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:

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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 kinetic term of Hamiltonian in {system} in the {real|momentum} 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:

$$H = \sum_s \sum_{i,j} t_s \left(\boldsymbol{R}_i - \boldsymbol{R}_j \right) c_{i,s}^\dagger c_{j,s}$$

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

where $\boldsymbol{R}_i$ represents the position of site i in a triangular lattice formed in the moir'e pattern [Fig.~\ref{fig:fig1}(a)], s is the spin index, and t and U are, respectively, the hopping parameter and the interaction strength. As proposed in Refs.~\cite{wu2018hubbard, wu2019topological, pan2020band}, the model in Eq.~\eqref{eq:hubbard} can be simulated in twisted TMD heterobilayers as well as homobilayers. For definiteness, we use twisted homobilayer WSe$_2$ (tWSe$_2$) as the model system in this work, and Eq.~\eqref{eq:hubbard} is then constructed following our previous work \cite{pan2020band} for low-energy holes in the first moir'e valence band at $\pm K$ valleys. Here we use $c_{i,s}^\dagger$ to represent the hole operator, and $s =\uparrow$ and $\downarrow$ are locked to $+K$ and $-K$ valleys, respectively. We define a filling factor ν as $(1/\mathcal{N}) \sum_{i,s} c_{i,s}^\dagger c_{i,s}$, which counts the number of holes per moir'e cell ($\mathcal{N}$ is the total number of moir'e sites in the system). The charge neutrality point of the semiconducting twisted bilayer corresponds to $\nu = 0$. For simplicity, we assume that no external out-of-plane displacement field is applied to WSe$_2$, and then the model in Eq.~\eqref{eq:hubbard} respects emergent spin SU(2) symmetry and C_6 point group symmetry. An important advantage of the moir'e platform is that both the hopping parameters and the interaction strength are highly tunable. Generally speaking, the moir'e bandwidth becomes narrower at smaller twist angle (larger moir'e period) and many-body interaction effects become more prominent~\cite{wu2018hubbard, wu2019topological, naik2018ultraflatbands}. We show the twist-angle dependence of t and U in the Supplemental Material \cite{SM} (see, also, Refs.~\cite{fukui2005chern,yu2011equivalent} therein). In the calculation of U, we project a screened Coulomb interaction $(e^2/\epsilon)(1/r - 1/\sqrt{r^2 + d^2})$ to the low-energy moir'e states, where ϵ is the background dielectric constant that is tunable by the dielectric environment and $d/2$ is the distance between the moir'e system and a nearby metallic gate. We take ϵ as a free parameter and d, which is also experimentally controllable, to be 60 nm in calculations.

Completion

You will be instructed to describe the kinetic term of Hamiltonian in twisted homobilayer WSe$_2$ (tWSe$_2$) in the real space in the second-quantized form.

The degrees of freedom of the system are: the position of site i in a triangular lattice formed in the moir'e pattern, and the spin index s.

The kinetic term is a tight-binding model composed of the following hopping process: site i and site j with the amplitude $t_s \left(\boldsymbol{R}_i - \boldsymbol{R}_j \right)$ 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:

$\boldsymbol{R}_i$ represents the position of site i in a triangular lattice formed in the moir'e pattern, s is the spin index, and t and U are, respectively, the hopping parameter and the interaction strength. $c_{i,s}^\dagger$ is used to represent the hole operator, and $s =\uparrow$ and $\downarrow$ are locked to $+K$ and $-K$ valleys, respectively. A filling factor ν is defined as $(1/\mathcal{N})\sum_{i,s} c_{i,s}^\dagger c_{i,s}$, which counts the number of holes per moir'e cell ($\mathcal{N}$ is the total number of moir'e sites in the system).

2   Identify interacting term (real space)

Prompt
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[..] 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 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:

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

where $\boldsymbol{R}_i$ represents the position of site i in a triangular lattice formed in the moir'e pattern [Fig.~\ref{fig:fig1}(a)], s is the spin index, and t and U are, respectively, the hopping parameter and the interaction strength. As proposed in Refs.~\cite{wu2018hubbard, wu2019topological, pan2020band}, the model in Eq.~\eqref{eq:hubbard} can be simulated in twisted TMD heterobilayers as well as homobilayers. For definiteness, we use twisted homobilayer WSe$_2$ (tWSe$_2$) as the model system in this work, and Eq.~\eqref{eq:hubbard} is then constructed following our previous work \cite{pan2020band} for low-energy holes in the first moir'e valence band at $\pm K$ valleys. Here we use $c_{i,s}^\dagger$ to represent the hole operator, and $s =\uparrow$ and $\downarrow$ are locked to $+K$ and $-K$ valleys, respectively. We define a filling factor ν as $(1/\mathcal{N})\sum_{i,s} c_{i,s}^\dagger c_{i,s}$, which counts the number of holes per moir'e cell ($\mathcal{N}$ is the total number of moir'e sites in the system). The charge neutrality point of the semiconducting twisted bilayer corresponds to $\nu = 0$. For simplicity, we assume that no external out-of-plane displacement field is applied to WSe$_2$, and then the model in Eq.~\eqref{eq:hubbard} respects emergent spin SU(2) symmetry and C_6 point group symmetry. An important advantage of the moir'e platform is that both the hopping parameters and the interaction strength are highly tunable. Generally speaking, the moir'e bandwidth becomes narrower at smaller twist angle (larger moir'e period) and many-body interaction effects become more prominent~\cite{wu2018hubbard, wu2019topological, naik2018ultraflatbands}. We show the twist-angle dependence of t and U in the Supplemental Material \cite{SM} (see, also, Refs.~\cite{fukui2005chern,yu2011equivalent} therein). In the calculation of U, we project a screened Coulomb interaction $(e^2/\epsilon)(1/r - 1/\sqrt{r^2 + d^2})$ to the low-energy moir'e states, where ϵ is the background dielectric constant that is tunable by the dielectric environment and $d/2$ is the distance between the moir'e system and a nearby metallic gate. We take ϵ as a free parameter and d, which is also experimentally controllable, to be 60 nm in calculations.

$$H_{\text{Coulomb}} = \frac{1}{2}\sum_{s,s'}\sum_{i,j} U(\boldsymbol{R}_i - \boldsymbol{R}_j) n_{i,s} n_{j,s'},$$

where $n_{i,s}$ is the binary occupancy number of site i. We choose proper supercells manually and minimize the total Coulomb energy per site by exploring various arrangement of occupied sites.

Completion

You will be instructed to construct the interaction part of the Hamiltonian, H_{Coulomb} in the real space in the second-quantized form.

The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian H.

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

Return the interaction term H_{Coulomb} in terms of $n_{i,s}$.

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): $\boldsymbol{R}_i$ represents the position of site i in a triangular lattice formed in the moir'e pattern, s is the spin index, $U(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is the interaction strength, $n_{i,s}$ is the binary occupancy number of site i, and $c^{\dagger}_{i,s}$ represents the hole operator.

3 Fourier transform noninteracting term to momentum space (lattice)

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 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:

$$H_0 = \sum_s \sum_{\boldsymbol{k}} \varepsilon_s(\boldsymbol{k}) c^{\dagger}_{\boldsymbol{k},s} c_{\boldsymbol{k},s},$$

where $\boldsymbol{k}$ is summed over the first Brillouin zone ($\mathbb{BZ}$) of the moir'e lattice, and $\varepsilon_s(\boldsymbol{k})$ is the noninteracting band energy dispersion calculated from the tight-binding model for spin s. The interaction term H_1 in the momentum space is

Completion

You will be instructed to convert the noninteracting Hamiltonian H_0 in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to $c^{\dagger}_{\boldsymbol{k},s}$ in the real space to the $c^{\dagger}_{\boldsymbol{k},s}$ in the momentum space, which is defined as $\varepsilon_s(\boldsymbol{k})$, where $\boldsymbol{k}$ 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_0 in terms of $c^{\dagger}_{\boldsymbol{k},s}$. Simplify any summation index if possible.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): H_0 is the noninteracting Hamiltonian, $\boldsymbol{k}$ is the momentum, $\varepsilon_s(\boldsymbol{k})$ is the non-interacting band energy dispersion, and $c^{\dagger}_{\boldsymbol{k},s}$ is the creation operator in momentum space.

4 Fourier transform interacting term to momentum space (lattice)

Prompt
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{{..}} 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 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:

$$H_1 = \frac{1}{2\mathcal{N}} \sum_{s,s'} \sum_{k} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} c^\dagger_{\boldsymbol{k}_\alpha,s} c^\dagger_{\boldsymbol{k}_\beta,s'} c_{\boldsymbol{k}_\gamma,s'} c_{\boldsymbol{k}_\delta,s},$$

where $\mathcal{N}$ is the number of total sites in the lattice, and $\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta$ are summed over the first $\mathbb{BZ}$. Here, the interaction in the momentum space (as shown in Fig.~\ref{fig:tU}(d)) is

$$U(\boldsymbol{q}) = \sum_{\boldsymbol{R}} U(\boldsymbol{R}) e^{i\boldsymbol{q}\cdot\boldsymbol{R}},$$

and

$$\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} = \sum_{\boldsymbol{G}} \delta(\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta - \boldsymbol{k}_\gamma - \boldsymbol{k}_\delta, \boldsymbol{G}),$$

where $\boldsymbol{G}$ is any moir'e reciprocal lattice vector, and $\delta(\dots)$ is the Kronecker delta function.
Completion
You will be instructed to convert the interacting Hamiltonian, H1, 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 $c^\dagger_{\boldsymbol{k}_\alpha,s}$ in the real space to the $c^\dagger_{\boldsymbol{k}_\alpha,s}$ in the momentum space, which is defined as $U(\boldsymbol{q}) = \sum_{\boldsymbol{R}} U(\boldsymbol{R}) e^{i\boldsymbol{q}\cdot\boldsymbol{R}}$, where $\boldsymbol{R}$ is integrated over all sites in the entire real space, and \bm{q} 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 H1 in terms of $c^\dagger_{\boldsymbol{k}_\alpha,s}$. 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.
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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:

\begin{widetext}

$$H_{\text{int}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta}$$

$$\left[\left\langle c^\dagger_{\boldsymbol{k}_\alpha, s} c_{\boldsymbol{k}_\delta, s} \right\rangle c^\dagger_{\boldsymbol{k}_\beta, s'} c_{\boldsymbol{k}_\gamma, s'} - \left\langle c^\dagger_{\boldsymbol{k}_\alpha, s} c_{\boldsymbol{k}_\gamma, s'} \right\rangle c^\dagger_{\boldsymbol{k}_\beta, s'} c_{\boldsymbol{k}_\delta, s} \right]$$

\end{widetext}

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, $\mathcal{N}$ is a normalization constant, s and s' are spin indices, $\boldsymbol{k}$ is the momentum vector, $U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$ is the interaction potential, $\delta_{\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta}$ is the Kronecker delta function, $c^\dagger_{\boldsymbol{k}_\alpha, s}$ and $c_{\boldsymbol{k}_\delta, s}$ are creation and annihilation operators respectively, and $\langle ... \rangle$ denotes expectation values.

6 Drop constant terms

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 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{widetext}

$$H_{\text{int}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta}$$

$$\left[\left\langle c_{\boldsymbol{k}_\alpha, s}^\dagger c_{\boldsymbol{k}_\delta, s} \right\rangle c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\gamma, s'} - \left\langle c_{\boldsymbol{k}_\alpha, s}^\dagger c_{\boldsymbol{k}_\gamma, s'} \right\rangle c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\delta, s} \right]$$

\end{widetext}

Completion

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

The quadratic terms mean terms that are proportional to $c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\gamma, s'}$ and $c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\delta, s}$, 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, $\mathcal{N}$ is a normalization factor, s and s' are spin indices, $\boldsymbol{k}$ is the momentum vector, $U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$ is the interaction potential, $\delta_{\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta}$ is the Kronecker delta function, $c_{\boldsymbol{k}_\alpha, s}^\dagger$ and $c_{\boldsymbol{k}_\delta, s}$ are creation and annihilation operators, and $\langle ... \rangle$ denotes expectation values.

7 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:

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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 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:

\begin{widetext}

$$H_{\text{int}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta}$$

$$\left[\left\langle c_{\boldsymbol{k}_\alpha, s}^\dagger c_{\boldsymbol{k}_\delta, s} \right\rangle c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\gamma, s'} - \left\langle c_{\boldsymbol{k}_\alpha, s}^\dagger c_{\boldsymbol{k}_\gamma, s'} \right\rangle c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\delta, s} \right]$$

\end{widetext}

Completion

You will be instructed to expand interaction term $V(q)$ in the MF quadratic term H_{int}. If you find the $V(q)$ 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 $V(q)$ by replacing q with the momentum $\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta$. Return H_{int} with expanded interaction.

8 Relabel the index

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

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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 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:

\begin{widetext}

$$H_{\mathrm{int}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{k}} U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta}$$

$$\left[\left\langle c_{\boldsymbol{k}_\alpha, s}^\dagger c_{\boldsymbol{k}_\delta, s} \right\rangle c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\gamma, s'} - \left\langle c_{\boldsymbol{k}_\alpha, s}^\dagger c_{\boldsymbol{k}_\gamma, s'} \right\rangle c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\delta, s} \right]$$

\end{widetext}

Completion

You will be instructed to simplify the quadratic term H_{int} through relabeling the index.

The logic is that the expected value ($\left\langle c_{\boldsymbol{k}_\alpha, s}^\dagger c_{\boldsymbol{k}_\delta, s} \right\rangle$ and $\left\langle c_{\boldsymbol{k}_\alpha, s}^\dagger c_{\boldsymbol{k}_\gamma, s'} \right\rangle$) in the first Hartree term ($c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\gamma, s'}$)

has the same form as the quadratic operators in the second Hartree term ($c_{\boldsymbol{k}_\beta, s'}^\dagger c_{\boldsymbol{k}_\delta, s}$), and vice versa. The same applies to the Fock term.

Namely, a replacement of $\boldsymbol{k}_\gamma \leftrightarrow \boldsymbol{k}_\delta$ is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes $\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta$.

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 $U(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) = U(-(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta))$, which is naturally satisfied in Coulomb interaction. You should follow the EXAMPLE below to simplify it through relabeling the index.

Return the simplified H_{int}.

9 Identify order parameters in Hartree term (extended BZ)

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 simplify the Hartree term in {Hartree_second_quantized_symbol} by reducing the momentum inside the expected value {expected_value}.

The expected value {expected_value} is only nonzero when the two momenta k_i, k_j are the same, namely, {expected_value_nonzero}.

You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i. Once you reduce one momentum inside the expected value $\langle \dots \rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.

You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.
Return the final simplified Hartree term {Hartree_second_quantized_symbol}.
Excerpt:

$$H_{\mathrm{HF}} = H_0 + H_{\mathrm{Hartree}} + H_{\mathrm{Fock}},$$

where the Hartree term is \begin{widetext}

$$H_{\mathrm{Hartree}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{q}_\alpha - \boldsymbol{q}_\delta) \delta_{\boldsymbol{q}_\alpha,\boldsymbol{q}_\beta,\boldsymbol{q}_\gamma,\boldsymbol{q}_\delta} \left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\delta,s} \right\rangle c^\dagger_{\boldsymbol{p}_\beta+\boldsymbol{q}_\beta,s'} c_{\boldsymbol{p}_\beta+\boldsymbol{q}_\gamma,s'}$$

\end{widetext}
Completion
You will be instructed to simplify the Hartree term in H_{Hartree} by reducing the momentum inside the expected value $\left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\delta,s} \right\rangle$.
The expected value $\left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\delta,s} \right\rangle$ is only nonzero when the two momenta $\boldsymbol{p}_\alpha + \boldsymbol{q}_\alpha, \boldsymbol{p}_\alpha + \boldsymbol{q}_\delta$ are the same, namely, $\left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} \right\rangle$.
You should use the property of Kronecker delta function $\delta_{\boldsymbol{q}_\alpha,\boldsymbol{q}_\beta,\boldsymbol{q}_\gamma,\boldsymbol{q}_\delta}$ to reduce one momentum $\boldsymbol{p}_\alpha + \boldsymbol{q}_\alpha$ but not $\boldsymbol{p}_\alpha + \boldsymbol{q}_\delta$. Once you reduce one momentum inside the expected value $\langle \ldots \rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.
You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.
Return the final simplified Hartree term H_{Hartree}.

10 Identify order parameters in Fock term (extended BZ)

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 Fock term in {Fock_second_quantized_symbol} by reducing the momentum inside the expected value {expected_value}.
The expected value {expected_value} is only nonzero when the two momenta k_i, k_j are the same, namely, {expected_value_nonzero}.
You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i.
Once you reduce one momentum inside the expected value $\langle \ldots \rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term.
Return the final simplified Fock term {Fock_second_quantized_symbol}.
Excerpt:
\begin{widetext}

$$H_{\mathrm{Fock}} = -\frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{p}_\alpha - \boldsymbol{p}_\beta + \boldsymbol{q}_\alpha - \boldsymbol{q}_\delta) \delta_{\boldsymbol{q}_\alpha,\boldsymbol{q}_\beta,\boldsymbol{q}_\gamma,\boldsymbol{q}_\delta} \left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\gamma,s'} \right\rangle c^\dagger_{\boldsymbol{p}_\beta+\boldsymbol{q}_\beta,s'} c_{\boldsymbol{p}_\beta+\boldsymbol{q}_\delta,s}.$$

\end{widetext}
Completion
You will be instructed to simplify the Fock term in H_{Fock} by reducing the momentum inside the expected value $\left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\gamma,s'} \right\rangle$.

The expected value $\left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\gamma,s'} \right\rangle$ is only nonzero when the two momenta $\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha$ and $\boldsymbol{p}_\alpha+\boldsymbol{q}_\gamma$ are the same, namely, $\left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s'} \right\rangle$.

You should use the property of Kronecker delta function $\delta_{\boldsymbol{q}_\alpha,\boldsymbol{q}_\beta,\boldsymbol{q}_\gamma,\boldsymbol{q}_\delta}$ to reduce one momentum $\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha$ but not $\boldsymbol{p}_\beta+\boldsymbol{q}_\beta$.

Once you reduce one momentum inside the expected value $\langle \dots \rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term. Return the final simplified Fock term H_{Fock}.

11 Final form of iteration in quadratic 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:

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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 now be instructed to combine the Hartree term {Hartree_symbol} and the Fock term {Fock_symbol}.

and the Fock term {Fock}.

You should perform the same trick of relabeling the index in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. The relabeling should be done with a swap : {swap_rule}. You should add them, relabel the index in Fock term, and simply their sum. Return the final sum of Hartree and Fock term.

Excerpt:

$$H_{\text{HF}} = H_0 + H_{\text{Hartree}} + H_{\text{Fock}},$$

where the Hartree term is \begin{widetext}

$$H_{\text{Hartree}} = \frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{q}_\alpha - \boldsymbol{q}_\delta) \delta_{\boldsymbol{q}_\alpha,\boldsymbol{q}_\beta,\boldsymbol{q}_\gamma,\boldsymbol{q}_\delta} \left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\delta,s} \right\rangle c^\dagger_{\boldsymbol{p}_\beta+\boldsymbol{q}_\beta,s'} c_{\boldsymbol{p}_\beta+\boldsymbol{q}_\gamma,s'}$$

\end{widetext} and the Fork term is \begin{widetext}

$$H_{\text{Fock}} = -\frac{1}{\mathcal{N}} \sum_{s,s'} \sum_{\boldsymbol{p},\boldsymbol{q}} U(\boldsymbol{p}_\alpha - \boldsymbol{p}_\beta + \boldsymbol{q}_\alpha - \boldsymbol{q}_\delta) \delta_{\boldsymbol{q}_\alpha,\boldsymbol{q}_\beta,\boldsymbol{q}_\gamma,\boldsymbol{q}_\delta} \left\langle c^\dagger_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\alpha,s} c_{\boldsymbol{p}_\alpha+\boldsymbol{q}_\gamma,s'} \right\rangle c^\dagger_{\boldsymbol{p}_\beta+\boldsymbol{q}_\beta,s'} c_{\boldsymbol{p}_\beta+\boldsymbol{q}_\delta,s}.$$

\end{widetext}

Completion

You will now be instructed to combine the Hartree term H_{Hartree} and the Fock term H_{Fock}.

You should perform the same trick of relabeling the index in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. The relabeling should be done with a swap : {swap_rule}. You should add them, relabel the index in Fock term, and simply their sum. Return the final sum of Hartree and Fock term.