

1 Identify kinetic term (continuum,first-quantized)

Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

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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 describe the kinetic term of Hamiltonian in {system} in the {real|momen-
tum} space in the {single-particle|second-quantized} form.

The degrees of freedom of the system are: {degrees_of_freedom}.

Express the Kinetic Hamiltonian {kinetic_symbol} using {variable} which are only on the diagonal terms, and arrange the basis in the order of {order}. [Note that the sublattice degrees of freedom is suppressed for now and will be stated later]

Use the following conventions for the symbols:

{definition_of_variables}

Excerpt:

We write the model's Bloch basis states in the form

$$\psi_{\mathbf{k}\kappa}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}(\mathbf{R}_i + \boldsymbol{\tau}_{\kappa})} \phi(\mathbf{r} - \mathbf{R}_i - \boldsymbol{\tau}_{\kappa}),$$

where N is the total number of unit cells in the system, $\phi(\mathbf{r})$ is the band's Wannier wavefunction, and κ labels the carbon site with position $\boldsymbol{\tau}_{\kappa}$ relative to a the triangular lattice vector \mathbf{R}_i . (We comment later on the possible role of screening effects from the p and s orbitals which form the σ and σ^* bonds neglected in this model.) Following the convention used in Refs.[\onlinecite{falko,hongki}], we use the notations {\em A}, {\em B}, \bar{A} , \bar{B} for the four sublattice indexes κ , where {\em B} and \bar{A} are the opposite-layer near-neighbor-pair sites.

Completion

You will be instructed to describe the kinetic term of Hamiltonian in the model's Bloch basis states in the real space in the second-quantized form.

The degrees of freedom of the system are: the total number of unit cells in the system, the band's Wannier wavefunction, and the carbon site with position relative to a the triangular lattice vector.

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

Use the following conventions for the symbols:

N is the total number of unit cells in the system, ϕ is the band's Wannier wavefunction, and κ labels the carbon site with position $\boldsymbol{\tau}_{\kappa}$ relative to a the triangular lattice vector \mathbf{R}_i . The notations A , B , \bar{A} , \bar{B} are used for the four sublattice indexes κ , where B and \bar{A} are the opposite-layer near-neighbor-pair sites.

2 Define energy dispersion (continuum)

Prompt

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Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to construct each term, namely {Energy_dispersion}.

For all energy dispersions, {Energy_dispersion}, it characterizes the {parabolic|Dirac|cos} dispersion for {electrons|holes}.

[In addition, a shift of {momentum_shift} in the momentum k_{symbol} for {shifted_Ek}, respectively.] You should follow the EXAMPLE below to obtain correct energy dispersion, select the correct EXAMPLE by noticing the type of dispersion.

Finally, in the real space, the momentum $k_{symbol} = -i\partial_{r_{symbol}}$. You should keep the form of k_{symbol} in the Hamiltonian for short notations but should remember k_{symbol} is an operator.

Return the expression for {Energy_dispersion} in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian {kinetic_symbol}.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):

{definition_of_variables}

Excerpt:

$$H_0 = \begin{pmatrix} 0 & \gamma_0 f & \gamma_4 f & \gamma_3 f^* \\ \gamma_0 f^* & 0 & \gamma_1 & \gamma_4 f \\ \gamma_4 f^* & \gamma_1 & 0 & \gamma_0 f \\ \gamma_3 f & \gamma_4 f^* & \gamma_0 f^* & 0 \end{pmatrix}$$

where

$$f(\mathbf{k}) = e^{ik_y a / \sqrt{3}} \left(1 + 2e^{-i3k_y a / 2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right) \right)$$

with $a = 2.46$ arises from a sum over the three near-neighbor hops within a layer. We have neglected differences in on-site energies and next nearest neighbor hopping processes which give rise to electron-hole asymmetry and do not play an important role in pseudospin ferromagnetism. The tight-binding model parameters γ_i should not be confused with the Slonczewski-Weiss, McClure \cite{swm} model parameters for bulk graphite, despite the obvious similarities in notation. In our calculations we adopt conventions similar to those of Ref.[\onlinecite{gamma3}] for bilayer graphene, taking the values $\gamma_0 = -3.12$ eV, $\gamma_1 = -0.377$, $\gamma_3 = -0.29$ eV and $\gamma_4 = -0.12$ eV for the hopping parameters. Only the intralayer nearest neighbor (γ_0) process and interlayer tunneling (γ_1) process are retained in the minimal tight-binding model. The trigonal warping (γ_3) process which connects the A and \tilde{B} sites is responsible for the leading circular symmetry breaking near the valley points, while the (γ_4) process which connects A and \tilde{A} sites influences the intralayer charge imbalance between sublattices A and B .

Completion

Template:

You will be instructed to construct each term, namely {H}_0.

For all energy dispersions, {H}_0, it characterizes the {parabolic|Dirac|cos} dispersion for {electrons|holes}.

[In addition, a shift of {momentum_shift} in the momentum {k} for {shifted_Ek}, respectively.]

You should follow the EXAMPLE below to obtain correct energy dispersion, select the correct EXAMPLE by noticing the type of dispersion.

Finally, in the real space, the momentum $k = -i\partial_r$. You should keep the form of k in the Hamiltonian for short notations but should remember k is an operator.

Return the expression for {H}_0 in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian {H}_0.

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):

$$f(\mathbf{k}) = e^{ik_y a / \sqrt{3}} \left(1 + 2e^{-i3k_y a / 2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right) \right)$$

with $a = 2.46$ arises from a sum over the three near-neighbor hops within a layer. We have neglected differences in on-site energies and next nearest neighbor hopping processes which give rise to electron-hole asymmetry and do not play an important role in pseudospin ferromagnetism. The tight-binding model parameters γ_i should not be confused with the Slonczewski-Weiss, McClure \cite{swm} model parameters for bulk graphite, despite the obvious similarities in notation. In our calculations we adopt conventions similar to those of Ref.[\onlinecite{gamma3}] for bilayer graphene, taking the values $\gamma_0 = -3.12$ eV, $\gamma_1 = -0.377$, $\gamma_3 = -0.29$ eV and $\gamma_4 = -0.12$ eV for the hopping parameters. Only the intralayer nearest neighbor (γ_0) process and interlayer tunneling (γ_1) process are retained in the minimal tight-binding model. The trigonal warping (γ_3) process which connects the A and \tilde{B} sites is responsible for the leading circular symmetry breaking near the valley points, while the (γ_4) process which connects A and \tilde{A} sites influences the intralayer charge imbalance between sublattices A and B . }

3 Second-quantization (matrix)

Prompt

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Template:

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

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

To construct the second quantized form of a Hamiltonian. You should construct the creation and annihilation operators from the basis explicitly. You should follow the EXAMPLE below to convert a Hamiltonian from the single-particle form to second-quantized form.

Finally by "total", it means you need to take a summation over the {real|momentum} space position {r|k}.

Return the second quantized form of the total noninteracting Hamiltonian {second_nonint_symbol}

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):

{definition_of_variables}

Excerpt:

We write the model's Bloch basis states in the form

$$\psi_{\mathbf{k}\kappa}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}(\mathbf{R}_i + \boldsymbol{\tau}_\kappa)} \phi(\mathbf{r} - \mathbf{R}_i - \boldsymbol{\tau}_\kappa),$$

where N is the total number of unit cells in the system, $\phi(\mathbf{r})$ is the band's Wannier wavefunction, and κ labels the carbon site with position $\boldsymbol{\tau}_\kappa$ relative to a the triangular lattice vector \mathbf{R}_i . (We comment later on the possible role of screening effects from the p and s orbitals which form the σ and σ^* bonds neglected in this model.) Following the convention used in Refs.[\onlinecite{falko,hongki}], we use the notations {\em A}, {\em B}, \tilde{A} , \tilde{B} for the four sublattice indexes κ , where {\em B} and \tilde{A} are the opposite-layer near-neighbor-pair sites. With this convention, the four band tight-binding model Hamiltonian of a graphene bilayer is:

$$H_0 = \begin{pmatrix} 0 & \gamma_0 f & \gamma_4 f & \gamma_3 f^* \\ \gamma_0 f^* & 0 & \gamma_1 & \gamma_4 f \\ \gamma_4 f^* & \gamma_1 & 0 & \gamma_0 f \\ \gamma_3 f & \gamma_4 f^* & \gamma_0 f^* & 0 \end{pmatrix}$$

where

$$f(\mathbf{k}) = e^{ik_y a / \sqrt{3}} \left(1 + 2e^{-i3k_y a / 2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right) \right)$$

with $a = 2.46$ arises from a sum over the three near-neighbor hops within a layer. We have neglected differences in on-site energies and next nearest neighbor hopping processes which give rise to electron-hole asymmetry and do not play an important role in pseudospin ferromagnetism. The tight-binding model parameters γ_i should not be confused with the Slonczewski-Weiss, McClure \cite{sww} model parameters for bulk graphite, despite the obvious similarities in notation. In our calculations we adopt conventions similar to those of Ref.[\onlinecite{gamma3}] for bilayer graphene, taking the values $\gamma_0 = -3.12$ eV, $\gamma_1 = -0.377$, $\gamma_3 = -0.29$ eV and $\gamma_4 = -0.12$ eV for the hopping parameters. Only the intralayer nearest neighbor (γ_0) process and interlayer tunneling (γ_1) process are retained in the minimal tight-binding model. The trigonal warping (γ_3) process which connects the A and \tilde{B} sites is responsible for the leading circular symmetry breaking near the valley points, while the (γ_4) process which connects A and \tilde{A} sites influences the intralayer charge imbalance between sublattices A and B .

Completion

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

The noninteracting Hamiltonian in the momentum space H_0 is the sum of Kinetic Hamiltonian and Potential Hamiltonian.

To construct the second quantized form of a Hamiltonian. You should construct the creation and annihilation operators from the basis explicitly. You should follow the EXAMPLE below to convert a Hamiltonian from the single-particle form to second-quantized form.

Finally by "total", it means you need to take a summation over the momentum space position k .

Return the second quantized form of the total noninteracting Hamiltonian.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):

The model's Bloch basis states are written as $\psi_{\mathbf{k}\kappa}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}(\mathbf{R}_i + \boldsymbol{\tau}_\kappa)} \phi(\mathbf{r} - \mathbf{R}_i - \boldsymbol{\tau}_\kappa)$, where N is the total number of unit cells in the system, $\phi(\mathbf{r})$ is the band's Wannier wavefunction, and κ labels the carbon site with position $\boldsymbol{\tau}_\kappa$ relative to a the triangular lattice vector \mathbf{R}_i . The four band tight-binding model Hamiltonian of a graphene bilayer is represented as H_0 . The tight-binding model parameters are represented as γ_i .

4 Second-quantization (summation)

Prompt

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Template:

You will be instructed to expand the second-quantized form Hamiltonian {second_nonint_symbol} using {matrix_element_symbol} and {basis_symbol}. You should follow the EXAMPLE below to expand the Hamiltonian.

You should use any previous knowledge to simplify it. For example, if any term of {matrix_element_symbol} is zero, you should remove it from the summation. Return the expanded form of {second_nonint_symbol} after simplification.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):

{definition_of_variables}

Excerpt:

We write the model's Bloch basis states in the form

$$\psi_{\mathbf{k}\kappa}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}(\mathbf{R}_i + \boldsymbol{\tau}_\kappa)} \phi(\mathbf{r} - \mathbf{R}_i - \boldsymbol{\tau}_\kappa),$$

where N is the total number of unit cells in the system, $\phi(\mathbf{r})$ is the band's Wannier wavefunction, and κ labels the carbon site with position $\boldsymbol{\tau}_\kappa$ relative to a the triangular lattice vector \mathbf{R}_i . (We comment later on the possible role of screening effects from the p and s orbitals which form the σ and σ^* bonds neglected in this model.) Following the convention used in Refs.[\onlinecite{falko,hongki}], we use the notations {\em A}, {\em B}, \tilde{A} , \tilde{B} for the four sublattice indexes κ , where {\em B} and \tilde{A} are the opposite-layer near-neighbor-pair sites. With this convention, the four band tight-binding model Hamiltonian of a graphene bilayer is:

$$H_0 = \begin{pmatrix} 0 & \gamma_0 f & \gamma_4 f & \gamma_3 f^* \\ \gamma_0 f^* & 0 & \gamma_1 & \gamma_4 f \\ \gamma_4 f^* & \gamma_1 & 0 & \gamma_0 f \\ \gamma_3 f & \gamma_4 f^* & \gamma_0 f^* & 0 \end{pmatrix}$$

where

$$f(\mathbf{k}) = e^{ik_y a / \sqrt{3}} \left(1 + 2e^{-i3k_y a / 2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right) \right)$$

with $a = 2.46$ arises from a sum over the three near-neighbor hops within a layer. We have neglected differences in on-site energies and next nearest neighbor hopping processes which give rise to

electron-hole asymmetry and do not play an important role in pseudospin ferromagnetism. The tight-binding model parameters γ_i should not be confused with the Slonczewski-Weiss, McClure \cite{swm} model parameters for bulk graphite, despite the obvious similarities in notation. In our calculations we adopt conventions similar to those of Ref.[\onlinecite{gamma3}] for bilayer graphene, taking the values $\gamma_0 = -3.12 \text{ eV}$, $\gamma_1 = -0.377$, $\gamma_3 = -0.29 \text{ eV}$ and $\gamma_4 = -0.12 \text{ eV}$ for the hopping parameters. Only the intralayer nearest neighbor (γ_0) process and interlayer tunneling (γ_1) process are retained in the minimal tight-binding model. The trigonal warping (γ_3) process which connects the A and \tilde{B} sites is responsible for the leading circular symmetry breaking near the valley points, while the (γ_4) process which connects A and \tilde{A} sites influences the intralayer charge imbalance between sublattices A and B .

Completion

You will be instructed to expand the second-quantized form Hamiltonian $\{H\}_0$ using $\{\gamma_{\text{mai}}\}$ and $\{\psi_{\{\bm{k}\}\kappa}\}$. You should follow the EXAMPLE below to expand the Hamiltonian.

You should use any previous knowledge to simplify it. For example, if any term of $\{\gamma_{\text{mai}}\}$ is zero, you should remove it from the summation. Return the expanded form of $\{H\}_0$ after simplification. Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):

$\{H\}_0$ is the four band tight-binding model Hamiltonian of a graphene bilayer, $\{\psi_{\{\bm{k}\}\kappa}\}$ is the model's Bloch basis states, and $\{\gamma_i\}$ are the tight-binding model parameters.

5 Identify interacting term (momentum space)

Prompt

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Template:

You will be instructed to construct the interaction part of the Hamiltonian $\{\text{second_int_symbol}\}$ in the momentum space.

The interaction Hamiltonian is a product of four parts. The first part is the product of four operators with two creation and two annihilation operators following the normal order, namely, creation operators are before annihilation operators. You should follow the order of 1, 2, 2, 1 for the $\{\text{index_of_operator}\}$, and 1, 2, 3, 4 for the $\{\text{momentum}\}$. The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators. [For each operator, the total momentum is the sum of moire reciprocal lattice $b_{\text{ }i}$ and momentum with in the first BZ $k_{\text{ }i}$]

The third part is the interaction form. You should use $\{\text{interaction}\}$ with $V(q) = \text{int_form}$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same $\{\text{index_of_operator}\}$, namely $q = k_1 - k_4$.

The fourth part is the normalization factor, you should use $\{\text{normalization_factor}\}$ here. Finally, the summation should be running over all $\{\text{index_of_operator}\}$, and $\{\text{momentum}\}$ Return the interaction term $\{\text{second_int_symbol}\}$ in terms of $\{\text{op}\}$ and $V(q)$ (with q expressed in terms of $\{\text{momentum}\}$).

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):

$\{\text{definition_of_variables}\}$

Excerpt:

a Hartree-Fock mean-field theory approximation \cite{ostlund} is a natural first step in considering electron-electron interaction effects. $V^{\{\kappa \kappa^{\prime}\}}(\{\bm{q}\}) = 2 \pi e^2 / \left(\left| \{\bm{q}\} \right| \epsilon_{\text{nr}} \right)$ \$ when κ and κ' refer to the same layer and $\left(2 \pi e^2 / \left(\left| \{\bm{q}\} \right| \epsilon_{\text{nr}} \right) \right) \exp \{ \left[- \left| \{\bm{q}\} \right| c \right] \}$ \$ when κ and κ' refer to the opposite layers. Here ϵ_r is the relative dielectric constant, $c = 3.35$ is the interlayer separation, A is the total area of the graphene sheet, and we use

$$\tilde{f}(q) = (1 - (r_0 q)^2) / ((1 + (r_0 q)^2)^4)$$

as a form factor which accounts for the spread of the π -orbital charge on each site. This simple form assumes an isotropic site-localized charge distribution. Eq.~(\ref{formfactor}) was obtained by Fourier transforming the radial charge distribution of a hydrogenic $2p$ orbital. The use of $r_0 = \tilde{a}_0 = a_0/\sqrt{30}$ would yield a root mean square radius corresponding to the covalent radius of the carbon atom $a_0 = 0.77$. If we consider screening from the σ band electrons neglected in our model and the fact that the charge density distribution of a p_z orbital is far from spherical we expect that larger values of r_0 , which effectively reduce onsite repulsion, would be more appropriate. For most of our calculations we have therefore used the value $r_0 = 3\tilde{a}_0$.

Completion

Template:

You will be instructed to construct the interaction part of the Hamiltonian $V^{\kappa\kappa'}$ in the momentum space.

The interaction Hamiltonian is a product of four parts. The first part is the product of four operators with two creation and two annihilation operators following the normal order, namely, creation operators are before annihilation operators. You should follow the order of $\kappa, \kappa', \kappa', \kappa$ for the index of operator, and 1, 2, 3, 4 for the momentum. The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators.

The third part is the interaction form. You should use the interaction form with $V(q) = 2\pi e^2/(|q|\epsilon_r)$ when κ and κ' refer to the same layer and $(2\pi e^2/(|q|\epsilon_r)) \exp\{-|q|c\}$ when κ and κ' refer to the opposite layers, where q is the transferred total momentum between a creation operator and an annihilation operator with the same index of operator, namely $q = k_1 - k_4$.

The fourth part is the normalization factor, you should use A here. Finally, the summation should be running over all index of operator κ, κ' , and momentum q . Return the interaction term $V^{\kappa\kappa'}$ in terms of creation and annihilation operators and $V(q)$ (with q expressed in terms of momentum).

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):

κ, κ' are the indices of operators, q is the momentum, $V^{\kappa\kappa'}$ is the interaction Hamiltonian, ϵ_r is the relative dielectric constant, $c = 3.35$ is the interlayer separation, A is the total area of the graphene sheet, $r_0 = 3\tilde{a}_0$ is the root mean square radius corresponding to the covalent radius of the carbon atom $a_0 = 0.77$.

6 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, $\{\text{second_int_symbol}\}$.

You should use Wick's theorem to expand the four-fermion term in $\{\text{second_int_symbol}\}$ 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 $\{\text{Hartree_Fock_symbol}\}$.

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):

$\{\text{definition_of_variables}\}$

Excerpt:

Hamiltonian take the form:

$$V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda\lambda'}^X c_{\mathbf{k}\lambda'}^\dagger c_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda'}$$

where λ is a composite label for sublattice κ and spin σ . The first term on the right hand side of Eq.~(\ref{hartreefock}) is the Hartree term:

$$N_\lambda = N_{\kappa\sigma} = \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$$

$$U_H^{\lambda\lambda'} = \frac{\delta_{\sigma,\sigma'}}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\} \left| \tilde{f}(|\mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{G}|), \quad ,$$

where \mathbf{G} is a reciprocal lattice vector. The second is the Fock (exchange) term:

$$W_{\mathbf{k}\lambda\lambda'}^X = \sum_{\mathbf{k}'} U_X^{\kappa\kappa'}(\mathbf{k}' - \mathbf{k}) \langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \rangle$$

$$U_X^{\kappa\kappa'}(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\} \\ \times \left| \tilde{f}(|\mathbf{q} - \mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{q} - \mathbf{G}|).$$

Completion

You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, V^{HF} .

You should use Wick's theorem to expand the four-fermion term in V^{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 V^{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):

λ is a composite label for sublattice κ and spin σ . N_λ is the Hartree term and $W_{\mathbf{k}\lambda\lambda'}^X$ is the Fock (exchange) term. \mathbf{G} is a reciprocal lattice vector.

7 Drop constant terms

Prompt

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Template:

You will be instructed to extract the quadratic terms in the $\{\text{Hartree_Fock_term_symbol}\}$.

The quadratic terms mean terms that are proportional to $\{\text{bilinear_op}\}$, which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in $\{\text{Hartree_Fock_term_symbol}\}$, denoted as $\{\text{Hartree_Fock_second_quantized_symbol}\}$.

Return $\{\text{Hartree_Fock_second_quantized_symbol}\}$.

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):

$\{\text{definition_of_variables}\}$

Excerpt:

Hamiltonian take the form:

$$V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda'\lambda}^X c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where λ is a composite label for sublattice κ and spin σ . The first term on the right hand side of Eq.~(\ref{hartreefock}) is the Hartree term:

$$N_\lambda = N_{\kappa\sigma} = \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$$

$$U_H^{\lambda\lambda'} = \frac{\delta_{\sigma,\sigma'}}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\} \left| \tilde{f}(|\mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{G}|), \quad ,$$

where \mathbf{G} is a reciprocal lattice vector. The second is the Fock (exchange) term:

$$W_{\mathbf{k}\lambda\lambda'}^X = \sum_{\mathbf{k}'} U_X^{\kappa\kappa'}(\mathbf{k}' - \mathbf{k}) \langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \rangle$$

$$U_X^{\kappa\kappa'}(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\} \times \left| \tilde{f}(|\mathbf{q} - \mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{q} - \mathbf{G}|).$$

Completion

You will be instructed to extract the quadratic terms in the Hamiltonian, denoted as V^{HF} .

The quadratic terms mean terms that are proportional to $c^\dagger\{\bm{k}\} \lambda^{\dag} c\{\bm{k}\} \lambda$, which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in V^{HF} , denoted as $V^{\text{HF}}_{\text{quadratic}}$.

Return $V^{\text{HF}}_{\text{quadratic}}$.

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):

λ is a composite label for sublattice κ and spin σ .

N_λ is the expectation value of the number operator.

$U_H^{\lambda\lambda'}$ is the Hartree term.

$W_X^{\{\bm{k}\} \lambda \lambda'}$ is the Fock (exchange) term.

$U_X^{\kappa\kappa'}$ is the exchange interaction.

\mathbf{G} is a reciprocal lattice vector.

8 Identify momentum transfer in interaction

Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

$\{..\}$ means a placeholder which you need to fill by extracting information from the excerpt.

$\{A|B\}$ means you need to make a choice between A and B

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

$\{\{..\}\}$ DOES NOT mean a placeholder. You should not change the content inside double curly braces $\{\{..\}\}$.

'You should recall that $\{..\}$.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $\{\text{Hartree_Fock_second_quantized_symbol}\}$. If you find the $V(q)$ in $\{\text{Hartree_Fock_second_quantized_symbol}\}$ does not contain any momentum that is not in the summation sign. The interaction term is already expanded. No action to perform on interaction term. Otherwise, you will expand $V(q)$ by replacing q with the momentum $\{\text{momentum}\}$. Return $\{\text{Hartree_Fock_second_quantized_symbol}\}$ with expanded interaction.

Excerpt:

Hamiltonian take the form:

$$V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda'\lambda}^X c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where λ is a composite label for sublattice κ and spin σ . The first term on the right hand side of Eq.~(\ref{hartreefock}) is the Hartree term:

$$N_{\lambda} = \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\lambda}^{\dagger} c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$$

$$U_H^{\lambda\lambda'} = \frac{\delta_{\sigma,\sigma'}}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_{\kappa} - \tau_{\kappa'})]\} \left| \tilde{f}(|\mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{G}|), \quad ,$$

where \mathbf{G} is a reciprocal lattice vector. The second is the Fock (exchange) term:

$$W_{\mathbf{k}\lambda\lambda'}^X = \sum_{\mathbf{k}'} U_X^{\kappa\kappa'}(\mathbf{k}' - \mathbf{k}) \langle c_{\mathbf{k}'\lambda'}^{\dagger} c_{\mathbf{k}'\lambda} \rangle$$

$$U_X^{\kappa\kappa'}(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_{\kappa} - \tau_{\kappa'})]\} \\ \times \left| \tilde{f}(|\mathbf{q} - \mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{q} - \mathbf{G}|).$$

Completion

You will be instructed to expand interaction term V^{HF} in the MF quadratic term $V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^{\dagger} c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda'\lambda}^X c_{\mathbf{k}\lambda}^{\dagger} c_{\mathbf{k}\lambda'}$. If you find the V^{HF} in $V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^{\dagger} c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda'\lambda}^X c_{\mathbf{k}\lambda}^{\dagger} c_{\mathbf{k}\lambda'}$ 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^{HF} by replacing q with the momentum \mathbf{k} . Return $V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^{\dagger} c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda'\lambda}^X c_{\mathbf{k}\lambda}^{\dagger} c_{\mathbf{k}\lambda'}$ with expanded interaction.

9 Combine Hartree/Fock terms

Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:

{..} means a placeholder which you need to fill by extracting information from the excerpt.

{A|B} means you need to make a choice between A and B

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

{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.

'You should recall that {..}.' : this sentence should be kept as is.

Finally, if you cannot figure out the placeholder, you should leave it as is.

Template:

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

The logic is that the expected value ({expected_value}) in the first Hartree term ({expression_Hartree_1}) has the same form as the quadratic operators in the second Hartree term ({expression_Hartree_2}), and vice versa. The same applies to the Fock term.

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

You should perform this trick of "relabeling the index" for both two Hartree terms and two Fock terms to reduce them to one Hartree term, and one Fock term.

Return the simplified {Hartree_Fock_second_quantized_symbol} which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term)

Excerpt:

Hamiltonian take the form:

$$V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^{\dagger} c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda'\lambda}^X c_{\mathbf{k}\lambda}^{\dagger} c_{\mathbf{k}\lambda'}$$

where λ is a composite label for sublattice κ and spin σ . The first term on the right hand side of Eq.~(\ref{hartreefock}) is the Hartree term:

$$N_{\lambda} = \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\lambda}^{\dagger} c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$$

$$U_H^{\lambda\lambda'} = \frac{\delta_{\sigma,\sigma'}}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_{\kappa} - \tau_{\kappa'})]\} \left| \tilde{f}(|\mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{G}|), \quad ,$$

where \mathbf{G} is a reciprocal lattice vector. The second is the Fock (exchange) term:

$$W_{\mathbf{k}\lambda\lambda'}^X = \sum_{\mathbf{k}'} U_X^{\kappa\kappa'}(\mathbf{k}' - \mathbf{k}) \langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \rangle$$

$$U_X^{\kappa\kappa'}(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\}$$

$$\times \left| \tilde{f}(|\mathbf{q} - \mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{q} - \mathbf{G}|).$$

Completion

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

The logic is that the expected value (N_λ in the first Hartree term and $\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \rangle$ in the second Fock term) in the first Hartree term ($U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda}$) has the same form as the quadratic operators in the second Hartree term ($W_{\mathbf{k}\lambda'\lambda}^X c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$), and vice versa. The same applies to the Fock term.

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

You should perform this trick of "relabeling the index" for both two Hartree terms and two Fock terms to reduce them to one Hartree term, and one Fock term.

Return the simplified V^{HF} which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term).

10 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:

{..} 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 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:

Hamiltonian take the form:

$$V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda'\lambda}^X c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where λ is a composite label for sublattice κ and spin σ . The first term on the right hand side of Eq.~(\ref{hartreefock}) is the Hartree term:

$$N_\lambda = N_{\kappa\sigma} = \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$$

$$U_H^{\lambda\lambda'} = \frac{\delta_{\sigma,\sigma'}}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\} \left| \tilde{f}(|\mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{G}|), \quad ,$$

where \mathbf{G} is a reciprocal lattice vector. The second is the Fock (exchange) term:

$$W_{\mathbf{k}\lambda\lambda'}^X = \sum_{\mathbf{k}'} U_X^{\kappa\kappa'}(\mathbf{k}' - \mathbf{k}) \langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \rangle$$

$$U_X^{\kappa\kappa'}(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\}$$

$$\times \left| \tilde{f}(|\mathbf{q} - \mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{q} - \mathbf{G}|).$$

Completion

You will be instructed to simplify the Hartree term in V^{HF} by reducing the momentum inside the expected value N_λ .

The expected value N_λ is only nonzero when the two momenta k_i, k_j are the same, namely, $N_\lambda = \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$.

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 V^{HF} .

11 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 $\{\text{Fock_second_quantized_symbol}\}$ by reducing the momentum inside the expected value $\{\text{expected_value}\}$.

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

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 Fock term, and another momentum in the quadratic term.

Return the final simplified Fock term $\{\text{Fock_second_quantized_symbol}\}$.

Excerpt:

Hamiltonian take the form:

$$V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda\lambda'}^X c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where λ is a composite label for sublattice κ and spin σ . The first term on the right hand side of Eq.~(\ref{hartreefock}) is the Hartree term:

$$N_\lambda = N_{\kappa\sigma} = \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$$

$$U_H^{\lambda\lambda'} = \frac{\delta_{\sigma,\sigma'}}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\} \left| \tilde{f}(|\mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{G}|), \quad ,$$

where \mathbf{G} is a reciprocal lattice vector. The second is the Fock (exchange) term:

$$W_{\mathbf{k}\lambda\lambda'}^X = \sum_{\mathbf{k}'} U_X^{\kappa\kappa'}(\mathbf{k}' - \mathbf{k}) \langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}\lambda} \rangle$$

$$U_X^{\kappa\kappa'}(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\}$$

$$\times \left| \tilde{f}(|\mathbf{q} - \mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{q} - \mathbf{G}|).$$

Completion

You will be instructed to simplify the Fock term in V^{HF} by reducing the momentum inside the expected value $\langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle$.

The expected value $\langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$.

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 Fock term, and another momentum in the quadratic term. Return the final simplified Fock term V^{HF} .

12 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:

Hamiltonian take the form:

$$V^{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} N_{\lambda'} c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda} - W_{\mathbf{k}\lambda\lambda'}^X c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where λ is a composite label for sublattice κ and spin σ . The first term on the right hand side of Eq.~(\ref{hartreefock}) is the Hartree term:

$$N_{\lambda} = \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\lambda}^\dagger c_{\mathbf{k}'\lambda} \rangle = \sum_{\mathbf{k}'} n_{\mathbf{k}'\lambda}$$

$$U_H^{\lambda\lambda'} = \frac{\delta_{\sigma,\sigma'}}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\} \left| \tilde{f}(|\mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{G}|), \quad ,$$

where \mathbf{G} is a reciprocal lattice vector. The second is the Fock (exchange) term:

$$W_{\mathbf{k}\lambda\lambda'}^X = \sum_{\mathbf{k}'} U_X^{\kappa\kappa'}(\mathbf{k}' - \mathbf{k}) \langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}\lambda} \rangle$$

$$U_X^{\kappa\kappa'}(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{G}} \exp\{[i\mathbf{G}(\tau_\kappa - \tau_{\kappa'})]\}$$

$$\times \left| \tilde{f}(|\mathbf{q} - \mathbf{G}|) \right|^2 V^{\kappa\kappa'}(|\mathbf{q} - \mathbf{G}|).$$

Completion

You will now be instructed to combine the Hartree term $U_H^{\lambda\lambda'}$ and the Fock term $W_{\mathbf{k}\lambda'\lambda}^X$.

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.