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:
and three-dimensional (3D) clusters/unit cells. In each case, the orbital basis includes both 3d e_g orbitals at each Ni site and the 2p$_\sigma$ orbital at each O site, as shown in Fig. \ref{Fig:clusters}. The microscopic Hamiltonian for the electronic degrees of freedom is $H = H_0 + H_{\rm int}$, where

$$H_0 = \sum_{i,\alpha} \epsilon_\alpha d^\dagger_{i,\alpha,\sigma} d_{i,\alpha,\sigma} + \sum_{i,j,\alpha,\beta,\sigma} t^{\alpha\beta}_{ij} d^\dagger_{i,\alpha,\sigma} d_{j,\beta,\sigma}$$

contains the non-interacting on-site and near-neighbor hopping terms, and

Completion

You will be instructed to describe the kinetic term of Hamiltonian in 3D clusters/unit cells in the real space in the second-quantized form.
The degrees of freedom of the system are: both 3d e_g orbitals at each Ni site and the 2p$_\sigma$ orbital at each O site.
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 space positions.
Return the Kinetic Hamiltonian H_0.
Use the following conventions for the symbols:
ϵ_α is the on-site energy of orbital α, $d^\dagger_{i,\alpha,\sigma}$ and $d_{i,\alpha,\sigma}$ are the creation and annihilation operators for an electron in orbital α at site i with spin σ, and $t^{\alpha\beta}_{ij}$ is the hopping amplitude between orbitals α and β at sites i and j.

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:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to construct the interaction part of the Hamiltonian, {second_int_symbol} in the 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:

$$\begin{aligned} H_{\text{int}} = & \sum_{i,\alpha,\sigma\neq\sigma'} \frac{U}{2} n_{i,\alpha,\sigma} n_{i,\alpha,\sigma'} + \sum_{i,\alpha\neq\alpha',\sigma,\sigma'} \frac{U'}{2} n_{i,\alpha,\sigma} n_{i,\alpha',\sigma'} \\ + & \sum_{i,\alpha,\alpha',\sigma,\sigma'} \frac{J}{2} d^\dagger_{i,\alpha,\sigma} d^\dagger_{i,\alpha',\sigma'} d_{i,\alpha,\sigma'} d_{i,\alpha',\sigma} \\ + & \sum_{i,\alpha\neq\alpha',\sigma\neq\sigma'} \frac{J'}{2} d^\dagger_{i,\alpha,\sigma} d^\dagger_{i,\alpha,\sigma'} d_{i,\alpha',\sigma'} d_{i,\alpha',\sigma} \end{aligned}$$

contains the on-site Coulomb interactions with $n_{i,\alpha,\sigma} = d^\dagger_{i,\alpha,\sigma} d_{i,\alpha,\sigma}$, where $ d^\dagger_{i,\alpha,\sigma}$ creates a spin-σ electron in one of the two e_g orbitals if i is a Ni site, or the $2p_\sigma$ orbital if i is an O site. In eV units we set $U_d = 7$, $J_d = J'_d = 0.9$, $U'_d = U_d - 2J_d$, $U_p = 5$, $\epsilon_d = 0$, $\epsilon_p = 2.25$, $(pd\sigma) = -1.8$, $(pp\sigma) = 0.6$, $(pd\pi) = -(pd\sigma)/2$, and $(pp\pi) = -(pp\sigma)/4$. For these parameters the ground state of an isolated NiO_6 octahedron is $|\Psi\rangle = \alpha |d^7\rangle +\beta|d^8\ligand\rangle + \gamma|d^9\ligand^2\rangle$ with $\beta^2 \approx 0.56$, i.e. the system is in the negative charge transfer regime and the ground state has predominantly $d^8\underline{\mathrm{L}}$ character, in agreement with experiment \cite{MizokawaPRB1995,AbbatePRB2002,HoribePRB2007,Bodenthin2011}.
Completion
You will be instructed to construct the interaction part of the Hamiltonian, H_{int} 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 U, U', J, and J' The summation should be taken over all spin and orbital degrees of freedom and all real space positions.
Return the interaction term H_{int} in terms of $n_{i,\alpha,\sigma}$.
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): $n_{i,\alpha,\sigma} = d^\dagger_{i,\alpha,\sigma} d_{i,\alpha,\sigma}$ where $d^\dagger_{i,\alpha,\sigma}$ creates a spin-σ electron in one of the two e_g orbitals if i is a Ni site, or the $2p_\sigma$ orbital if i is an O site.

3 Fourier transform noninteracting term to momentum space (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 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:
Hamiltonian given in the main text.
Our treatment follows that of Ref. \onlinecite{MeanField}, which we summarize here for completeness. We work in momentum space where the microscopic Hamiltonian can be rewritten in the form

$$H = \sum_{\mathbf{k},\alpha,\beta,\sigma} T_{\alpha,\beta}(\mathbf{k}) d^\dagger_{\mathbf{k},\alpha,\sigma} d_{\mathbf{k},\beta,\sigma} + \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U^{\sigma,\sigma'}_{\alpha,\alpha',\beta,\beta'}(\mathbf{q}) d^\dagger_{\mathbf{k},\alpha,\sigma} d^\dagger_{\mathbf{k}',\alpha',\sigma'} d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} d_{\mathbf{k}+\mathbf{q},\beta,\sigma}.$$

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 d in the real space to the d in the momentum space, which is defined as $T_{\alpha,\beta}(\mathbf{k}) d^\dagger_{\mathbf{k},\alpha,\sigma} d_{\mathbf{k},\beta,\sigma}$, where $\mathbf{k}$ 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 in terms of d. 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 is the Hamiltonian, $\mathbf{k}$ is the momentum, α and β are the indices for the basis in momentum space, σ is the spin index, $T_{\alpha,\beta}(\mathbf{k})$ is the Fourier transformation, and $d^\dagger_{\mathbf{k},\alpha,\sigma}$ and $d_{\mathbf{k},\beta,\sigma}$ are the creation and annihilation operators in momentum space respectively.

4 Fourier transform interacting term to momentum space (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 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:
Hamiltonian given in the main text.
Our treatment follows that of Ref. \onlinecite{MeanField}, which we summarize here for completeness. We work in momentum space where the microscopic Hamiltonian can be rewritten in the form

$$H = \sum_{\mathbf{k},\alpha,\beta,\sigma} T_{\alpha,\beta}(\mathbf{k}) d^\dagger_{\mathbf{k},\alpha,\sigma} d_{\mathbf{k},\beta,\sigma} + \sum_{\alpha,\alpha',\beta,\beta',\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U^{\sigma,\sigma'}_{\alpha,\alpha',\beta,\beta'}(\mathbf{q}) d^\dagger_{\mathbf{k},\alpha,\sigma} d^\dagger_{\mathbf{k}',\alpha',\sigma'} d_{\mathbf{k}'-\mathbf{q},\beta',\sigma'} d_{\mathbf{k}+\mathbf{q},\beta,\sigma}.$$

where the interaction on a Ni site is given by

$$\begin{aligned} U^{\sigma\sigma'}_{\alpha,\alpha',\beta,\beta'} = & \quad \frac{U}{2}\delta_{-\sigma,\sigma'}\delta_{\alpha,\alpha'}\delta_{\alpha\beta}\delta_{\alpha\beta'} + \frac{U'}{2}(1-\delta_{\alpha\alpha'})\delta_{\alpha\beta}\delta_{\alpha'\beta'} \\ + & \quad \frac{J}{2}(1-\delta_{\alpha\alpha'})\delta_{\alpha\beta'}\delta_{\alpha'\beta} + \frac{J'}{2}\delta_{\alpha\alpha'}\delta_{\beta\beta'}(1-\delta_{\sigma\sigma'})(1-\delta_{\alpha\beta}). \end{aligned}$$

The interaction on an O site is like the first term with U replaced by U_p.
Completion
You will be instructed to convert the interacting Hamiltonian, $U^{\sigma\sigma'}_{\alpha,\alpha',\beta,\beta'}$, 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 $d^\dagger_{\mathbf{k},\alpha,\sigma}$ in the real space to the $d^\dagger_{\mathbf{k},\alpha,\sigma}$ in the momentum space, which is defined as $H=\sum_{\mathbf{k},\alpha,\beta,\sigma} T_{\alpha,\beta}(\mathbf{k}) d^\dagger_{\mathbf{k},\alpha,\sigma} d_{\mathbf{k},\beta,\sigma}$, where $\mathbf{k}$ is integrated over all sites in the entire real space, and α,β,σ 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 $U^{\sigma\sigma'}_{\alpha,\alpha',\beta,\beta'}$ in terms of $d^\dagger_{\mathbf{k},\alpha,\sigma}$. Simplify any summation index if possible.

5 Wick's theorem expansion

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, {second_int_symbol}.
You should use Wick's theorem to expand the four-fermion term in {second_int_symbol} into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without †, and be extremely cautious about the order of the index and sign before each term.
You should only preserve the normal terms. Here, the normal terms mean the product of a creation operator and an annihilation operator.
Return the expanded interaction term after Hartree-Fock approximation as {Hartree_Fock_symbol}.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{definition_of_variables}
Excerpt:

$$
\begin{aligned}
M_{\alpha\beta}(\mathbf{k}) = T_{\alpha,\beta}(\mathbf{k}) + & \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta',\sigma'} \left[U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}\right] \langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle \\
- & \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta'} \left[U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}\right] \langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle
\end{aligned}
$$

where the average $\langle\rangle$ defines the self-consistent HF fields, which are found iteratively. It should be noted that the dependence on the static lattice displacement is introduced through the kinetic term $T_{\alpha,\beta}(\mathbf{k})$, see main text.
Completion
You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $M_{\alpha\beta}(\mathbf{k})$.
You should use Wick's theorem to expand the four-fermion term in $M_{\alpha\beta}(\mathbf{k})$ 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 $\langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$ and $\langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$.
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):

$M_{\alpha\beta}(\mathbf{k})$ is the interaction term, $T_{\alpha,\beta}(\mathbf{k})$ is the kinetic term, $\langle\rangle$ defines the self-consistent Hartree-Fock fields, $U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'}$ and $U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}$ are the interaction terms, and $d^{\dagger}_{\mathbf{q},\alpha',\sigma'}$ and $d_{\mathbf{q},\beta',\sigma'}$ are the creation and annihilation operators respectively.

6 Drop constant terms

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to extract the quadratic terms in the {Hartree_Fock_term_symbol}.
The quadratic terms mean terms that are proportional to {bilinear_op}, which excludes terms that are solely expectations or products of expectations.
You should only preserve the quadratic terms in {Hartree_Fock_term_symbol}, denoted as {Hartree_Fock_second_quantized_symbol}.
Return {Hartree_Fock_second_quantized_symbol}.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{definition_of_variables}
Excerpt:

$$M_{\alpha\beta}(\mathbf{k}) = T_{\alpha,\beta}(\mathbf{k}) + \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta',\sigma'} \left[U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}\right] \langle d^{\dagger}_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$$
$$- \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta'} \left[U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}\right] \langle d^{\dagger}_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$$

where the average $\langle\rangle$ defines the self-consistent HF fields, which are found iterationally. It should be noted that the dependence on the static lattice displacement is introduced through the kinetic term $T_{\alpha,\beta}(\mathbf{k})$, see main text.
Completion
You will be instructed to extract the quadratic terms in the $M_{\alpha\beta}(\mathbf{k})$.
The quadratic terms mean terms that are proportional to $d^{\dagger}_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}$, which excludes terms that are solely expectations or products of expectations.
You should only preserve the quadratic terms in $M_{\alpha\beta}(\mathbf{k})$, denoted as $M^{(2)}_{\alpha\beta}(\mathbf{k})$.
Return $M^{(2)}_{\alpha\beta}(\mathbf{k})$.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
$\mathbf{k}$ is the momentum vector, α and β are band indices, σ and σ' are spin indices, $\mathbf{q}$ is the wave vector, $d^{\dagger}_{\mathbf{q},\alpha',\sigma'}$ and $d_{\mathbf{q},\beta',\sigma'}$ are creation and annihilation operators respectively, $U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'}$ and $U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}$ are interaction terms, and $T_{\alpha,\beta}(\mathbf{k})$ is the kinetic term. The average $\langle\rangle$ defines the self-consistent Hartree-Fock fields.

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:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to expand interaction term $V(q)$ in the MF quadratic term {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:

$$\begin{aligned} M_{\alpha\beta}(\mathbf{k}) = T_{\alpha,\beta}(\mathbf{k}) + & \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta',\sigma'} \left[U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}\right] \langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle \\ - & \quad \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta'} \left[U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}\right] \langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle \end{aligned}$$

where the average $\langle\rangle$ defines the self-consistent HF fields, which are found iteratively. It should be noted that the dependence on the static lattice displacement is introduced through the kinetic term $T_{\alpha,\beta}(\mathbf{k})$, see main text.
Completion
You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $M_{\alpha\beta}(\mathbf{k})$. If you find the $V(q)$ in $M_{\alpha\beta}(\mathbf{k})$ 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 $\mathbf{q}$. Return $M_{\alpha\beta}(\mathbf{k})$ 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:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to simplify the quadratic term {Hartree_Fock_second_quantized_symbol} through relabeling the index.
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:

$$\begin{aligned} M_{\alpha\beta}(\mathbf{k}) = T_{\alpha,\beta}(\mathbf{k}) + & \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta',\sigma'} \left[U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}\right] \langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle \\ - & \quad \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta'} \left[U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}\right] \langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle \end{aligned}$$

where the average $\langle\rangle$ defines the self-consistent HF fields, which are found iteratively. It should be noted that the dependence on the static lattice displacement is introduced through the kinetic term $T_{\alpha,\beta}(\mathbf{k})$, see main text.
Completion

You will be instructed to simplify the quadratic term $M_{\alpha\beta}(\mathbf{k})$ through relabeling the index.
The logic is that the expected value ($\langle d^{\dagger}_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$) in the first Hartree term ($U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}$) has the same form as the quadratic operators in the second Hartree term ($U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}$), and vice versa. The same applies to the Fock term.
Namely, a replacement of $\alpha', \beta, \beta', \alpha$ is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes $\mathbf{q}, \sigma, \sigma'$.
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 $M_{\alpha\beta}(\mathbf{k})$.

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:
{..} 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 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 $\langle\dots\rangle$. 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:

$$M_{\alpha\beta}(\mathbf{k}) = T_{\alpha,\beta}(\mathbf{k}) + \frac{1}{2} \sum_{\mathbf{q},\alpha',\beta',\sigma'} \left[U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}\right] \langle d^{\dagger}_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle - \frac{1}{2} \sum_{\mathbf{q},\alpha',\beta'} \left[U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}\right] \langle d^{\dagger}_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$$

where the average $\langle\rangle$ defines the self-consistent HF fields, which are found iterationally. It should be noted that the dependence on the static lattice displacement is introduced through the kinetic term $T_{\alpha,\beta}(\mathbf{k})$, see main text.
Completion
You will be instructed to simplify the Hartree term, $M_{\alpha\beta}(\mathbf{k})$, by reducing the momentum inside the expected value $\langle d^{\dagger}_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$ and $\langle d^{\dagger}_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$.
The expected value $\langle d^{\dagger}_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$ and $\langle d^{\dagger}_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\mathbf{q} = \mathbf{q}$.
You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum $\mathbf{q}$. Once you reduce one momentum inside the expected value $\langle d^{\dagger}_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$ and $\langle d^{\dagger}_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$. 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 $M_{\alpha\beta}(\mathbf{k})$.

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 $\langle\dots\rangle$. 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 {Fock_second_quantized_symbol}.
Excerpt:

$$\begin{aligned} M_{\alpha\beta}(\mathbf{k}) = T_{\alpha,\beta}(\mathbf{k}) + & \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta',\sigma'} \left[U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}\right] \langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle \\ - & \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta'} \left[U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}\right] \langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle \end{aligned}$$

where the average $\langle\rangle$ defines the self-consistent HF fields, which are found iterationally. It should be noted that the dependence on the static lattice displacement is introduced through the kinetic term $T_{\alpha,\beta}(\mathbf{k})$, see main text.
Completion
You will be instructed to simplify the Fock term in $M_{\alpha\beta}(\mathbf{k})$ by reducing the momentum inside the expected value $\langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$ and $\langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$.
The expected value $\langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$ and $\langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$ is only nonzero when the two momenta $\mathbf{q}, \mathbf{q}$ are the same, namely, $\langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$ and $\langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$.
You should use the property of Kronecker delta function $\delta_{\mathbf{q},\mathbf{q}}$ to reduce one momentum $\mathbf{q}$.
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 $M_{\alpha\beta}(\mathbf{k})$.

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:

$$M_{\alpha\beta}(\mathbf{k}) = T_{\alpha,\beta}(\mathbf{k}) + \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta',\sigma'}\left[U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}\right]\langle d^\dagger_{\mathbf{q},\alpha',\sigma'} d_{\mathbf{q},\beta',\sigma'}\rangle$$
$$- \frac{1}{2}\sum_{\mathbf{q},\alpha',\beta'}\left[U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}\right]\langle d^\dagger_{\mathbf{q},\alpha',\sigma} d_{\mathbf{q},\beta',\sigma}\rangle$$

where the average $\langle\rangle$ defines the self-consistent HF fields, which are found iteratively. It should be noted that the dependence on the static lattice displacement is introduced through the kinetic term $T_{\alpha,\beta}(\mathbf{k})$, see main text.

Completion

You will now be instructed to combine the Hartree term $U^{\sigma\sigma'}_{\beta,\alpha',\alpha,\beta'} + U^{\sigma'\sigma}_{\alpha',\beta,\beta',\alpha}$ and the Fock term $U^{\sigma\sigma}_{\alpha',\beta,\alpha,\beta'} + U^{\sigma\sigma}_{\beta,\alpha',\beta',\alpha}$.
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 : $\alpha', \beta, \alpha, \beta'$ to $\beta, \alpha', \beta', \alpha$. You should add them, relabel the index in Fock term, and simply their sum. Return the final sum of Hartree and Fock term.