Use the following conventions for the symbols:

{definition\_of\_variables}

Excerpt:

$$H_{\tau} = \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r}) & \Delta_{T,\tau}(\mathbf{r}) \\ \Delta_{T,\tau}^{\dagger}(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt} \end{pmatrix},$$

where  $\tau = \pm 1$  represents  $\pm K$  valleys, and  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone. For each valley, the  $2 \times 2$  Hamiltonian hybridizes the bottom layer (b) and top layer (t), where the off diagonal terms describe the interlayer tunneling  $\Delta_{T,\tau}$ , and the diagonal terms describe the momentum-shifted kinetic energy with the effective mass  $(m_b, m_t) = (0.65, 0.35)m_e$  ( $m_e$  is the rest electron mass), plus the intralayer potential  $\Delta_{b/t}$ , and a band offset  $V_{zt}$  [Fig.~\ref{fig:1}(b)]. Our  $H_{\tau}$  differs from that in Ref.~\onlinecite{zhang2021spintextured} by a gauge transformation.

## Completion

You will be instructed to describe the kinetic term of Hamiltonian in a system with two layers in the momentum space in the second-quantized form.

The degrees of freedom of the system are: valleys, layers, and momentum.

Express the Kinetic Hamiltonian  $H_{\tau}$  using variables which are only on the diagonal terms, and arrange the basis in the order of bottom layer and top layer. Note that the sublattice degrees of freedom is suppressed for now and will be stated later.

Use the following conventions for the symbols:

$\tau = \pm 1$  represents  $\pm K$  valleys,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone. The  $2 \times 2$  Hamiltonian hybridizes the bottom layer (b) and top layer (t), where the off diagonal terms describe the interlayer tunneling  $\Delta_{T,\tau}$ , and the diagonal terms describe the momentum-shifted kinetic energy with the effective mass  $(m_b, m_t) = (0.65, 0.35)m_e$  ( $m_e$  is the rest electron mass), plus the intralayer potential  $\Delta_{b/t}$ , and a band offset  $V_{zt}$ .

# 2 Define energy dispersion (continuum)

## Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

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{A|B} means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to construct each term, namely {Energy\_dispersion}.

For all energy dispersions, {Energy\_dispersion}, it characterizes the {parabolic|Dirac|cos} dispersion for {electrons|holes}.

[In addition, a shift of  $\{\text{momentum\_shift}\}$  in the momentum  $k_{symbol}$  for  $\{\text{shifted\_Ek}\}$ , 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  $k_{symbol} = -i\partial_{r_{symbol}}$ . You should keep the form of  $k_{symbol}$  in the Hamiltonian for short notations but should remember  $k_{symbol}$  is an operator.

Return the expression for  $\{\text{Energy\_dispersion}\}$  in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian  $\{\text{kinetic\_symbol}\}$ .

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):

$\{\text{definition\_of\_variables}\}$

Excerpt:

$$H_\tau = \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r}) & \Delta_{T,\tau}(\mathbf{r}) \\ \Delta_{T,\tau}^\dagger(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k} - \tau \boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt} \end{pmatrix},$$

where  $\tau = \pm 1$  represents  $\pm K$  valleys, and  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1, 0)$  is at a corner of the moir'e Brillouin zone. For each valley, the  $2 \times 2$  Hamiltonian hybridizes the bottom layer (b) and top layer (t), where the off diagonal terms describe the interlayer tunneling  $\Delta_{T,\tau}$ , and the diagonal terms describe the momentum-shifted kinetic energy with the effective mass  $(m_b, m_t) = (0.65, 0.35)m_e$  ( $m_e$  is the rest electron mass), plus the intralayer potential  $\Delta_{b/t}$ , and a band offset  $V_{zt}$  [Fig.~\ref{fig:1}(b)]. Our  $H_\tau$  differs from that in Ref.~\onlinecite{zhang2021spintextured} by a gauge transformation.

$$\begin{aligned} \hat{\mathcal{H}}_0 &= \sum_{\tau=\pm} \int d^2\mathbf{r} \Psi_\tau^\dagger(\mathbf{r}) H_\tau \Psi_\tau(\mathbf{r}), \\ H_\tau &= \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r}) & \Delta_{T,\tau}(\mathbf{r}) \\ \Delta_{T,\tau}^\dagger(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k} - \tau \boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt} \end{pmatrix}, \\ \Psi_+(\mathbf{r}) &= \begin{pmatrix} \psi_{b,\uparrow,+}(\mathbf{r}) \\ \psi_{t,\downarrow,+}(\mathbf{r}) \end{pmatrix}, \quad \Psi_-(\mathbf{r}) = \begin{pmatrix} \psi_{b,\downarrow,-}(\mathbf{r}) \\ \psi_{t,\uparrow,-}(\mathbf{r}) \end{pmatrix}, \end{aligned}$$

where  $\tau = \pm$  represents  $\pm K$  valleys,  $\hbar \mathbf{k} = -i\hbar \partial_{\mathbf{r}}$  is the momentum operator,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1, 0)$  is at a corner of the moir'e Brillouin zone ({as shown in Fig.~\ref{fig:BZ}}), and  $a_M$  is the moir'e lattice constant. Note that the spin index of the fermion operators  $\Psi_\tau$  is both layer and valley dependent.

### Completion

You will be instructed to construct each term, namely  $H_\tau$ .

For all energy dispersions,  $H_\tau$ , it characterizes the parabolic dispersion for electrons.

In addition, a shift of  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1, 0)$  in the momentum  $\mathbf{k}$  for  $\mathbf{k} - \tau \boldsymbol{\kappa}$ , 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  $\mathbf{k} = -i\partial_{\mathbf{r}}$ . You should keep the form of  $\mathbf{k}$  in the Hamiltonian for short notations but should remember  $\mathbf{k}$  is an operator.

Return the expression for  $H_\tau$  in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian  $\hat{\mathcal{H}}_0$ .

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

$\tau = \pm 1$  represents  $\pm K$  valleys,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1, 0)$  is at a corner of the moir'e Brillouin zone, the  $2 \times 2$  Hamiltonian hybridizes the bottom layer (b) and top layer (t), the off diagonal terms describe the interlayer tunneling  $\Delta_{T,\tau}$ , and the diagonal terms describe the momentum-shifted kinetic energy with the effective mass  $(m_b, m_t) = (0.65, 0.35)m_e$  ( $m_e$  is the rest electron mass), plus the intralayer potential  $\Delta_{b/t}$ , and a band offset  $V_{zt}$ .

## 3 Identify potential term (continuum)

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

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$\{A|B\}$  means you need to make a choice between A and B

$[..]$  means optional sentence. You should decide whether to use it depending on the excerpt.

$\{\{..\}\}$  DOES NOT mean a placeholder. You should not change the content inside double curly braces  $\{\{..\}\}$ .

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to describe the potential term of Hamiltonian {potential\_symbol} in the {real|momentum} space in the {single-particle|second-quantized} form.

The potential Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian.

The diagonal terms are {diagonal\_potential}.

The off-diagonal terms are the coupling between {interaction\_degrees\_of\_freedom}, {offdiagonal\_potential}, which should be kept hermitian.

All others terms are zero. Express the potential Hamiltonian {potential\_symbol} using {diagonal\_potential} and {offdiagonal\_potential}.

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):

{definition\_of\_variables}

Excerpt:

$$H_{\tau} = \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r}) & \Delta_{T,\tau}(\mathbf{r}) \\ \Delta_{T,\tau}^{\dagger}(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt} \end{pmatrix},$$

where  $\tau = \pm 1$  represents  $\pm K$  valleys, and  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone. For each valley, the  $2 \times 2$  Hamiltonian hybridizes the bottom layer (b) and top layer (t), where the off diagonal terms describe the interlayer tunneling  $\Delta_{T,\tau}$ , and the diagonal terms describe the momentum-shifted kinetic energy with the effective mass  $(m_b, m_t) = (0.65, 0.35)m_e$  ( $m_e$  is the rest electron mass), plus the intralayer potential  $\Delta_{b/t}$ , and a band offset  $V_{zt}$  [Fig.~\ref{fig:1}(b)]. Our  $H_{\tau}$  differs from that in Ref.~\onlinecite{zhang2021spintextured} by a gauge transformation.

$$\hat{\mathcal{H}}_0 = \sum_{\tau=\pm} \int d^2\mathbf{r} \Psi_{\tau}^{\dagger}(\mathbf{r}) H_{\tau} \Psi_{\tau}(\mathbf{r}),$$

$$H_{\tau} = \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_{b,\tau}(\mathbf{r}) & \Delta_{T,\tau}(\mathbf{r}) \\ \Delta_{T,\tau}^{\dagger}(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_{t,\tau}(\mathbf{r}) + V_{zt} \end{pmatrix},$$

$$\Psi_{+}(\mathbf{r}) = \begin{pmatrix} \psi_{b,\uparrow,+}(\mathbf{r}) \\ \psi_{t,\downarrow,+}(\mathbf{r}) \end{pmatrix}, \quad \Psi_{-}(\mathbf{r}) = \begin{pmatrix} \psi_{b,\downarrow,-}(\mathbf{r}) \\ \psi_{t,\uparrow,-}(\mathbf{r}) \end{pmatrix},$$

where  $\tau = \pm$  represents  $\pm K$  valleys,  $\hbar\mathbf{k} = -i\hbar\partial_{\mathbf{r}}$  is the momentum operator,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone (as shown in Fig.~\ref{fig:BZ}), and  $a_M$  is the moir'e lattice constant. Note that the spin index of the fermion operators  $\Psi_{\tau}$  is both layer and valley dependent.

### Completion

You will be instructed to describe the potential term of Hamiltonian  $H_{\tau}$  in the momentum space in the second-quantized form.

The potential Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian. The diagonal terms are  $-\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r})$  and  $-\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt}$ .

The off-diagonal terms are the coupling between the bottom layer (b) and top layer (t),  $\Delta_{T,\tau}(\mathbf{r})$  and  $\Delta_{T,\tau}^{\dagger}(\mathbf{r})$ , which should be kept hermitian.

All others terms are zero. Express the potential Hamiltonian  $H_{\tau}$  using  $-\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r})$  and  $-\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt}$  and  $\Delta_{T,\tau}(\mathbf{r})$  and  $\Delta_{T,\tau}^{\dagger}(\mathbf{r})$ .

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):

$\tau = \pm 1$  represents  $\pm K$  valleys,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone, the effective mass  $(m_b, m_t) = (0.65, 0.35)m_e$  ( $m_e$  is the rest electron mass), and the intralayer potential  $\Delta_{b/t}$ , and a band offset  $V_{zt}$ .

## 4 Define potential term (continuum)

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

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'You should recall that {...}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to construct each term {potential\_symbol}, namely, {Potential\_variables}.

The expression for diagonal terms are: {expression\_diag}.

The expression for off-diagonal terms are: {expression\_offdiag}.

Return the expressions for {Potential\_variables}, and substitute it into the potential Hamiltonian {potential\_symbol}.

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):

{definition\_of\_variables}

Excerpt:

$$H_\tau = \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r}) & \Delta_{T,\tau}(\mathbf{r}) \\ \Delta_{T,\tau}^\dagger(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt} \end{pmatrix},$$

where  $\tau = \pm 1$  represents  $\pm K$  valleys, and  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1, 0)$  is at a corner of the moir'e Brillouin zone. For each valley, the  $2 \times 2$  Hamiltonian hybridizes the bottom layer (b) and top layer (t), where the off diagonal terms describe the interlayer tunneling  $\Delta_{T,\tau}$ , and the diagonal terms describe the momentum-shifted kinetic energy with the effective mass  $(m_b, m_t) = (0.65, 0.35)m_e$  ( $m_e$  is the rest electron mass), plus the intralayer potential  $\Delta_{b/t}$ , and a band offset  $V_{zt}$  [Fig.~\ref{fig:1}(b)]. Our  $H_\tau$  differs from that in Ref.~\onlinecite{zhang2021spintextured} by a gauge transformation.

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

where  $V_b$  and  $\psi_b$  respectively characterize the amplitude and spatial pattern of the potential, and  $\mathbf{g}_j = \frac{4\pi}{\sqrt{3}a_M} \left( -\sin \frac{\pi(j-1)}{3}, \cos \frac{\pi(j-1)}{3} \right)$  are the moir'e reciprocal lattice vectors in the first shell. We set  $\Delta_t(\mathbf{r}) = 0$ , since the low-energy physics only involves the band maximum of  $\text{WSe}_2$  \cite{zhang2021spintextured}. The interlayer tunneling term is

$$\Delta_{T,\tau}(\mathbf{r}) = \tau w (1 + \omega^\tau e^{i\tau \mathbf{g}_2 \cdot \mathbf{r}} + \omega^{2\tau} e^{i\tau \mathbf{g}_3 \cdot \mathbf{r}}),$$

where  $w$  describes the tunneling strength, and  $\omega = e^{i\frac{2\pi}{3}}$  following the  $C_{3z}$  symmetry \cite{zhang2021spintextured}. The valley dependence of  $\Delta_{T,\tau}$  is constrained by  $\mathcal{T}$  symmetry. Here  $\Delta_{T,\tau}$  couples states with opposite spins, which is symmetry allowed because the heterobilayer breaks the  $z \rightarrow -z$  mirror symmetry. For parameters in  $H_\tau$ , we take  $\psi_b = -14^\circ$  such that the potential maximum of  $\Delta_b(\mathbf{r})$  is at the MM site \cite{zhang2021spintextured};  $V_{zt}$  is a parameter that is experimentally controllable by an applied out-of-plane displacement field;  $V_b$  and  $w$  are taken as theoretical parameters that can be adjusted to study different phases. We note that the interlayer tunneling strength  $w$  can be modified by pressure.

$$\begin{aligned} \hat{\mathcal{H}}_0 &= \sum_{\tau=\pm} \int d^2\mathbf{r} \Psi_\tau^\dagger(\mathbf{r}) H_\tau \Psi_\tau(\mathbf{r}), \\ H_\tau &= \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r}) & \Delta_{T,\tau}(\mathbf{r}) \\ \Delta_{T,\tau}^\dagger(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt} \end{pmatrix}, \\ \Psi_+(\mathbf{r}) &= \begin{pmatrix} \psi_{b,\uparrow,+}(\mathbf{r}) \\ \psi_{t,\downarrow,+}(\mathbf{r}) \end{pmatrix}, \quad \Psi_-(\mathbf{r}) = \begin{pmatrix} \psi_{b,\downarrow,-}(\mathbf{r}) \\ \psi_{t,\uparrow,-}(\mathbf{r}) \end{pmatrix}, \end{aligned}$$

where  $\tau = \pm$  represents  $\pm K$  valleys,  $\hbar \mathbf{k} = -i\hbar \partial_{\mathbf{r}}$  is the momentum operator,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1, 0)$  is at a corner of the moir'e Brillouin zone (as shown in Fig.~\ref{fig:BZ}), and  $a_M$  is the moir'e lattice constant. Note that the spin index of the fermion operators  $\Psi_\tau$  is both layer and valley dependent.

### Completion

You will be instructed to construct each term  $H_\tau$ , namely,  $\Delta_b(\mathbf{r})$ ,  $\Delta_{T,\tau}(\mathbf{r})$ ,  $-\frac{\hbar^2 \mathbf{k}^2}{2m_b}$ ,  $-\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t}$ , and  $V_{zt}$ .

The expression for diagonal terms are:  $-\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_b(\mathbf{r})$  and  $-\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_t(\mathbf{r}) + V_{zt}$ .

The expression for off-diagonal terms are:  $\Delta_{T,\tau}(\mathbf{r})$  and  $\Delta_{T,\tau}^\dagger(\mathbf{r})$ .

Return the expressions for  $\Delta_b(\mathbf{r})$ ,  $\Delta_{T,\tau}(\mathbf{r})$ ,  $-\frac{\hbar^2 \mathbf{k}^2}{2m_b}$ ,  $-\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t}$ , and  $V_{zt}$ , and substitute it into the potential Hamiltonian  $H_\tau$ .

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

$\tau = \pm 1$  represents  $\pm K$  valleys,  $\kappa = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moiré Brillouin zone,  $m_b$  and  $m_t$  are the effective masses of the bottom and top layer respectively with values  $(0.65, 0.35)m_e$  where  $m_e$  is the rest electron mass,  $\Delta_b(\mathbf{r})$  and  $\Delta_{T,\tau}(\mathbf{r})$  are the intralayer potential and interlayer tunneling term respectively,  $V_{zt}$  is a band offset, and  $V_b$  and  $w$  are theoretical parameters that can be adjusted to study different phases.

## 5 Second-quantization (matrix)

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

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$\{A|B\}$  means you need to make a choice between A and B

$[..]$  means optional sentence. You should decide whether to use it depending on the excerpt.

$\{\{..\}\}$  DOES NOT mean a placeholder. You should not change the content inside double curly braces  $\{\{..\}\}$ .

'You should recall that  $\{..\}$ .' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to construct the second quantized form of the total noninteracting Hamiltonian in the  $\{\text{real|momentum}\}$  space.

The noninteracting Hamiltonian in the  $\{\text{real|momentum}\}$  space  $\{\text{nonint\_symbol}\}$  is the sum of Kinetic Hamiltonian  $\{\text{kinetic\_symbol}\}$  and Potential Hamiltonian  $\{\text{potential\_symbol}\}$ .

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  $\{\text{real|momentum}\}$  space position  $\{r|k\}$ .

Return the second quantized form of the total noninteracting Hamiltonian  $\{\text{second\_nonint\_symbol}\}$   
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):

$\{\text{definition\_of\_variables}\}$

Excerpt:

$$\hat{\mathcal{H}}_0 = \sum_{\tau=\pm} \int d^2\mathbf{r} \Psi_{\tau}^{\dagger}(\mathbf{r}) H_{\tau} \Psi_{\tau}(\mathbf{r}),$$

$$H_{\tau} = \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_{b,\tau}(\mathbf{r}) & \Delta_{T,\tau}(\mathbf{r}) \\ \Delta_{T,\tau}^{\dagger}(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k}-\tau\kappa)^2}{2m_t} + \Delta_{t,\tau}(\mathbf{r}) + V_{zt} \end{pmatrix},$$

$$\Psi_{+}(\mathbf{r}) = \begin{pmatrix} \psi_{b,\uparrow,+}(\mathbf{r}) \\ \psi_{t,\downarrow,+}(\mathbf{r}) \end{pmatrix}, \quad \Psi_{-}(\mathbf{r}) = \begin{pmatrix} \psi_{b,\downarrow,-}(\mathbf{r}) \\ \psi_{t,\uparrow,-}(\mathbf{r}) \end{pmatrix},$$

where  $\tau = \pm$  represents  $\pm K$  valleys,  $\hbar\mathbf{k} = -i\hbar\partial_r$  is the momentum operator,  $\kappa = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moiré Brillouin zone (as shown in Fig.~\ref{fig:BZ}), and  $a_M$  is the moiré lattice constant. Note that the spin index of the fermion operators  $\Psi_{\tau}$  is both layer and valley dependent.

### Completion

You will be instructed to construct the second quantized form of the total noninteracting Hamiltonian in the real space.

The noninteracting Hamiltonian in the real space  $\hat{\mathcal{H}}_0$  is the sum of Kinetic Hamiltonian  $-\frac{\hbar^2 \mathbf{k}^2}{2m_b}$  and  $-\frac{\hbar^2 (\mathbf{k}-\tau\kappa)^2}{2m_t}$  and Potential Hamiltonian  $\Delta_{b,\tau}(\mathbf{r})$ ,  $\Delta_{T,\tau}(\mathbf{r})$ ,  $\Delta_{T,\tau}^{\dagger}(\mathbf{r})$ ,  $\Delta_{t,\tau}(\mathbf{r})$ , and  $V_{zt}$ .

To construct the second quantized form of a Hamiltonian. You should construct the creation and annihilation operators from the basis explicitly. You should follow the EXAMPLE below to convert a Hamiltonian from the single-particle form to second-quantized form.

Finally by "total", it means you need to take a summation over the real space position  $r$ .

Return the second quantized form of the total noninteracting Hamiltonian  $\{\text{second\_nonint\_symbol}\}$   
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):

$\tau = \pm$  represents  $\pm K$  valleys,  $\hbar\mathbf{k} = -i\hbar\partial_{\mathbf{r}}$  is the momentum operator,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone, and  $a_M$  is the moir'e lattice constant. Note that the spin index of the fermion operators  $\Psi_{\tau}$  is both layer and valley dependent.

## 6 Second-quantization (summation)

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

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$\{A|B\}$  means you need to make a choice between A and B

$[..]$  means optional sentence. You should decide whether to use it depending on the excerpt.

$\{\{..\}\}$  DOES NOT mean a placeholder. You should not change the content inside double curly braces  $\{\{..\}\}$ .

'You should recall that  $\{..\}$ .' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to expand the second-quantized form Hamiltonian  $\{\text{second\_nonint\_symbol}\}$  using  $\{\text{matrix\_element\_symbol}\}$  and  $\{\text{basis\_symbol}\}$ . 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  $\{\text{matrix\_element\_symbol}\}$  is zero, you should remove it from the summation. Return the expanded form of  $\{\text{second\_nonint\_symbol}\}$  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):

$\{\text{definition\_of\_variables}\}$

Excerpt:

$$\hat{\mathcal{H}}_0 = \sum_{\tau=\pm} \int d^2\mathbf{r} \Psi_{\tau}^{\dagger}(\mathbf{r}) H_{\tau} \Psi_{\tau}(\mathbf{r}),$$

$$H_{\tau} = \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_{b,\tau}(\mathbf{r}) & \Delta_{t,\tau}(\mathbf{r}) \\ \Delta_{t,\tau}^{\dagger}(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_{t,\tau}(\mathbf{r}) + V_{zt} \end{pmatrix},$$

$$\Psi_{+}(\mathbf{r}) = \begin{pmatrix} \psi_{b,\uparrow,+}(\mathbf{r}) \\ \psi_{t,\downarrow,+}(\mathbf{r}) \end{pmatrix}, \quad \Psi_{-}(\mathbf{r}) = \begin{pmatrix} \psi_{b,\downarrow,-}(\mathbf{r}) \\ \psi_{t,\uparrow,-}(\mathbf{r}) \end{pmatrix},$$

where  $\tau = \pm$  represents  $\pm K$  valleys,  $\hbar\mathbf{k} = -i\hbar\partial_{\mathbf{r}}$  is the momentum operator,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone (as shown in Fig.~\ref{fig:BZ}), and  $a_M$  is the moir'e lattice constant. Note that the spin index of the fermion operators  $\Psi_{\tau}$  is both layer and valley dependent.

### Completion

You will be instructed to expand the second-quantized form Hamiltonian  $\hat{\mathcal{H}}_0$  using  $H_{\tau}$  and  $\Psi_{\tau}$ . 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  $H_{\tau}$  is zero, you should remove it from the summation. Return the expanded form of  $\hat{\mathcal{H}}_0$  after simplification.

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

$\hat{\mathcal{H}}_0$  is the second-quantized form Hamiltonian,  $H_{\tau}$  is the matrix element, and  $\Psi_{\tau}$  is the basis.  $\tau = \pm$  represents  $\pm K$  valleys,  $\hbar\mathbf{k} = -i\hbar\partial_{\mathbf{r}}$  is the momentum operator,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone, and  $a_M$  is the moir'e lattice constant. The spin index of the fermion operators  $\Psi_{\tau}$  is both layer and valley dependent.

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

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

$\{..\}$  means a placeholder which you need to fill by extracting information from the excerpt.

$\{A|B\}$  means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.  
 {{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

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 {real\_creation\_op} in the real space to the {momentum\_creation\_op} in the momentum space, which is defined as {definition\_of\_Fourier\_Transformation}, where {real\_variable} is integrated over the {entire\_real|first\_Brillouin\_Zone}. You should follow the EXAMPLE below to apply the Fourier transformation.

Express the total noninteracting Hamiltonian {second\_nonint\_symbol} in terms of {momentum\_creation\_op}. 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):

{definition\_of\_variables}

Excerpt:

$$\hat{\mathcal{H}}_0 = \sum_{\tau=\pm} \int d^2\mathbf{r} \Psi_{\tau}^{\dagger}(\mathbf{r}) H_{\tau} \Psi_{\tau}(\mathbf{r}),$$

$$H_{\tau} = \begin{pmatrix} -\frac{\hbar^2 \mathbf{k}^2}{2m_b} + \Delta_{b,\tau}(\mathbf{r}) & \Delta_{t,\tau}(\mathbf{r}) \\ \Delta_{t,\tau}^{\dagger}(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k}-\tau\boldsymbol{\kappa})^2}{2m_t} + \Delta_{t,\tau}(\mathbf{r}) + V_{zt} \end{pmatrix},$$

$$\Psi_{+}(\mathbf{r}) = \begin{pmatrix} \psi_{b,\uparrow,+}(\mathbf{r}) \\ \psi_{t,\downarrow,+}(\mathbf{r}) \end{pmatrix}, \quad \Psi_{-}(\mathbf{r}) = \begin{pmatrix} \psi_{b,\downarrow,-}(\mathbf{r}) \\ \psi_{t,\uparrow,-}(\mathbf{r}) \end{pmatrix},$$

where  $\tau = \pm$  represents  $\pm K$  valleys,  $\hbar\mathbf{k} = -i\hbar\partial_{\mathbf{r}}$  is the momentum operator,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone ({as shown in Fig.~\ref{fig:BZ}}), and  $a_M$  is the moir'e lattice constant. Note that the spin index of the fermion operators  $\Psi_{\tau}$  is both layer and valley dependent.

$$\hat{\mathcal{H}}_0 = \sum_{\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}} \sum_{l_{\alpha}, l_{\beta}} \sum_{\tau} h_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}}^{(\tau)} c_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau}^{\dagger} c_{\mathbf{k}_{\beta}, l_{\beta}, \tau},$$

where  $h^{(\tau)}$  is the Hamiltonian  $H_{\tau}$  expanded in the plane-wave basis, and the momentum  $\mathbf{k}$  is defined in the extended Brillouin zone {that spans the full momentum space, i.e.,  $\mathbf{k} \in \mathbb{R}^2$ }. {Here, the subscripts  $\alpha, \beta$  are index for momenta.} Due to Bloch's theorem,  $h_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}}^{(\tau)}$  is nonzero only when  $\mathbf{k}_{\alpha} - \mathbf{k}_{\beta}$  is equal to {the linear combination of any multiples of} one of the moir'e reciprocal lattice vectors (including the zero vector).

### Completion

You will be instructed to convert the total noninteracting Hamiltonian in the second quantized form from the basis in real space to the basis by momentum space.

To do that, you should apply the Fourier transformation to  $\Psi_{\tau}^{\dagger}(\mathbf{r})$  in the real space to  $c_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau}^{\dagger}$  in the momentum space, which is defined as  $\hat{\mathcal{H}}_0 = \sum_{\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}} \sum_{l_{\alpha}, l_{\beta}} \sum_{\tau} h_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}}^{(\tau)} c_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau}^{\dagger} c_{\mathbf{k}_{\beta}, l_{\beta}, \tau}$ , where  $\mathbf{r}$  is integrated over the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation.

Express the total noninteracting Hamiltonian  $\hat{\mathcal{H}}_0$  in terms of  $c_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau}^{\dagger}$ . Simplify any summation index if possible.

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

$\tau = \pm$  represents  $\pm K$  valleys,  $\hbar\mathbf{k} = -i\hbar\partial_{\mathbf{r}}$  is the momentum operator,  $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$  is at a corner of the moir'e Brillouin zone, and  $a_M$  is the moir'e lattice constant. The spin index of the fermion operators  $\Psi_{\tau}$  is both layer and valley dependent.  $h^{(\tau)}$  is the Hamiltonian  $H_{\tau}$  expanded in the plane-wave basis, and the momentum  $\mathbf{k}$  is defined in the extended Brillouin zone that spans the full momentum space, i.e.,  $\mathbf{k} \in \mathbb{R}^2$ . The subscripts  $\alpha, \beta$  are index for momenta. Due to Bloch's theorem,  $h_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}}^{(\tau)}$  is nonzero only when  $\mathbf{k}_{\alpha} - \mathbf{k}_{\beta}$  is equal to the linear combination of any multiples of one of the moir'e reciprocal lattice vectors (including the zero vector).

## 8 Particle-hole transformation

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

{..} means a placeholder which you need to fill by extracting information from the excerpt.

{A|B} means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to perform a particle-hole transformation.

Define a hole operator, {hole\_op}, which equals {particle\_op}.

You should replace {particle\_creation\_op} with {hole\_creation\_op}, and {particle\_annihilation\_op} with {hole\_annihilation\_op}. You should follow the EXAMPLE below to apply the particle-hole transformation.

Return the {second\_nonint\_symbol} in the hole operators.

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

{definition\_of\_variables}

Excerpt:

We define the hole operator as  $b_{\mathbf{k},l,\tau} = c_{\mathbf{k},l,\tau}^\dagger$ , and  $\hat{\mathcal{H}}_0$  in the hole basis is

$$\hat{\mathcal{H}}_0 = \sum_{\tau} \text{Tr} h^{(\tau)} - \sum_{\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}} \sum_{l_{\alpha}, l_{\beta}} \sum_{\tau} [h^{(\tau)}]_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}} b_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau}^\dagger b_{\mathbf{k}_{\beta}, l_{\beta}, \tau}$$

### Completion

You will be instructed to perform a particle-hole transformation.

Define a hole operator,  $b_{\mathbf{k},l,\tau}$ , which equals  $c_{\mathbf{k},l,\tau}^\dagger$ .

You should replace  $c_{\mathbf{k},l,\tau}^\dagger$  with  $b_{\mathbf{k},l,\tau}$ , and  $c_{\mathbf{k},l,\tau}$  with  $b_{\mathbf{k},l,\tau}^\dagger$ . You should follow the EXAMPLE below to apply the particle-hole transformation.

Return the  $\hat{\mathcal{H}}_0$  in the hole operators.

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

The hole operator is defined as  $b_{\mathbf{k},l,\tau} = c_{\mathbf{k},l,\tau}^\dagger$ . The Hamiltonian in the hole basis is represented as  $\hat{\mathcal{H}}_0$ .

## 9 Simplify the Hamiltonian in the particle-hole basis

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

{..} means a placeholder which you need to fill by extracting information from the excerpt.

{A|B} means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to simplify the {second\_nonint\_symbol} in the hole basis.

You should use canonical commutator relation for fermions to reorder the hole operator to the normal order. Normal order means that creation operators always appear before the annihilation operators. You should follow the EXAMPLE below to simplify it to the normal order.

Express the {second\_nonint\_symbol} in the normal order of {hole\_op} and also make {index\_1} always appear before {index\_2} in the index of {op} and {Ham\_op}.

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):

{definition\_of\_variables}



Excerpt:

We define the hole operator as  $b_{\mathbf{k},l,\tau} = c_{\mathbf{k},l,\tau}^\dagger$ , and  $\hat{\mathcal{H}}_0$  in the hole basis is

$$\hat{\mathcal{H}}_0 = \sum_{\tau} \text{Tr } h^{(\tau)} - \sum_{\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}} \sum_{l_{\alpha}, l_{\beta}} \sum_{\tau} [h^{(\tau)}]_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}}^\top b_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau}^\dagger b_{\mathbf{k}_{\beta}, l_{\beta}, \tau}$$

### Completion

You will be instructed to simplify the  $\hat{\mathcal{H}}_0$  in the hole basis.

You should use canonical commutator relation for fermions to reorder the hole operator to the normal order. Normal order means that creation operators always appear before the annihilation operators. You should follow the EXAMPLE below to simplify it to the normal order.

Express the  $\hat{\mathcal{H}}_0$  in the normal order of  $b_{\mathbf{k},l,\tau}$  and also make  $\mathbf{k}_{\alpha}$  always appear before  $\mathbf{k}_{\beta}$  in the index of  $b_{\mathbf{k},l,\tau}$  and  $[h^{(\tau)}]_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}}^\top$ .

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

The hole operator is defined as  $b_{\mathbf{k},l,\tau} = c_{\mathbf{k},l,\tau}^\dagger$ , and  $\hat{\mathcal{H}}_0$  is defined as  $\hat{\mathcal{H}}_0 = \sum_{\tau} \text{Tr } h^{(\tau)} - \sum_{\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}} \sum_{l_{\alpha}, l_{\beta}} \sum_{\tau} [h^{(\tau)}]_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}}^\top b_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau}^\dagger b_{\mathbf{k}_{\beta}, l_{\beta}, \tau}$ .

## 10 Identify interacting term (momentum space)

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

{..} means a placeholder which you need to fill by extracting information from the excerpt.

{A|B} means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to construct the interaction part of the Hamiltonian {second\_int\_symbol} 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 {index\_of\_operator}, and 1, 2, 3, 4 for the {momentum}. The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators. [For each operator, the total momentum is the sum of moire reciprocal lattice  $b_i$  and momentum with in the first BZ  $k_i$ ]

The third part is the interaction form. You should use {interaction} with  $V(q) = \text{int\_form}$ , where  $q$  is the transferred total momentum between a creation operator and an annihilation operator with the same {index\_of\_operator}, namely  $q = k_1 - k_4$ .

The fourth part is the normalization factor, you should use {normalization\_factor} here. Finally, the summation should be running over all {index\_of\_operator}, and {momentum} Return the interaction term {second\_int\_symbol} in terms of {op} and  $V(q)$  (with  $q$  expressed in terms of {momentum}).

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

{definition\_of\_variables}

Excerpt:

$$\begin{aligned} \hat{\mathcal{H}} &= \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_{\text{int}}, \\ \hat{\mathcal{H}}_1 &= \sum_{\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}} \sum_{l_{\alpha}, l_{\beta}} \sum_{\tau} \tilde{h}_{\mathbf{k}_{\alpha} l_{\alpha}, \mathbf{k}_{\beta} l_{\beta}}^{(\tau)} b_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau}^\dagger b_{\mathbf{k}_{\beta}, l_{\beta}, \tau}, \\ \hat{\mathcal{H}}_{\text{int}} &= \frac{1}{2A} \sum_{\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}, \mathbf{k}_{\gamma}, \mathbf{k}_{\delta}} \sum_{l_{\alpha}, l_{\beta}, l_{\gamma}, l_{\delta}} \sum_{\tau_{\alpha}, \tau_{\beta}} V(\mathbf{k}_{\alpha} - \mathbf{k}_{\delta}) b_{\mathbf{k}_{\alpha}, l_{\alpha}, \tau_{\alpha}}^\dagger b_{\mathbf{k}_{\beta}, l_{\beta}, \tau_{\beta}}^\dagger b_{\mathbf{k}_{\gamma}, l_{\gamma}, \tau_{\gamma}} b_{\mathbf{k}_{\delta}, l_{\delta}, \tau_{\delta}} \delta_{\mathbf{k}_{\alpha} + \mathbf{k}_{\beta}, \mathbf{k}_{\gamma} + \mathbf{k}_{\delta}}, \end{aligned}$$

where  $\tilde{h}^{(\tau)} = -[h^{(\tau)}]^\top$ , the dual-gate screened Coulomb interaction  $V(\mathbf{k}) = 2\pi e^2 \tanh(|\mathbf{k}|d)/(\epsilon|\mathbf{k}|)$ ,  $d$  is the sample-to-gate distance, and  $\epsilon$  is the dielectric constant.

## Completion

You will be instructed to construct the interaction part of the Hamiltonian  $\hat{\mathcal{H}}_{\text{int}}$  in the momentum space.

The interaction Hamiltonian is a product of four parts. The first part is the product of four operators with two creation and two annihilation operators following the normal order, namely, creation operators are before annihilation operators. You should follow the order of  $l_\alpha, l_\beta, l_\beta, l_\alpha$  for the index of operator, and  $\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta$  for the momentum. The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators.

The third part is the interaction form. You should use dual-gate screened Coulomb interaction with  $V(\mathbf{k}) = 2\pi e^2 \tanh(|\mathbf{k}|d)/(\epsilon|\mathbf{k}|)$ , where  $\mathbf{k}$  is the transferred total momentum between a creation operator and an annihilation operator with the same index of operator, namely  $\mathbf{k} = \mathbf{k}_\alpha - \mathbf{k}_\delta$ .

The fourth part is the normalization factor, you should use  $\frac{1}{2A}$  here. Finally, the summation should be running over all index of operator, and momentum. Return the interaction term  $\hat{\mathcal{H}}_{\text{int}}$  in terms of  $b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger, b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger, b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta}, b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha}$  and  $V(\mathbf{k})$  (with  $\mathbf{k}$  expressed in terms of momentum).

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

$\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta$  are the momenta,  $l_\alpha, l_\beta$  are the indices of operators,  $\tau_\alpha, \tau_\beta$  are the spin indices,  $V(\mathbf{k})$  is the dual-gate screened Coulomb interaction,  $d$  is the sample-to-gate distance, and  $\epsilon$  is the dielectric constant.

## 11 Wick's theorem expansion

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

{..} means a placeholder which you need to fill by extracting information from the excerpt.

{A|B} means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, {second\_int\_symbol}.

You should use Wick's theorem to expand the four-fermion term in {second\_int\_symbol} 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.

Return the expanded interaction term after Hartree-Fock approximation as {Hartree\_Fock\_symbol}.

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):

{definition\_of\_variables}

Excerpt:

$$\begin{aligned}\hat{\mathcal{H}}^{\text{HF}} &= \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_{\text{int}}^{\text{HF}}, \\ \hat{\mathcal{H}}_{\text{int}}^{\text{HF}} &= \frac{1}{A} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} \sum_{l_\alpha, l_\beta} \sum_{\tau_\alpha, \tau_\beta} V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \left( \left\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \right\rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right. \\ &\quad \left. - \left\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right\rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \right) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\delta + \mathbf{k}_\gamma}.\end{aligned}$$

### Completion

You will be instructed to perform a Hartree-Fock approximation to expand the interaction term,  $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$ .

You should use Wick's theorem to expand the four-fermion term in  $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$  into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without  $^\dagger$ , 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.

Return the expanded interaction term after Hartree-Fock approximation as  $\hat{\mathcal{H}}^{\text{HF}}$ .

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

$\hat{\mathcal{H}}^{\text{HF}}$  is the Hartree-Fock Hamiltonian,  $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$  is the interaction term in the Hartree-Fock Hamiltonian,  $\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta$  are the momentum vectors,  $l_\alpha, l_\beta$  are the orbital quantum numbers,  $\tau_\alpha, \tau_\beta$  are the spin quantum numbers,  $V(\mathbf{k}_\alpha - \mathbf{k}_\delta)$  is the interaction potential,  $b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger$  and  $b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha}$  are the creation and annihilation operators, and  $\langle \dots \rangle$  denotes the expectation value.

## 12 Drop constant terms

### Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

{..} means a placeholder which you need to fill by extracting information from the excerpt.

{A|B} means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to extract the quadratic terms in the {Hartree\_Fock\_term\_symbol}.

The quadratic terms mean terms that are proportional to {bilinear\_op}, which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in {Hartree\_Fock\_term\_symbol}, denoted as {Hartree\_Fock\_second\_quantized\_symbol}.

Return {Hartree\_Fock\_second\_quantized\_symbol}.

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):

{definition\_of\_variables}

Excerpt:

$$\begin{aligned}\hat{\mathcal{H}}^{\text{HF}} &= \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_{\text{int}}^{\text{HF}}, \\ \hat{\mathcal{H}}_{\text{int}}^{\text{HF}} &= \frac{1}{A} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} \sum_{l_\alpha, l_\beta} \sum_{\tau_\alpha, \tau_\beta} V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \left( \left\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \right\rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right. \\ &\quad \left. - \left\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right\rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \right) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\delta + \mathbf{k}_\gamma}.\end{aligned}$$

### Completion

You will be instructed to extract the quadratic terms in the Hartree-Fock term symbol, denoted as  $\hat{\mathcal{H}}^{\text{HF}}$ .

The quadratic terms mean terms that are proportional to  $b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta}$  and  $b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha}$ , which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in  $\hat{\mathcal{H}}^{\text{HF}}$ , denoted as  $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$ .

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

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

$\hat{\mathcal{H}}^{\text{HF}}$  is the Hartree-Fock term symbol,  $\hat{\mathcal{H}}_{\text{int}}^{\text{HF}}$  is the Hartree-Fock second quantized symbol, and

$b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta}$  and  $b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha}$  are the bilinear operators.

# 13 Combine Hartree/Fock terms

## Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

{..} means a placeholder which you need to fill by extracting information from the excerpt.

{A|B} means you need to make a choice between A and B

[..] means optional sentence. You should decide whether to use it depending on the excerpt.

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to simplify the quadratic term {Hartree\_Fock\_second\_quantized\_symbol} through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.

The logic is that the expected value ({expected\_value}) in the first Hartree term ({expression\_Hartree\_1}) has the same form as the quadratic operators in the second Hartree term ({expression\_Hartree\_2}), 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.

Return the simplified {Hartree\_Fock\_second\_quantized\_symbol} which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term)

Excerpt:

$$\begin{aligned}\hat{\mathcal{H}}^{\text{HF}} &= \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_{\text{int}}^{\text{HF}}, \\ \hat{\mathcal{H}}_{\text{int}}^{\text{HF}} &= \frac{1}{A} \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma, \mathbf{k}_\delta} \sum_{l_\alpha, l_\beta} \sum_{\tau_\alpha, \tau_\beta} V(\mathbf{k}_\alpha - \mathbf{k}_\delta) \left( \left\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \right\rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right. \\ &\quad \left. - \left\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \right\rangle b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \right) \delta_{\mathbf{k}_\alpha + \mathbf{k}_\beta, \mathbf{k}_\delta + \mathbf{k}_\gamma}.\end{aligned}$$

## Completion

You will be instructed to simplify the quadratic term  $\hat{\mathcal{H}}^{\text{HF}}$  through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.

The logic is that the expected value ( $\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha} \rangle$  and  $\langle b_{\mathbf{k}_\alpha, l_\alpha, \tau_\alpha}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta} \rangle$ ) in the first Hartree term ( $b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\gamma, l_\beta, \tau_\beta}$ ) has the same form as the quadratic operators in the second Hartree term ( $b_{\mathbf{k}_\beta, l_\beta, \tau_\beta}^\dagger b_{\mathbf{k}_\delta, l_\alpha, \tau_\alpha}$ ), 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.

Return the simplified  $\hat{\mathcal{H}}^{\text{HF}}$  which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term).