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|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:
of TBG, $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\mathrm{C}}$, where

$$\mathcal{H}_0 = \sum_{\alpha\beta}\sum_{ij} h_{\alpha\beta}(\boldsymbol{R}_i - \boldsymbol{R}_j)d^{\dagger}_{\alpha,i,\sigma}d_{\beta,j,\sigma}$$

is the hopping term, with $d_{\alpha,i,\sigma}$ the annihilation operator of an electron with spin $\sigma = \uparrow, \downarrow$ on sublattice α of unit cell i, and $h_{\alpha\beta}(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is the corresponding tight-binding matrix element between sublattices α and β located in unit cells centered at $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$ respectively. The second term describes a screened

Completion
You will be instructed to describe the kinetic term of Hamiltonian in TBG in the real space in the second-quantized form.
The degrees of freedom of the system are: spin and sublattice
The kinetic term is a tight-binding model composed of the following hopping process: site i and site j with the amplitude $h_{\alpha\beta}(R_i - R_j)$ [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_0.
Use the following conventions for the symbols:
$d_{\alpha,i,\sigma}$ is the annihilation operator of an electron with spin σ= ↑,↓ on sublattice α of unit cell i, and $h_{\alpha\beta}(R_i - R_j)$ is the corresponding tight-binding matrix element between sublattices α and β located in unit cells centered at R_i and R_j respectively.

2 Identify interacting term (real space)

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 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:

Coulomb interaction between any two lattice sites,

$$\mathcal{H}_{\mathrm{C}} = \frac{1}{2} \sum_{\alpha\beta} \sum_{ij} \hat{n}_{\alpha,i} V_{\alpha\beta}(\boldsymbol{R}_i - \boldsymbol{R}_j) \hat{n}_{\beta,j},$$

where $\hat{n}_{\alpha,i} = \sum_\sigma d^\dagger_{\alpha,i,\sigma} d_{\alpha,i,\sigma}$ is the local density operator and $V_{\alpha\beta}(\boldsymbol{R}) = e^2/(\varepsilon\xi) \sum_{m=-\infty}^{\infty} (-1)^m [(|\boldsymbol{\tau}_\alpha - \boldsymbol{\tau}_\beta + \boldsymbol{R}|/\xi)^2 + m^2]^{-\frac{1}{2}}$ is the screened form of the interaction in the presence of symmetric gates located at the top and bottom of the TBG heterostructure \cite{Throckmorton,Bernevig2}, with e the electron charge and $\boldsymbol{\tau}_\alpha$ the position of a site in sublattice α measured from the center of its unit cell. $\xi \approx 10\,$nm is the distance between the plates of the metallic gates in most experiments \cite{Stepanov,Saito}, and ε is the background dielectric constant, which we treat as a free adjustable parameter. The value of the dielectric constant of graphene encapsulated in hexagonal boron nitride (hBN) is $\varepsilon \approx 6$, although polarization effects due to remote bands in TBG could effectively make it several times larger \cite{Potasz,Gonzalez}. We regularize the on-site Coulomb interaction by choosing the onsite Hubbard term $V_{\alpha\alpha}(\boldsymbol{R}=0) = 12.4/\varepsilon$ eV of single layer graphene \cite{Wehling} and then smoothly interpolating it with Eq.~\eqref{eq:Hc} through $V_{\alpha\beta}(\boldsymbol{R}) \approx 1.438/[\varepsilon(0.116+|\boldsymbol{\tau}_\alpha - \boldsymbol{\tau}_\beta + \boldsymbol{R}|)]$ eV \cite{Radamaker}. Although this choice is not unique, the results do not depend on the details of the regularization.

Completion

You will be instructed to construct the interaction part of the Hamiltonian, $\mathcal{H}_{\mathrm{C}}$ 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 $V_{\alpha\beta}(\boldsymbol{R}_i - \boldsymbol{R}_j)$ The summation should be taken over all $\alpha\beta$ and all real space positions.

Return the interaction term $\mathcal{H}_{\mathrm{C}}$ in terms of $\hat{n}_{\alpha,i}$.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): $\hat{n}_{\alpha,i} = \sum_\sigma d^\dagger_{\alpha,i,\sigma} d_{\alpha,i,\sigma}$ is the local density operator and $V_{\alpha\beta}(\boldsymbol{R}) = e^2/(\varepsilon\xi) \sum_{m=-\infty}^{\infty} (-1)^m [(|\boldsymbol{\tau}_\alpha - \boldsymbol{\tau}_\beta + \boldsymbol{R}|/\xi)^2 + m^2]^{-\frac{1}{2}}$ is the screened form of the interaction in the presence of symmetric gates located at the top and bottom of the TBG heterostructure.

3 Fourier transform noninteracting term to momentum space (lattice)

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 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:
absence of strain effects and rewrite the Hamiltonian in momentum representation,

$$\mathcal{H} = \sum_{\alpha\beta} \sum_{\boldsymbol{k},\sigma} h_{\alpha\beta}(\boldsymbol{k}) d^{\dagger}_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma} + \mathcal{H}_{\mathrm{C}},$$

Completion
You will be instructed to convert the noninteracting Hamiltonian \mathcal{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 d*{\alpha,\bm{k},\sigma}^{\dagger} in the real space to the d*{\alpha,\bm{k},\sigma}^{\dagger} 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 \mathcal{H} in terms of d_{\alpha,\bm{k},\sigma}^{\dagger}. Simplify any summation index if possible. Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): {definition_of_variables}

4 Fourier transform interacting 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 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:

$$\mathcal{H}_{\mathrm{C}} = \frac{1}{2} \sum_{\alpha\beta} \sum_{\boldsymbol{q}} \hat{n}_{\alpha}(\boldsymbol{q}) V_{\alpha\beta}(\boldsymbol{q}) \hat{n}_{\beta}(-\boldsymbol{q}),$$

with $V_{\alpha\beta}(\boldsymbol{q})$ being the Fourier transform of the Coulomb interaction in Eq.~\eqref{eq:Hc}.
Completion
You will be instructed to convert the interacting Hamiltonian, $\mathcal{H}_{\mathrm{C}}$, 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 $\hat{n}_{\alpha}$ in the real space to $\hat{n}_{\alpha}(\boldsymbol{q})$ in the momentum space, which is defined as $V_{\alpha\beta}(\boldsymbol{q})$, where α is integrated over all sites in the entire real space, and $\boldsymbol{q}$ 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 $\mathcal{H}_{\mathrm{C}}$ in terms of $\hat{n}_{\alpha}(\boldsymbol{q})$. 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 †, 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:

$$\mathcal{H}_{\mathrm{HF}} = \sum_{\boldsymbol{k},\sigma} \sum_{\alpha\beta} \bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) d^\dagger_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma}.$$

Here $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) = h_{\alpha\beta}(\boldsymbol{k}) + h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) + h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree,

$$h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) = \delta_{\alpha\beta} \sum_{\gamma,\boldsymbol{k}',\sigma'} V_{\beta\gamma}(0)\rho_{\gamma\gamma}(\boldsymbol{k}',\sigma'),$$

and Fock contributions,

$$h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma) = -\sum_{\boldsymbol{k}'} V_{\alpha\beta}(\boldsymbol{k}-\boldsymbol{k}')\rho_{\alpha\beta}(\boldsymbol{k}',\sigma).$$

Each contribution can be cast in terms of the $N_b \times N_b$ zero-temperature density matrix for a given momentum and spin,

$$\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \sum_{n}^{\mathrm{occupied}} \phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)\phi^{(n)*}_{\beta,\boldsymbol{k}}(\sigma),$$

which is defined as a sum over all occupied bands, with $n = 1, \ldots, N_b$. The N_b-component spinors $\phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)$ describe the exact eigenvectors of Eq.~\eqref{eq:H_HF}, which need to be calculated self-consistently while enforcing a fixed total number of particles per unit cell.

Completion
Template:
You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $\mathcal{H}_{\mathrm{HF}}$.
You should use Wick's theorem to expand the four-fermion term in $\mathcal{H}_{\mathrm{HF}}$ into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without †, 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 $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma)$.
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):

$\mathcal{H}_{\mathrm{HF}}$ is the Hartree-Fock Hamiltonian, $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree and Fock contributions, $h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ and $h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ are the Hartree and Fock contributions respectively, $\rho_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the zero-temperature density matrix for a given momentum and spin, and $\phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)$ are the exact eigenvectors of $\mathcal{H}_{\mathrm{HF}}$.

6 Drop constant terms

Prompt
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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:

$$\mathcal{H}_{\mathrm{HF}} = \sum_{\boldsymbol{k},\sigma} \sum_{\alpha\beta} \bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) d^{\dagger}_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma}.$$

Here $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) = h_{\alpha\beta}(\boldsymbol{k}) + h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) + h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree,

$$h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) = \delta_{\alpha\beta} \sum_{\gamma,\boldsymbol{k}',\sigma'} V_{\beta\gamma}(0)\rho_{\gamma\gamma}(\boldsymbol{k}',\sigma'),$$

and Fock contributions,

$$h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma) = -\sum_{\boldsymbol{k}'} V_{\alpha\beta}(\boldsymbol{k}-\boldsymbol{k}')\rho_{\alpha\beta}(\boldsymbol{k}',\sigma).$$

Each contribution can be cast in terms of the $N_b \times N_b$ zero-temperature density matrix for a given momentum and spin,

$$\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \sum_{n}^{\mathrm{occupied}} \phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)\phi^{(n)*}_{\beta,\boldsymbol{k}}(\sigma),$$

which is defined as a sum over all occupied bands, with $n = 1,\ldots,N_b$. The N_b-component spinors $\phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)$ describe the exact eigenvectors of Eq.~\eqref{eq:H_HF}, which need to be calculated self-consistently while enforcing a fixed total number of particles per unit cell.
Completion
You will be instructed to extract the quadratic terms in the Hartree-Fock term.
The quadratic terms mean terms that are proportional to $d^{\dagger}_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma}$, which excludes terms that are solely expectations or products of expectations.
You should only preserve the quadratic terms in the Hartree-Fock term, denoted as $\mathcal{H}_{\mathrm{HF}}$.
Return $\mathcal{H}_{\mathrm{HF}}$.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
$\mathcal{H}_{\mathrm{HF}}$ is the Hartree-Fock term, $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree and Fock contributions, $d^{\dagger}_{\alpha,\boldsymbol{k},\sigma}$ and $d_{\beta,\boldsymbol{k},\sigma}$ are creation and annihilation operators respectively, and $\rho_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the zero-temperature density matrix for a given momentum and spin.

7 Identify momentum transfer in interaction

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 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:

$$\mathcal{H}_{\mathrm{HF}} = \sum_{\boldsymbol{k},\sigma} \sum_{\alpha\beta} \bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) d^{\dagger}_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma}.$$

Here $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) = h_{\alpha\beta}(\boldsymbol{k}) + h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) + h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree,

$$h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) = \delta_{\alpha\beta} \sum_{\gamma,\boldsymbol{k}',\sigma'} V_{\beta\gamma}(0)\rho_{\gamma\gamma}(\boldsymbol{k}',\sigma'),$$

and Fock contributions,

$$h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma) = -\sum_{\boldsymbol{k}'} V_{\alpha\beta}(\boldsymbol{k}-\boldsymbol{k}')\rho_{\alpha\beta}(\boldsymbol{k}',\sigma).$$

Each contribution can be cast in terms of the $N_b \times N_b$ zero-temperature density matrix for a given momentum and spin,

$$\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \sum_{n}^{\mathrm{occupied}} \phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)\phi^{(n)*}_{\beta,\boldsymbol{k}}(\sigma),$$

which is defined as a sum over all occupied bands, with $n = 1,\ldots,N_b$. The N_b-component spinors $\phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)$ describe the exact eigenvectors of Eq.~\eqref{eq:H_HF}, which need to be calculated self-consistently while enforcing a fixed total number of particles per unit cell.

Completion
You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $\mathcal{H}_{\mathrm{HF}}$. If you find the $V(q)$ in $\mathcal{H}_{\mathrm{HF}}$ 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 $\boldsymbol{k}$. Return $\mathcal{H}_{\mathrm{HF}}$ with expanded interaction.

8 Relabel the index

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 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:

$$\mathcal{H}_{\mathrm{HF}} = \sum_{\boldsymbol{k},\sigma} \sum_{\alpha\beta} \bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) d^{\dagger}_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma}.$$

Here $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) = h_{\alpha\beta}(\boldsymbol{k}) + h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) + h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree,

$$h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) = \delta_{\alpha\beta} \sum_{\gamma,\boldsymbol{k}',\sigma'} V_{\beta\gamma}(0) \rho_{\gamma\gamma}(\boldsymbol{k}',\sigma'),$$

and Fock contributions,

$$h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma) = -\sum_{\boldsymbol{k}'} V_{\alpha\beta}(\boldsymbol{k}-\boldsymbol{k}') \rho_{\alpha\beta}(\boldsymbol{k}',\sigma).$$

Each contribution can be cast in terms of the $N_b \times N_b$ zero-temperature density matrix for a given momentum and spin,

$$\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \sum_{n}^{\mathrm{occupied}} \phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma) \phi^{(n)*}_{\beta,\boldsymbol{k}}(\sigma),$$

which is defined as a sum over all occupied bands, with $n = 1, \ldots, N_b$. The N_b-component spinors $\phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)$ describe the exact eigenvectors of Eq.~\eqref{eq:H_HF}, which need to be calculated self-consistently while enforcing a fixed total number of particles per unit cell.

Completion

You will be instructed to simplify the quadratic term $\mathcal{H}_{\mathrm{HF}}$ through relabeling the index.

The logic is that the expected value ($\rho_{\alpha\beta}(\boldsymbol{k},\sigma)$) in the first Hartree term ($h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma)$) has the same form as the quadratic operators in the second Hartree term ($h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma)$), and vice versa. The same applies to the Fock term.

Namely, a replacement of {α and β} is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes {$\boldsymbol{k},\sigma$}.

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 $\mathcal{H}_{\mathrm{HF}}$.

9 Identify order parameters in Hartree term

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, {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. 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 {Hartree_second_quantized_symbol}.

Excerpt:

$$\mathcal{H}_{\mathrm{HF}} = \sum_{\boldsymbol{k},\sigma} \sum_{\alpha\beta} \bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) d^{\dagger}_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma}.$$

Here $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) = h_{\alpha\beta}(\boldsymbol{k}) + h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) + h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree,

$$h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) = \delta_{\alpha\beta} \sum_{\gamma,\boldsymbol{k}',\sigma'} V_{\beta\gamma}(0)\rho_{\gamma\gamma}(\boldsymbol{k}',\sigma'),$$

and Fock contributions,

$$h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma) = -\sum_{\boldsymbol{k}'} V_{\alpha\beta}(\boldsymbol{k} - \boldsymbol{k}')\rho_{\alpha\beta}(\boldsymbol{k}',\sigma).$$

Each contribution can be cast in terms of the $N_b \times N_b$ zero-temperature density matrix for a given momentum and spin,

$$\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \sum_{n}^{\mathrm{occupied}} \phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)\phi^{(n)*}_{\beta,\boldsymbol{k}}(\sigma),$$

which is defined as a sum over all occupied bands, with $n = 1, \ldots, N_b$. The N_b-component spinors $\phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)$ describe the exact eigenvectors of Eq.~\eqref{eq:H_HF}, which need to be calculated self-consistently while enforcing a fixed total number of particles per unit cell.

Completion

You will be instructed to simplify the Hartree term, $h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma)$, by reducing the momentum inside the expected value $\rho_{\alpha\beta}(\boldsymbol{k},\sigma)$.

The expected value $\rho_{\alpha\beta}(\boldsymbol{k},\sigma)$ is only nonzero when the two momenta $\boldsymbol{k}, \boldsymbol{k}'$ are the same, namely, $\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \delta_{\alpha\beta} \sum_{\gamma,\boldsymbol{k}',\sigma'} V_{\beta\gamma}(0)\rho_{\gamma\gamma}(\boldsymbol{k}',\sigma')$.

You should use the property of Kronecker delta function $\delta_{\boldsymbol{k},\boldsymbol{k}'}$ to reduce one momentum $\boldsymbol{k}$. 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 $h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma)$.

10 Identify order parameters in Fock term

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. 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:

$$\mathcal{H}_{\mathrm{HF}} = \sum_{\boldsymbol{k},\sigma} \sum_{\alpha\beta} \bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) d^{\dagger}_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma}.$$

Here $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) = h_{\alpha\beta}(\boldsymbol{k}) + h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) + h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree,

$$h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) = \delta_{\alpha\beta} \sum_{\gamma,\boldsymbol{k}',\sigma'} V_{\beta\gamma}(0)\rho_{\gamma\gamma}(\boldsymbol{k}',\sigma'),$$

and Fock contributions,

$$h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma) = -\sum_{\boldsymbol{k}'} V_{\alpha\beta}(\boldsymbol{k}-\boldsymbol{k}')\rho_{\alpha\beta}(\boldsymbol{k}',\sigma).$$

Each contribution can be cast in terms of the $N_b \times N_b$ zero-temperature density matrix for a given momentum and spin,

$$\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \sum_{n}^{\mathrm{occupied}} \phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)\phi^{(n)*}_{\beta,\boldsymbol{k}}(\sigma),$$

which is defined as a sum over all occupied bands, with $n = 1,\ldots,N_b$. The N_b-component spinors $\phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)$ describe the exact eigenvectors of Eq.~\eqref{eq:H_HF}, which need to be calculated self-consistently while enforcing a fixed total number of particles per unit cell.
Completion
You will be instructed to simplify the Fock term in $h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ by reducing the momentum inside the expected value $\rho_{\alpha\beta}(\boldsymbol{k},\sigma)$.
The expected value $\rho_{\alpha\beta}(\boldsymbol{k},\sigma)$ is only nonzero when the two momenta $\boldsymbol{k},\boldsymbol{k}'$ are the same, namely, $\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \sum_{n}^{\mathrm{occupied}} \phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)\phi^{(n)*}_{\beta,\boldsymbol{k}}(\sigma)$.
You should use the property of Kronecker delta function $\delta_{\boldsymbol{k},\boldsymbol{k}'}$ to reduce one momentum $\boldsymbol{k}$.
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 $h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$.

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:
{..} 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 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:

$$\mathcal{H}_{\mathrm{HF}} = \sum_{\boldsymbol{k},\sigma} \sum_{\alpha\beta} \bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) d^{\dagger}_{\alpha,\boldsymbol{k},\sigma} d_{\beta,\boldsymbol{k},\sigma}.$$

Here $\bar{h}_{\alpha\beta}(\boldsymbol{k},\sigma) = h_{\alpha\beta}(\boldsymbol{k}) + h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) + h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ is the renormalized matrix elements due to both Hartree,

$$h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma) = \delta_{\alpha\beta} \sum_{\gamma,\boldsymbol{k}',\sigma'} V_{\beta\gamma}(0)\rho_{\gamma\gamma}(\boldsymbol{k}',\sigma'),$$

and Fock contributions,

$$h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma) = -\sum_{\boldsymbol{k}'} V_{\alpha\beta}(\boldsymbol{k}-\boldsymbol{k}')\rho_{\alpha\beta}(\boldsymbol{k}',\sigma).$$

Each contribution can be cast in terms of the $N_b \times N_b$ zero-temperature density matrix for a given momentum and spin,

$$\rho_{\alpha\beta}(\boldsymbol{k},\sigma) = \sum_n^{\mathrm{occupied}} \phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)\phi^{(n)*}_{\beta,\boldsymbol{k}}(\sigma),$$

which is defined as a sum over all occupied bands, with $n = 1,\ldots,N_b$. The N_b-component spinors $\phi^{(n)}_{\alpha,\boldsymbol{k}}(\sigma)$ describe the exact eigenvectors of Eq.~\eqref{eq:H_HF}, which need to be calculated self-consistently while enforcing a fixed total number of particles per unit cell.

Completion

You will now be instructed to combine the Hartree term $h^{\mathrm{H}}_{\alpha\beta}(\boldsymbol{k},\sigma)$ and the Fock term $h^{\mathrm{F}}_{\alpha\beta}(\boldsymbol{k},\sigma)$.
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.