

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:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r}) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta_D & 0 \\ 0 & -\Delta_D \end{pmatrix},$$

where the intralayer and interlayer moir'e 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 moir'e reciprocal lattice vectors with a_M being the moir'e 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 Δ_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

You will be instructed to describe the kinetic term of Hamiltonian in the system in the real space in the second-quantized form.

The degrees of freedom of the system are: intralayer and interlayer moir'e potentials, moir'e reciprocal lattice vectors, mBZ corners, effective mass, and out-of-plane electric field.

Express the Kinetic Hamiltonian H_K using variables which are only on the diagonal terms, and arrange the basis in the order of the matrix provided. Note that the sublattice degrees of freedom is suppressed for now and will be stated later.

Use the following conventions for the symbols:

- $\Delta_{b/t}$ represents the intralayer and interlayer moir'e potentials
- \mathbf{G}_i represents the moir'e reciprocal lattice vectors
- $\boldsymbol{\kappa}_+$ and $\boldsymbol{\kappa}_-$ represent the mBZ corners
- m^* represents the effective mass
- Δ_D represents the layer-differentiating potential proportional to the out-of-plane electric field.

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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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 {momentum_shift} in the momentum k_{symbol} for {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 {Energy_dispersion} in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian {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):

{definition_of_variables}

Excerpt:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r}) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta_D & 0 \\ 0 & -\Delta_D \end{pmatrix},$$

where the intralayer and interlayer moir'e 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 moir'e reciprocal lattice vectors with a_M being the moir'e 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 Δ_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

You will be instructed to construct each term, namely $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r})$ and $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r})$.

For all energy dispersions, $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r})$ and $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r})$, it characterizes the parabolic dispersion for electrons.

In addition, a shift of $\boldsymbol{\kappa}_+$ and $\boldsymbol{\kappa}_-$ in the momentum \mathbf{k} for $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r})$ and $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r})$, 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 $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r})$ and $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r})$ 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):

\mathbf{k} is the momentum, $\boldsymbol{\kappa}_+$ and $\boldsymbol{\kappa}_-$ are the mBZ corners, m^* is the effective mass and is taken as $0.6m_e$, where m_e is the free electron mass, $\Delta_b(\mathbf{r})$ and $\Delta_t(\mathbf{r})$ are the intralayer and interlayer moir'e potentials, respectively, \mathbf{G}_i are moir'e reciprocal lattice vectors with a_M being the moir'e lattice constant, Δ_D is the layer-differentiating potential included in H_K to take into account the out-of-plane electric field.

3 Identify potential term (continuum)

Prompt

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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:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r}) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta_D & 0 \\ 0 & -\Delta_D \end{pmatrix},$$

where the intralayer and interlayer moir'e 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 moir'e reciprocal lattice vectors with a_M being the moir'e 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 Δ_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

You will be instructed to describe the potential term of Hamiltonian H_K in the real space in the second-quantized 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 the intralayer and interlayer moir'e potentials, $\Delta_T(\mathbf{r})$ and $\Delta_T^\dagger(\mathbf{r})$, which should be kept hermitian.

All others terms are zero. Express the potential Hamiltonian H_K using $\Delta_b(\mathbf{r})$, $\Delta_t(\mathbf{r})$, $\Delta_T(\mathbf{r})$ 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 moir'e 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 moir'e reciprocal lattice vectors with a_M being the moir'e 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 Δ_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 .

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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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:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r}) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta_D & 0 \\ 0 & -\Delta_D \end{pmatrix},$$

where the intralayer and interlayer moir'e 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 moir'e reciprocal lattice vectors with a_M being the moir'e 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 Δ_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

You will be instructed to construct each term H_K , namely, $\Delta_{b/t}$, Δ_T , and Δ_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 $\Delta_T^\dagger(\mathbf{r})$.

Return the expressions for $\Delta_{b/t}$, Δ_T , and Δ_D , and substitute it into the potential 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 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 Δ_D is the layer-differentiating potential.

5 Second-quantization (matrix)

Prompt

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Template:

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

The noninteracting Hamiltonian in the {real|momentum} space {nonint_symbol} is the sum of Kinetic Hamiltonian {kinetic_symbol} and Potential Hamiltonian {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 {real|momentum} space position {r|k}.

Return the second quantized form of the total noninteracting Hamiltonian {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):

{definition_of_variables}

Excerpt:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r}) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta_D & 0 \\ 0 & -\Delta_D \end{pmatrix},$$

where the intralayer and interlayer moir'e 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 moir'e reciprocal lattice vectors with a_M being the moir'e 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 Δ_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

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

The noninteracting Hamiltonian in the momentum space H_K is the sum of Kinetic Hamiltonian $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r})$ and Potential Hamiltonian $\Delta_T(\mathbf{r})$.

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 momentum space position k .

Return the second quantized form of the total noninteracting Hamiltonian {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):

H_K is the noninteracting Hamiltonian in the momentum space, $-\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r})$ is the Kinetic Hamiltonian, $\Delta_T(\mathbf{r})$ is the Potential Hamiltonian, and k is the momentum space position.

6 Second-quantization (summation)

Prompt

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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 {second_nonint_symbol} using {matrix_element_symbol} and {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 {matrix_element_symbol} is zero, you should remove it from the summation. Return the expanded form of {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):

{definition_of_variables}

Excerpt:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r}) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta_D & 0 \\ 0 & -\Delta_D \end{pmatrix},$$

where the intralayer and interlayer moir'e 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 moir'e reciprocal lattice vectors with a_M being the moir'e 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 Δ_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

You will be instructed to expand the second-quantized form Hamiltonian H_K using $\Delta_{b/t}$, Δ_T , Δ_D , and G_i . 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 $\Delta_{b/t}$, Δ_T , Δ_D , and G_i is zero, you should remove it from the summation. Return the expanded form of H_K 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):

The intralayer and interlayer moiré potentials are represented by $\Delta_{b/t} = 2V \sum_{i=1,3,5} \cos(\mathbf{G}_i \cdot \mathbf{r} \pm \phi)$ 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. $\kappa_+ = 2\mathbf{G}_1/3 - \mathbf{G}_2/3$ and $\kappa_- = \mathbf{G}_1/3 + \mathbf{G}_2/3$ 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 Δ_D is included in H_K to take into account the out-of-plane electric field.

7 Fourier transform noninteracting term to momentum space (continuum)

Prompt

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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 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:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\kappa_+)^2}{2m^*} + \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & -\frac{\hbar^2(\mathbf{k}-\kappa_-)^2}{2m^*} + \Delta_t(\mathbf{r}) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta_D & 0 \\ 0 & -\Delta_D \end{pmatrix},$$

where 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. $\kappa_+ = 2\mathbf{G}_1/3 - \mathbf{G}_2/3$ and $\kappa_- = \mathbf{G}_1/3 + \mathbf{G}_2/3$ 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 Δ_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

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:

$$H_K = \begin{pmatrix} -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & -\frac{\hbar^2(\mathbf{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\mathbf{r}) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta_D & 0 \\ 0 & -\Delta_D \end{pmatrix},$$

where the intralayer and interlayer moir'e 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 moir'e reciprocal lattice vectors with a_M being the moir'e 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 Δ_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 .

8 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:

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

where A is the area of the system, l and l' label layers and τ and τ' label valleys. The Coulomb interaction takes the form \cite{chatterjee2020symmetry}

$$V_{ll'}(\mathbf{q}) = \frac{e^2}{2\epsilon\epsilon_0|\mathbf{q}|} \left[\tanh(d_{\text{gate}}|\mathbf{q}|) + (1 - \delta_{ll'})(e^{-d|\mathbf{q}|} - 1) \right],$$

where ϵ is the relative dielectric constant, ϵ_0 is the vacuum permittivity, d_{gate} is the distance between the sample and the symmetric metal gate, and d is the distance between the two monolayers. The interlayer Coulomb interaction is reduced from the intralayer Coulomb interaction by $e^{-d|\mathbf{q}|} - 1$. This correction is only valid for $d \ll d_{\text{gate}}$ \cite{chatterjee2020symmetry}. The self-consistent Hartree-Fock calculations are performed in the reciprocal space without projecting the interaction to bands near the charge neutrality point.

Completion

You will be instructed to construct the interaction part of the Hamiltonian H_{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, l', τ, τ' for the index of operator, and $\mathbf{k}, \mathbf{k}', \mathbf{q}$ 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 Coulomb interaction with $V_{ll'}(\mathbf{q}) = \frac{e^2}{2\epsilon\epsilon_0|\mathbf{q}|} [\tanh(d_{\text{gate}}|\mathbf{q}|) + (1 - \delta_{ll'})(e^{-d|\mathbf{q}|} - 1)]$ 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 $\frac{1}{2A}$ here. Finally, the summation should be running over all index of operator, and momentum. Return the interaction term H_{int} in terms of $c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger$, $c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger$, $c_{l'\tau'\mathbf{k}'}$ and $c_{l\tau\mathbf{k}}$ and $V_{ll'}(\mathbf{q})$ (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):

A is the area of the system, l and l' label layers and τ and τ' label valleys. ϵ is the relative dielectric constant, ϵ_0 is the vacuum permittivity, d_{gate} is the distance between the sample and the symmetric metal gate, and d is the distance between the two monolayers.

9 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 † , 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:

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

where A is the area of the system, l and l' label layers and τ and τ' label valleys. The Coulomb interaction takes the form \cite{chatterjee2020symmetry}

$$V_{ll'}(\mathbf{q}) = \frac{e^2}{2\epsilon\epsilon_0|q|} \left[\tanh(d_{\text{gate}}|q|) + (1 - \delta_{ll'})(e^{-d|q|} - 1) \right],$$

where ϵ is the relative dielectric constant, ϵ_0 is the vacuum permittivity, d_{gate} is the distance between the sample and the symmetric metal gate, and d is the distance between the two monolayers. The interlayer Coulomb interaction is reduced from the intralayer Coulomb interaction by $e^{-d|q|} - 1$. This correction is only valid for $d \ll d_{\text{gate}}$ \cite{chatterjee2020symmetry}. The self-consistent Hartree-Fock calculations are performed in the reciprocal space without projecting the interaction to bands near the charge neutrality point.

Completion

You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, H_{int} .

You should use Wick's theorem to expand the four-fermion term in H_{int} into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without † , and be extremely cautious about the order of the index and sign before each term.

You should only preserve the normal terms. Here, the normal terms mean the product of a creation operator and an annihilation operator.

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):

H_{int} is the interaction term, A is the area of the system, l and l' label layers, τ and τ' 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.

10 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:

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

where A is the area of the system, l and l' label layers and τ and τ' label valleys. The Coulomb interaction takes the form \cite{chatterjee2020symmetry}

$$V_{ll'}(\mathbf{q}) = \frac{e^2}{2\epsilon\epsilon_0|\mathbf{q}|} \left[\tanh(d_{\text{gate}}|\mathbf{q}|) + (1 - \delta_{ll'})(e^{-d|\mathbf{q}|} - 1) \right],$$

where ϵ is the relative dielectric constant, ϵ_0 is the vacuum permittivity, d_{gate} is the distance between the sample and the symmetric metal gate, and d is the distance between the two monolayers. The interlayer Coulomb interaction is reduced from the intralayer Coulomb interaction by $e^{-d|\mathbf{q}|} - 1$. This correction is only valid for $d \ll d_{\text{gate}}$ \cite{chatterjee2020symmetry}. The self-consistent Hartree-Fock calculations are performed in the reciprocal space without projecting the interaction to bands near the charge neutrality point.

Completion

You will be instructed to extract the quadratic terms in the H_{int} .

The quadratic terms mean terms that are proportional to $c_{l\tau\mathbf{k}+\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'-\mathbf{q}}^\dagger c_{l'\tau'\mathbf{k}'} c_{l\tau\mathbf{k}}$, which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in H_{int} , denoted as $H_{\text{int}}^{(2)}$.

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_{int} is the interaction Hamiltonian, A is the area of the system, l and l' label layers, τ and τ' 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.

11 Identify momentum transfer in interaction

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 expand interaction term $V(q)$ in the MF quadratic term $\{\text{Hartree_Fock_second_quantized_symbol}\}$. If you find the $V(q)$ in $\{\text{Hartree_Fock_second_quantized_symbol}\}$ 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 $\{\text{momentum}\}$. Return $\{\text{Hartree_Fock_second_quantized_symbol}\}$ with expanded interaction.

Excerpt:

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

where A is the area of the system, l and l' label layers and τ and τ' label valleys. The Coulomb interaction takes the form \cite{chatterjee2020symmetry}

$$V_{ll'}(\mathbf{q}) = \frac{e^2}{2\epsilon\epsilon_0|\mathbf{q}|} \left[\tanh(d_{\text{gate}}|\mathbf{q}|) + (1 - \delta_{ll'})(e^{-d|\mathbf{q}|} - 1) \right],$$

where ϵ is the relative dielectric constant, ϵ_0 is the vacuum permittivity, d_{gate} is the distance between the sample and the symmetric metal gate, and d is the distance between the two monolayers. The interlayer Coulomb interaction is reduced from the intralayer Coulomb interaction by $e^{-d|\mathbf{q}|} - 1$. This correction is only valid for $d \ll d_{\text{gate}}$ \cite{chatterjee2020symmetry}. The self-consistent Hartree-Fock calculations are performed in the reciprocal space without projecting the interaction to bands near the charge neutrality point.

Completion

You will be instructed to expand interaction term $V_{ll'}(\mathbf{q})$ in the MF quadratic term H_{int} . If you find the $V_{ll'}(\mathbf{q})$ in H_{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 $V_{ll'}(\mathbf{q})$ by replacing \mathbf{q} with the momentum \mathbf{k} and \mathbf{k}' . Return H_{int} with expanded interaction.

12 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 $V(\mathbf{q}) = V(-\mathbf{q})$, 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:

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

where A is the area of the system, l and l' label layers and τ and τ' label valleys. The Coulomb interaction takes the form \cite{chatterjee2020symmetry}

$$V_{ll'}(\mathbf{q}) = \frac{e^2}{2\epsilon\epsilon_0|\mathbf{q}|} \left[\tanh(d_{\text{gate}}|\mathbf{q}|) + (1 - \delta_{ll'})(e^{-d|\mathbf{q}|} - 1) \right],$$

where ϵ is the relative dielectric constant, ϵ_0 is the vacuum permittivity, d_{gate} is the distance between the sample and the symmetric metal gate, and d is the distance between the two monolayers. The interlayer Coulomb interaction is reduced from the intralayer Coulomb interaction by $e^{-d|\mathbf{q}|} - 1$. This correction is only valid for $d \ll d_{\text{gate}}$ \cite{chatterjee2020symmetry}. The self-consistent Hartree-Fock calculations are performed in the reciprocal space without projecting the interaction to bands near the charge neutrality point.

Completion

You will be instructed to simplify the quadratic term H_{int} through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.

The logic is that the expected value in the first Hartree term has the same form as the quadratic operators in the second Hartree term, 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 $V(\mathbf{q}) = V(-\mathbf{q})$, 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 H_{int} which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term).