

# 1 Identify kinetic term (lattice)

## 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}

The kinetic term is a tight-binding model composed of the following hopping process: {site i and site  
j with the amplitude hopping} [You should ensure the hermiticity of the Hamiltonian] The summation  
should be taken over all {degrees\_of\_freedom} and all {real|momentum} space positions.

Return the Kinetic Hamiltonian {kinetic\_symbol}.

Use the following conventions for the symbols:

{definition\_of\_variables}

Excerpt:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where {the hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ )}. Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone~\cite{pan2020band}. {Both}  $t$  and  $U$  involve distant nearest neighbors (i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites)), refer to Refs.~\onlinecite{pan2020band,pan2020quantum,wu2018hubbard,wu2019topological} for the motivation and derivation of Eq.~\eqref{eq:hubbard} as the basic description for the interacting moir'e physics in TTMD systems. Although the theory based on Eq.~\eqref{eq:hubbard} should apply to all TTMD systems, our specific numerical results are for the WSe<sub>2</sub> based TTMD structures currently being studied at Columbia University~\cite{wang2020correlated}. Details of the numerical model for Eq.~\eqref{eq:hubbard} {are available in Refs.}~\onlinecite{pan2020band,pan2020quantum}. We emphasize that Eq.~\eqref{eq:hubbard} cannot be thought of as either a Hubbard (or extended Hubbard) model or a {WC} (or generalized WC) model. Equation~\eqref{eq:hubbard} is a semirealistic model for the actual interacting TTMD 2D moir'e materials.

## Completion

You will be instructed to describe the kinetic term of Hamiltonian in the TTMD 2D moir'e materials in the real space in the second-quantized form.

The degrees of freedom of the system are: valley index  $s$ , spin-up or down, coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone.

The kinetic term is a tight-binding model composed of the following hopping process: between site  $i$  and site  $j$  with the amplitude hopping  $t_s$ . You should ensure the hermiticity of the Hamiltonian. The summation should be taken over all degrees of freedom and all real space positions.

Return the Kinetic Hamiltonian  $H$ .

Use the following conventions for the symbols:

$t_s$  represents band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ ). Both  $t$  and  $U$  involve distant nearest neighbors (i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites).

# 2 Identify interacting term (real 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:

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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 the interaction part of the Hamiltonian, {second\_int\_symbol} in the real space in the second-quantized form.

The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian {kinetic\_symbol}.

The interaction is a density-density interaction composed of the following process: {site i and site j with the interaction strength} The summation should be taken over all {degrees\_of\_freedom} and all real space positions.

Return the interaction term {second\_int\_symbol} in terms of {density\_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:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where {the hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ )}. Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone~\cite{pan2020band}. {Both}  $t$  and  $U$  involve distant nearest neighbors ({i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites}), refer to Refs.~\onlinecite{pan2020band,pan2020quantum,wu2018hubbard,wu2019topological} for the motivation and derivation of Eq.~\eqref{eq:hubbard} as the basic description for the interacting moir'e physics in TTMD systems. Although the theory based on Eq.~\eqref{eq:hubbard} should apply to all TTMD systems, our specific numerical results are for the WSe<sub>2</sub> based TTMD structures currently being studied at Columbia University~\cite{wang2020correlated}. Details of the numerical model for Eq.~\eqref{eq:hubbard} {are available in Refs.}~\onlinecite{pan2020band,pan2020quantum}. We emphasize that Eq.~\eqref{eq:hubbard} cannot be thought of as either a Hubbard (or extended Hubbard) model or a {WC} (or generalized WC) model. Equation~\eqref{eq:hubbard} is a semirealistic model for the actual interacting TTMD 2D moir'e materials.

### Completion

You will be instructed to construct the interaction part of the Hamiltonian,  $H$  in the real space in the second-quantized form.

The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian  $\sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s}$ .

The interaction is a density-density interaction composed of the following process: site  $i$  and site  $j$  with the interaction strength  $U(\mathbf{R}_i - \mathbf{R}_j)$ . The summation should be taken over all valley indices  $s$  and  $s'$  and all real space positions.

Return the interaction term  $H$  in terms of  $c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s}$ .

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):  $t_s$  represents band structures,  $U$  represents the correlation effect,  $c_{i,s}^\dagger$  and  $c_{j,s'}$  are creation and annihilation operators, respectively, and  $\mathbf{R}_i$  and  $\mathbf{R}_j$  are real space positions.

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

**Prompt**

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Template:

You will be instructed to convert the noninteracting Hamiltonian {nonint\_symbol} in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to {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 all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that hopping have no position dependence now.] Express the total noninteracting Hamiltonian {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:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where {the hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ )}. Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone~\cite{pan2020band}. {Both}  $t$  and  $U$  involve distant nearest neighbors ({i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites}), refer to Refs.~\onlinecite{pan2020band,pan2020quantum,wu2018hubbard,wu2019topological} for the motivation and derivation of Eq.~\eqref{eq:hubbard} as the basic description for the interacting moir'e physics in TTMD systems. Although the theory based on Eq.~\eqref{eq:hubbard} should apply to all TTMD systems, our specific numerical results are for the WSe<sub>2</sub> based TTMD structures currently being studied at Columbia University~\cite{wang2020correlated}. Details of the numerical model for Eq.~\eqref{eq:hubbard} {are available in Refs.}~\onlinecite{pan2020band,pan2020quantum}. We emphasize that Eq.~\eqref{eq:hubbard} cannot be thought of as either a Hubbard (or extended Hubbard) model or a {WC} (or generalized WC) model. Equation~\eqref{eq:hubbard} is a semirealistic model for the actual interacting TTMD 2D moir'e materials.

### Completion

You will be instructed to convert the noninteracting Hamiltonian  $H$  in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to  $c_{i,s}^\dagger$  in the real space to the {momentum\_creation\_op} in the momentum space, which is defined as {definition\_of\_Fourier\_Transformation}, where  $i$  is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that hopping have no position dependence now.] Express the total noninteracting Hamiltonian  $H$  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): The hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ ). Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone. Both  $t$  and  $U$  involve distant nearest neighbors (i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites).

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

### Prompt

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Template:

You will be instructed to convert the interacting Hamiltonian, {second\_int\_symbol}, in the {single-particle|second-quantized} form the basis in real space to the basis in 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 all sites in the entire real space, and {momentum\_var} is defined within the first Brillouin zone. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that interaction have no position dependence now]

Express {second\_int\_symbol} in terms of {momentum\_creation\_op}. Simplify any summation index if possible.

Excerpt:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where {the hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ )}. Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone~\cite{pan2020band}. {Both}  $t$  and  $U$  involve distant nearest neighbors ({i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites}), refer to Refs.~\onlinecite{pan2020band,pan2020quantum,wu2018hubbard,wu2019topological} for the motivation and derivation of Eq.~\eqref{eq:hubbard} as the basic description for the interacting moir'e physics in TTMD systems. Although the theory based on Eq.~\eqref{eq:hubbard} should apply to all TTMD systems, our specific numerical results are for the WSe<sub>2</sub> based TTMD structures currently being studied at Columbia University~\cite{wang2020correlated}. Details of the numerical model for Eq.~\eqref{eq:hubbard} {are available in Refs.}~\onlinecite{pan2020band,pan2020quantum}. We emphasize that Eq.~\eqref{eq:hubbard} cannot be thought of as either a Hubbard (or extended Hubbard) model or a {WC} (or generalized WC) model. Equation~\eqref{eq:hubbard} is a semirealistic model for the actual interacting TTMD 2D moir'e materials.

### Completion

You will be instructed to convert the interacting Hamiltonian,  $H$ , in the second-quantized form the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to  $c_{i,s}^\dagger$  in the real space to the {momentum\_creation\_op} in the momentum space, which is defined as {definition\_of\_Fourier\_Transformation}, where  $i$  is integrated over all sites in the entire real space, and {momentum\_var} is defined within the first Brillouin zone. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that interaction have no position dependence now] Express  $H$  in terms of {momentum\_creation\_op}. Simplify any summation index if possible.

## 5 Wick's theorem expansion

### 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 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:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where {the hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ )}. Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone~\cite{pan2020band}. {Both}  $t$  and  $U$  involve distant nearest neighbors ({i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites}), refer to Refs.~\onlinecite{pan2020band,pan2020quantum,wu2018hubbard,wu2019topological} for the motivation and derivation of Eq.~\eqref{eq:hubbard} as the basic description for the interacting moir'e physics in TTMD systems. Although the theory based on Eq.~\eqref{eq:hubbard} should apply to all TTMD systems, our specific numerical results are for the WSe<sub>2</sub> based TTMD structures currently being studied at Columbia University~\cite{wang2020correlated}. Details of the numerical model for Eq.~\eqref{eq:hubbard} {are available in Refs.}~\onlinecite{pan2020band,pan2020quantum}. We emphasize that Eq.~\eqref{eq:hubbard} cannot be thought of as either a Hubbard (or extended Hubbard) model or a {WC} (or generalized WC) model. Equation~\eqref{eq:hubbard} is a semirealistic model for the actual interacting TTMD 2D moir'e materials.

### Completion

You will be instructed to perform a Hartree-Fock approximation to expand the interaction term,  $\frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s}$ .

You should use Wick's theorem to expand the four-fermion term in  $\frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s}$  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):

The hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ ). Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone. Both  $t$  and  $U$  involve distant nearest neighbors.

## 6 Drop constant terms

### 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 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:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where {the hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ )}. Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone~\cite{pan2020band}. {Both}  $t$  and  $U$  involve distant nearest neighbors ({i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites}), refer to Refs.~\onlinecite{pan2020band,pan2020quantum,wu2018hubbard,wu2019topological} for the motivation and derivation of Eq.~\eqref{eq:hubbard} as the basic description for the interacting moir'e physics in TTMD systems. Although the theory based on Eq.~\eqref{eq:hubbard} should apply to all TTMD systems, our specific numerical results are for the WSe<sub>2</sub> based TTMD structures currently being studied at Columbia University~\cite{wang2020correlated}. Details of the numerical model for Eq.~\eqref{eq:hubbard} {are available in Refs.}~\onlinecite{pan2020band,pan2020quantum}. We emphasize that Eq.~\eqref{eq:hubbard} cannot be thought of as either a Hubbard (or extended Hubbard) model or a {WC} (or generalized WC) model. Equation~\eqref{eq:hubbard} is a semirealistic model for the actual interacting TTMD 2D moir'e materials.

### Completion

You will be instructed to extract the quadratic terms in the Hubbard Hamiltonian.

The quadratic terms mean terms that are proportional to  $c_{i,s}^\dagger c_{j,s}$ , which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in the Hubbard Hamiltonian, denoted as  $H$ .

Return  $H$ .

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):

$t_s$  represents the hopping terms which are band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ ). Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone. Both  $t$  and  $U$  involve distant nearest neighbors.

## 7 Identify momentum transfer in interaction

### Prompt

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

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Template:

You will be instructed to expand interaction term  $V(q)$  in the MF quadratic term {Hartree\_Fock\_second\_quantized\_symbol}. If you find the  $V(q)$  in {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 {momentum}. Return {Hartree\_Fock\_second\_quantized\_symbol} with expanded interaction.

Excerpt:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where {the hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ )}. Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone~\cite{pan2020band}. {Both}  $t$  and  $U$  involve distant nearest neighbors ({i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites}), refer to Refs.~\onlinecite{pan2020band,pan2020quantum,wu2018hubbard,wu2019topological} for the motivation and derivation of Eq.~\eqref{eq:hubbard} as the basic description for the interacting moir'e physics in TTMD systems. Although the theory based on Eq.~\eqref{eq:hubbard} should apply to all TTMD systems, our specific numerical results are for the WSe<sub>2</sub> based TTMD structures currently being studied at Columbia University~\cite{wang2020correlated}. Details of the numerical model for Eq.~\eqref{eq:hubbard} {are available in Refs.}~\onlinecite{pan2020band,pan2020quantum}. We emphasize that Eq.~\eqref{eq:hubbard} cannot be thought of as either a Hubbard (or extended Hubbard) model or a {WC} (or generalized WC) model. Equation~\eqref{eq:hubbard} is a semirealistic model for the actual interacting TTMD 2D moir'e materials.

### Completion

You will be instructed to expand interaction term  $U(\mathbf{R}_i - \mathbf{R}_j)$  in the MF quadratic term  $H$ . If you find the  $U(\mathbf{R}_i - \mathbf{R}_j)$  in  $H$  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  $U(\mathbf{R}_i - \mathbf{R}_j)$  by replacing  $\mathbf{R}_i - \mathbf{R}_j$  with the momentum  $\mathbf{R}_i - \mathbf{R}_j$ . Return  $H$  with expanded interaction.

## 8 Relabel the index

### Prompt

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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 simplify the quadratic term {Hartree\_Fock\_second\_quantized\_symbol} through relabeling the index.

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.

Namely, a replacement of {relabel} is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes {Unsummed\_Indices}. This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree or Fock term, you can make the second Hartree or Fock term look identical to the first Hartree or Fock term, as long as  $V(q) = V(-q)$ , which is naturally satisfied in Coulomb interaction. You should follow the EXAMPLE below to simplify it through relabeling the index.

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

Excerpt:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where {the hopping terms  $t_s$  represent band structures (depending on  $\theta$ ), and effective interparticle Coulomb interactions  $U$  represent the correlation effect (depending on  $\epsilon$ )}. Valley index  $s$ , spin-up or down, is coupled with  $+K$  or  $-K$  valley, respectively, in the Brillouin zone~\cite{pan2020band}. {Both}  $t$  and  $U$  involve distant nearest neighbors ({i.e., our parametrization of Eq.~\eqref{eq:hubbard} includes hopping up to the third nearest neighbors and Coulomb coupling term  $U$  up to 1993 distant sites}), refer to Refs.~\onlinecite{pan2020band,pan2020quantum,wu2018hubbard,wu2019topological} for the motivation and derivation of Eq.~\eqref{eq:hubbard} as the basic description for the interacting moir'e physics in TTMD systems. Although the theory based on Eq.~\eqref{eq:hubbard} should apply to all TTMD systems, our specific numerical results are for the WSe<sub>2</sub> based TTMD structures currently being studied at Columbia University~\cite{wang2020correlated}. Details of the numerical model for Eq.~\eqref{eq:hubbard} {are available in Refs.}~\onlinecite{pan2020band,pan2020quantum}. We emphasize that Eq.~\eqref{eq:hubbard} cannot be thought of as either a Hubbard (or extended Hubbard) model or a {WC} (or generalized WC) model. Equation~\eqref{eq:hubbard} is a semirealistic model for the actual interacting TTMD 2D moir'e materials.

### Completion

You will be instructed to simplify the quadratic term  $H$  through relabeling the index.

The logic is that the expected value ( $\langle t_s \rangle$ ) in the first Hartree term ( $\langle c_{i,s}^\dagger c_{j,s} \rangle$ ) has the same form as the quadratic operators in the second Hartree term ( $\langle c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s} \rangle$ ), and vice versa. The same applies to the Fock term.

Namely, a replacement of {relabel} is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes {Unsummed\_Indices}.

This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree or Fock term, you can make the second Hartree or Fock term look identical to the first Hartree or Fock term, as long as  $V(q) = V(-q)$ , which is naturally satisfied in Coulomb interaction. You should follow the EXAMPLE below to simplify it through relabeling the index.

Return the simplified  $H$ .