1 Identify kinetic term (continuum,second-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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{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}.

Express the Kinetic Hamiltonian {kinetic_symbol} using {dispersion_symbol}, {annihilation_op}, and {creation_op}, where the summation of $k|r$ should be running over the {entire_space|first_Brillouin_zone}.

Use the following conventions for the symbols:

{definition_of_variables}

Excerpt:

The field operators are four-component spinors $\psi_{\boldsymbol{k}} = (a_{c\uparrow\boldsymbol{k}}, a_{v\uparrow\boldsymbol{k}}, a_{c\downarrow\boldsymbol{k}}, a_{v\downarrow\boldsymbol{k}})^T$, where c and v denote the conduction and valence bands, and $\uparrow$ and $\downarrow$ denote two opposite spins. The single-particle physics of the system under an in-plane magnetic field is described by the modified BHZ Hamiltonian \cite{Hu2016,hu2017topological}

$$H_{\mathrm{BHZ}} = \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}}^\dagger \begin{pmatrix} h_\uparrow(\boldsymbol{k}) & 0 \\ 0 & h_\downarrow(\boldsymbol{k}) \end{pmatrix} \psi_{\boldsymbol{k}},$$

where the two 2×2 matrices $h_\uparrow$ and $h_\downarrow$ can be explicitly expressed as

$$h_\uparrow(\boldsymbol{k}) = \begin{pmatrix} \frac{\hbar^2}{2m_e}(\boldsymbol{k} - \frac{\boldsymbol{Q}}{2})^2 + \frac{E_g}{2} & A(k_x + ik_y) \\ A(k_x - ik_y) & -\frac{\hbar^2}{2m_h}(\boldsymbol{k} + \frac{\boldsymbol{Q}}{2})^2 - \frac{E_g}{2} \end{pmatrix},$$

$$h_\downarrow(\boldsymbol{k}) = \begin{pmatrix} \frac{\hbar^2}{2m_e}(\boldsymbol{k} - \frac{\boldsymbol{Q}}{2})^2 + \frac{E_g}{2} & -A(k_x - ik_y) \\ -A(k_x + ik_y) & -\frac{\hbar^2}{2m_h}(\boldsymbol{k} + \frac{\boldsymbol{Q}}{2})^2 - \frac{E_g}{2} \end{pmatrix}.$$

m_e and m_h are the effective masses of electrons and holes, E_g is the band gap, A is the strength of hybridization between the conduction and valence bands, and $\boldsymbol{Q}$ is the momentum shift due to the in-plane magnetic field. Without the magnetic field, $\boldsymbol{Q} = 0$ and $h_\uparrow, h_\downarrow$ are time-reversal partners:

$$h_\uparrow(\boldsymbol{k}) = h_\downarrow^*(-\boldsymbol{k}).$$

When an in-plane magnetic field $\boldsymbol{B} = B\hat{y}$ is applied to electron and hole layers separated by an interlayer distance d, the conduction and valence bands are shifted in momentum by $\mp\boldsymbol{Q} = \mp(eBd/\hbar)\hat{x}$ by Peierls substitution. The in-plane magnetic field breaks the time-reversal symmetry of the system and induces orbital moments. The electrons and holes interact via the Coulomb interaction

Completion

You will be instructed to describe the kinetic term of Hamiltonian in a system under an in-plane magnetic field in the momentum space in the single-particle form.

The degrees of freedom of the system are: four-component spinors $\psi_{\boldsymbol{k}} = (a_{c\uparrow\boldsymbol{k}}, a_{v\uparrow\boldsymbol{k}}, a_{c\downarrow\boldsymbol{k}}, a_{v\downarrow\boldsymbol{k}})^T$, where c and v denote the conduction and valence bands, and $\uparrow$ and $\downarrow$ denote two opposite spins.

Express the Kinetic Hamiltonian H_{BHZ} using $h_\uparrow$, $h_\downarrow$, $\psi_{\boldsymbol{k}}^\dagger$, and $\psi_{\boldsymbol{k}}$, where the summation of k should be running over the entire space.

Use the following conventions for the symbols:

$h_\uparrow$ and $h_\downarrow$ are the two 2×2 matrices that can be explicitly expressed as given in the excerpt. m_e and m_h are the effective masses of electrons and holes, E_g is the band gap, A is the strength of hybridization between the conduction and valence bands, and $\boldsymbol{Q}$ is the momentum shift due to the in-plane magnetic field. Without the magnetic field, $\boldsymbol{Q} = 0$ and $h_\uparrow, h_{downarrow}$ are time-reversal partners.

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:
The field operators are four-component spinors $\psi_{\boldsymbol{k}} = (a_{c\uparrow\boldsymbol{k}}, a_{v\uparrow\boldsymbol{k}}, a_{c\downarrow\boldsymbol{k}}, a_{v\downarrow\boldsymbol{k}})^T$, where c and v denote the conduction and valence bands, and $\uparrow$ and $\downarrow$ denote two opposite spins. The single-particle physics of the system under an in-plane magnetic field is described by the modified BHZ Hamiltonian \cite{Hu2016,hu2017topological}

$$H_{\mathrm{BHZ}} = \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}}^{\dagger} \begin{pmatrix} h_{\uparrow}(\boldsymbol{k}) & 0 \\ 0 & h_{\downarrow}(\boldsymbol{k}) \end{pmatrix} \psi_{\boldsymbol{k}},$$

where the two 2×2 matrices $h_{\uparrow}$ and $h_{\downarrow}$ can be explicitly expressed as

$$h_{\uparrow}(\boldsymbol{k}) = \begin{pmatrix} \frac{\hbar^2}{2m_e}(\boldsymbol{k} - \frac{\boldsymbol{Q}}{2})^2 + \frac{E_g}{2} & A(k_x + ik_y) \\ A(k_x - ik_y) & -\frac{\hbar^2}{2m_h}(\boldsymbol{k} + \frac{\boldsymbol{Q}}{2})^2 - \frac{E_g}{2} \end{pmatrix},$$

$$h_{\downarrow}(\boldsymbol{k}) = \begin{pmatrix} \frac{\hbar^2}{2m_e}(\boldsymbol{k} - \frac{\boldsymbol{Q}}{2})^2 + \frac{E_g}{2} & -A(k_x - ik_y) \\ -A(k_x + ik_y) & -\frac{\hbar^2}{2m_h}(\boldsymbol{k} + \frac{\boldsymbol{Q}}{2})^2 - \frac{E_g}{2} \end{pmatrix}.$$

m_e and m_h are the effective masses of electrons and holes, E_g is the band gap, A is the strength of hybridization between the conduction and valence bands, and $\boldsymbol{Q}$ is the momentum shift due to the in-plane magnetic field. Without the magnetic field, $\boldsymbol{Q} = 0$ and $h_{\uparrow}, h_{\downarrow}$ are time-reversal partners:

$$h_{\uparrow}(\boldsymbol{k}) = h_{\downarrow}^*(-\boldsymbol{k}).$$

When an in-plane magnetic field $\boldsymbol{B} = B\hat{y}$ is applied to electron and hole layers separated by an interlayer distance d, the conduction and valence bands are shifted in momentum by $\mp\boldsymbol{Q} = \mp(eBd/\hbar)\hat{x}$ by Peierls substitution. The in-plane magnetic field breaks the time-reversal symmetry of the system and induces orbital moments. The electrons and holes interact via the Coulomb interaction

Completion
You will be instructed to construct each term, namely $h_{\uparrow}(\boldsymbol{k})$ and $h_{\downarrow}(\boldsymbol{k})$.
For all energy dispersions, $h_{\uparrow}(\boldsymbol{k})$ and $h_{\downarrow}(\boldsymbol{k})$, it characterizes the parabolic dispersion for electrons and holes.
In addition, a shift of $\boldsymbol{Q}$ in the momentum $\boldsymbol{k}$ for $h_{\uparrow}(\boldsymbol{k})$ and $h_{\downarrow}(\boldsymbol{k})$, 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 $\boldsymbol{k} = -i\partial_{\boldsymbol{r}}$. You should keep the form of $\boldsymbol{k}$ in the Hamiltonian for short notations but should remember $\boldsymbol{k}$ is an operator.
Return the expression for $h_{\uparrow}(\boldsymbol{k})$ and $h_{\downarrow}(\boldsymbol{k})$ in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian H_{BHZ}.

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):

$\psi_{\boldsymbol{k}}$: field operators, c and v: conduction and valence bands, $\uparrow$ and $\downarrow$: two opposite spins, $h_\uparrow$ and $h_\downarrow$: two 2×2 matrices, m_e and m_h: effective masses of electrons and holes, E_g: band gap, A: strength of hybridization between the conduction and valence bands, $\boldsymbol{Q}$: momentum shift due to the in-plane magnetic field.

3 Identify interacting term (momentum space)

Prompt

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

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

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

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

Template:

You will be instructed to construct the interaction part of the Hamiltonian {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 {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. [For each operator, the total momentum is the sum of moire reciprocal lattice b_i and momentum with in the first BZ k_i]

The third part is the interaction form. You should use {interaction} with $V(q) = int\_form$, 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 {normalization_factor} here. Finally, the summation should be running over all {index_of_operator}, and {momentum} Return the interaction term {second_int_symbol} in terms of {op} 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):

{definition_of_variables}

Excerpt:

$$H_I = \frac{1}{2S} \sum_{bb'ss'} \sum_{\boldsymbol{kk'q}} V_{bb'}(q) a^\dagger_{bs\boldsymbol{k+q}} a^\dagger_{b's'\boldsymbol{k'-q}} a_{b's'\boldsymbol{k'}} a_{bs\boldsymbol{k}},$$

where S is the area of the two-dimensional system, b, b' and s, s' are band and spin indices respectively, $V_{cc}(q) = V_{vv}(q) = V(q) = 2\pi e^2/\epsilon q$ is the intralayer Coulomb interaction, $V_{cv}(q) = V_{vc}(q) = U(q) = V(q) \exp(-qd)$ is the interlayer Coulomb interaction at interlayer distance d, and ϵ is the dielectric constant of the surrounding three-dimensional material.

Completion

You will be instructed to construct the interaction part of the Hamiltonian H_I 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 b, b', s', b' for the band and spin indices, and k, k', q 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 intralayer Coulomb interaction and interlayer Coulomb interaction with $V(q) = 2\pi e^2/\epsilon q$ and $U(q) = V(q) \exp(-qd)$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same band and spin indices, namely $q = k - k'$.

The fourth part is the normalization factor, you should use $1/2S$ here. Finally, the summation should be running over all band and spin indices, and momentum. Return the interaction term H_I in terms of $a^\dagger_{bs\bm{k}+\bm{q}}$, $a^\dagger_{b's'\bm{k}'-\bm{q}}$, $a_{b's'\bm{k}'}$, $a_{bs\bm{k}}$ and $V(q)$, $U(q)$ (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):

S is the area of the two-dimensional system, b, b' and s, s' are band and spin indices respectively, $V_{cc}(q) = V_{vv}(q) = V(q) = 2\pi e^2/\epsilon q$ is the intralayer Coulomb interaction, $V_{cv}(q) = V_{vc}(q) = U(q) = V(q)\exp(-qd)$ is the interlayer Coulomb interaction at interlayer distance d, and ϵ is the dielectric constant of the surrounding three-dimensional material.

4 Wick's theorem expansion

Prompt

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Template:

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

You should use Wick's theorem to expand the four-fermion term in {second_int_symbol} into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without †, and be extremely cautious about the order of the index and sign before each term.

You should only preserve the normal terms. Here, the normal terms mean the product of a creation operator and an annihilation operator.

Return the expanded interaction term after Hartree-Fock approximation as {Hartree_Fock_symbol}.

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

{definition_of_variables}

Excerpt:

$$\Sigma_H = \frac{1}{S} \sum_{\substack{bb' \\ ss'}} \sum_{\substack{nn'n'' \\ \bm{k}\bm{k}'}} V_{bb'}((n'-n)\bm{Q})$$
$$\times \rho^{b's'\,n''+n'-n}_{b's'\,n''}(\bm{k}')\, a^\dagger_{bsn'\bm{k}} a_{bsn\bm{k}},$$

where the density matrix ρ is defined relative to the density matrix with valence bands filled and conduction bands empty:

$$\rho^{bsn}_{b's'n'}(\bm{k}) = \langle a^\dagger_{b's'n'\bm{k}} a_{bsn\bm{k}} \rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}.$$

For $n' = n$, the Hartree term accounts for the electrostatic potential energy difference $4\pi e^2 n_x d/\epsilon$ between the electron and hole layers, where

$$n_x = \frac{1}{S} \sum_{sn\bm{k}} \rho^{csn}_{csn}(\bm{k})$$
$$= -\frac{1}{S} \sum_{sn\bm{k}} \rho^{vsn}_{vsn}(\bm{k})$$

is the exciton density. The Fock term

$$\Sigma_F = -\frac{1}{S} \sum_{\substack{bb' \\ ss'}} \sum_{\substack{nn'n'' \\ \bm{k}\bm{k}'}} V_{bb'}((n''-n)\bm{Q} + \bm{k}' - \bm{k})$$
$$\times \rho^{b's'\,n''+n'-n}_{bs\,n''}(\bm{k}') a^\dagger_{b's'n'\bm{k}} a_{bsn\bm{k}}.$$

accounts for the exchange interaction. Together, the system is described by the mean-field Hamiltonian

$$H_{\mathrm{MF}} = H_{\mathrm{BHZ}} + \Sigma_H + \Sigma_F.$$

Completion

You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, Σ_H and Σ_F.

You should use Wick's theorem to expand the four-fermion term in Σ_H and Σ_F 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 H_{MF}.

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):

Σ_H and Σ_F are the Hartree and Fock terms respectively, $V_{bb'}$ is the interaction potential, $\rho_{b's'n''}^{b's'n''+n'-n}$ is the density matrix, $a_{bsn'\boldsymbol{k}}^\dagger$ and $a_{bsn\boldsymbol{k}}$ are the creation and annihilation operators, H_{BHZ} is the base Hamiltonian, and H_{MF} is the mean-field Hamiltonian.

5 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:

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

Template:

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

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

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

Return {Hartree_Fock_second_quantized_symbol}.

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

{definition_of_variables}

Excerpt:

$$\Sigma_H = \frac{1}{S} \sum_{\substack{bb'\\ss'}} \sum_{\substack{nn'n''\\\boldsymbol{kk'}}} V_{bb'}((n'-n)\boldsymbol{Q})$$
$$\times \rho_{b's'n''}^{b's'n''+n'-n}(\boldsymbol{k'})\, a_{bsn'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}},$$

where the density matrix ρ is defined relative to the density matrix with valence bands filled and conduction bands empty:

$$\rho_{b's'n'}^{bsn}(\boldsymbol{k}) = \langle a_{b's'n'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}} \rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}.$$

For $n' = n$, the Hartree term accounts for the electrostatic potential energy difference $4\pi e^2 n_x d/\epsilon$ between the electron and hole layers, where

$$n_x = \frac{1}{S} \sum_{sn\boldsymbol{k}} \rho_{csn}^{csn}(\boldsymbol{k})$$
$$= -\frac{1}{S} \sum_{sn\boldsymbol{k}} \rho_{vsn}^{vsn}(\boldsymbol{k})$$

is the exciton density. The Fock term

$$\Sigma_F = -\frac{1}{S} \sum_{\substack{bb' \\ ss'}} \sum_{\substack{nn'n'' \\ \boldsymbol{k}\boldsymbol{k}'}} V_{bb'}((n''-n)\boldsymbol{Q} + \boldsymbol{k}' - \boldsymbol{k})$$
$$\times \rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')a_{b's'n'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}}.$$

accounts for the exchange interaction. Together, the system is described by the mean-field Hamiltonian

$$H_{\mathrm{MF}} = H_{\mathrm{BHZ}} + \Sigma_H + \Sigma_F.$$

Completion
You will be instructed to extract the quadratic terms in the Hartree and Fock terms.
The quadratic terms mean terms that are proportional to $a_{bsn'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}}$, which excludes terms that are solely expectations or products of expectations.
You should only preserve the quadratic terms in Hartree and Fock terms, denoted as Σ_H and Σ_F.
Return Σ_H and Σ_F.
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):
Σ_H and Σ_F are the Hartree and Fock terms respectively. $a_{bsn'\boldsymbol{k}}^\dagger$ and $a_{bsn\boldsymbol{k}}$ are creation and annihilation operators. $\rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$ is the density matrix. $V_{bb'}((n'-n)\boldsymbol{Q})$ and $V_{bb'}((n''-n)\boldsymbol{Q}+\boldsymbol{k}'-\boldsymbol{k})$ are the interaction potentials. H_{BHZ} is the BHZ Hamiltonian. H_{MF} is the mean-field Hamiltonian.

6 Identify momentum transfer in interaction

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
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'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to expand interaction term $V(q)$ in the MF quadratic term {Hartree_Fock_second_quantized_symbol}. If you find the $V(q)$ in {Hartree_Fock_second_quantized_symbol} does not contain any momentum that is not in the summation sign. The interaction term is already expanded. No action to perform on interaction term. Otherwise, you will expand $V(q)$ by replacing q with the momentum {momentum}. Return {Hartree_Fock_second_quantized_symbol} with expanded interaction.
Excerpt:

$$\Sigma_H = \frac{1}{S} \sum_{\substack{bb' \\ ss'}} \sum_{\substack{nn'n'' \\ \boldsymbol{k}\boldsymbol{k}'}} V_{bb'}((n'-n)\boldsymbol{Q})$$
$$\times \rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')\, a_{bsn'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}},$$

where the density matrix ρ is defined relative to the density matrix with valence bands filled and conduction bands empty:

$$\rho_{b's'n'}^{bsn}(\boldsymbol{k}) = \langle a_{b's'n'\boldsymbol{k}}^\dagger a_{bsn\boldsymbol{k}} \rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}.$$

For $n' = n$, the Hartree term accounts for the electrostatic potential energy difference $4\pi e^2 n_x d/\epsilon$ between the electron and hole layers, where

$$n_x = \frac{1}{S} \sum_{sn\boldsymbol{k}} \rho_{csn}^{csn}(\boldsymbol{k})$$
$$= -\frac{1}{S} \sum_{sn\boldsymbol{k}} \rho_{vsn}^{vsn}(\boldsymbol{k})$$

is the exciton density. The Fock term

$$\Sigma_F = -\frac{1}{S} \sum_{\substack{bb' \\ ss'}} \sum_{\substack{nn'n'' \\ \boldsymbol{k}\boldsymbol{k}'}} V_{bb'}((n''-n)\boldsymbol{Q}+\boldsymbol{k}'-\boldsymbol{k})$$

$$\times \rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}') a_{b's'n'\boldsymbol{k}}^{\dagger} a_{bsn\boldsymbol{k}}.$$

accounts for the exchange interaction. Together, the system is described by the mean-field Hamiltonian

$$H_{\mathrm{MF}} = H_{\mathrm{BHZ}} + \Sigma_H + \Sigma_F.$$

Completion
You will be instructed to expand interaction term $V_{bb'}((n'-n)\boldsymbol{Q})$ and $V_{bb'}((n''-n)\boldsymbol{Q}+\boldsymbol{k}'-\boldsymbol{k})$ in the MF quadratic term Σ_H and Σ_F. If you find the $V_{bb'}((n'-n)\boldsymbol{Q})$ and $V_{bb'}((n''-n)\boldsymbol{Q}+\boldsymbol{k}'-\boldsymbol{k})$ in Σ_H and Σ_F 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 $V_{bb'}((n'-n)\boldsymbol{Q})$ and $V_{bb'}((n''-n)\boldsymbol{Q}+\boldsymbol{k}'-\boldsymbol{k})$ by replacing q with the momentum $(n'-n)\boldsymbol{Q}$ and $(n''-n)\boldsymbol{Q}+\boldsymbol{k}'-\boldsymbol{k}$. Return Σ_H and Σ_F with expanded interaction.

7 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:
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[..] means optional sentence. You should decide whether to use it depending on the excerpt.
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'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to simplify the quadratic term {Hartree_Fock_second_quantized_symbol} through relabeling the index 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:

$$\Sigma_H = \frac{1}{S} \sum_{\substack{bb' \\ ss'}} \sum_{\substack{nn'n'' \\ \boldsymbol{k}\boldsymbol{k}'}} V_{bb'}((n'-n)\boldsymbol{Q})$$

$$\times \rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}') \, a_{bsn'\boldsymbol{k}}^{\dagger} a_{bsn\boldsymbol{k}},$$

where the density matrix ρ is defined relative to the density matrix with valence bands filled and conduction bands empty:

$$\rho_{b's'n'}^{bsn}(\boldsymbol{k}) = \langle a_{b's'n'\boldsymbol{k}}^{\dagger} a_{bsn\boldsymbol{k}} \rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}.$$

For $n' = n$, the Hartree term accounts for the electrostatic potential energy difference $4\pi e^2 n_x d/\epsilon$ between the electron and hole layers, where

$$n_x = \frac{1}{S} \sum_{sn\boldsymbol{k}} \rho_{csn}^{csn}(\boldsymbol{k})$$

$$= -\frac{1}{S} \sum_{sn\boldsymbol{k}} \rho_{vsn}^{vsn}(\boldsymbol{k})$$

is the exciton density. The Fock term

$$\Sigma_F = -\frac{1}{S} \sum_{\substack{bb' \\ ss'}} \sum_{\substack{nn'n'' \\ \boldsymbol{k}\boldsymbol{k}'}} V_{bb'}((n''-n)\boldsymbol{Q} + \boldsymbol{k}' - \boldsymbol{k})$$

$$\times \rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}') a_{b's'n'\boldsymbol{k}}^{\dagger} a_{bsn\boldsymbol{k}}.$$

accounts for the exchange interaction. Together, the system is described by the mean-field Hamiltonian

$$H_{\mathrm{MF}} = H_{\mathrm{BHZ}} + \Sigma_H + \Sigma_F.$$

Completion
You will be instructed to simplify the quadratic term H_{MF} through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.
The logic is that the expected value ($\rho_{b's'\,n'}^{b's'\,n''+n'-n}(\boldsymbol{k}')$) in the first Hartree term (Σ_H) has the same form as the quadratic operators in the second Hartree term (Σ_F), 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 H_{MF} which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term).

8 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 $\langle \ldots \rangle$. 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:

$$\Sigma_H = \frac{1}{S} \sum_{\substack{bb' \\ ss'}} \sum_{\substack{nn'n'' \\ \boldsymbol{k}\boldsymbol{k}'}} V_{bb'}((n'-n)\boldsymbol{Q})$$

$$\times \rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}') \, a_{bsn'\boldsymbol{k}}^{\dagger} a_{bsn\boldsymbol{k}},$$

where the density matrix ρ is defined relative to the density matrix with valence bands filled and conduction bands empty:

$$\rho_{b's'n'}^{bsn}(\boldsymbol{k}) = \langle a_{b's'n'\boldsymbol{k}}^{\dagger} a_{bsn\boldsymbol{k}} \rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}.$$

For $n' = n$, the Hartree term accounts for the electrostatic potential energy difference $4\pi e^2 n_x d/\epsilon$ between the electron and hole layers, where

$$n_x = \frac{1}{S}\sum_{snk}\rho_{csn}^{csn}(\boldsymbol{k})$$

$$= -\frac{1}{S}\sum_{snk}\rho_{vsn}^{vsn}(\boldsymbol{k})$$

is the exciton density. The Fock term

$$\Sigma_F = -\frac{1}{S}\sum_{\substack{bb'\\ss'}}\sum_{\substack{nn'n''\\kk'}} V_{bb'}((n''-n)\boldsymbol{Q}+\boldsymbol{k'}-\boldsymbol{k})$$

$$\times \rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k'})a_{b's'n'\boldsymbol{k}}^{\dagger}a_{bsn\boldsymbol{k}}.$$

accounts for the exchange interaction. Together, the system is described by the mean-field Hamiltonian

$$H_{\mathrm{MF}} = H_{\mathrm{BHZ}} + \Sigma_H + \Sigma_F.$$

Completion
You will be instructed to simplify the Hartree term in Σ_H by reducing the momentum inside the expected value $\rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k'})$.
The expected value $\rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k'})$ is only nonzero when the two momenta k_i, k_j are the same, namely,
$\rho_{b's'n'}^{bsn}(\boldsymbol{k}) = \langle a_{b's'n'\boldsymbol{k}}^{\dagger}a_{bsn\boldsymbol{k}}\rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}$.
You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i. Once you reduce one momentum inside the expected value $\langle\ldots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.
You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.
Return the final simplified Hartree term Σ_H.

9 Identify order parameters in Fock term (extended BZ)

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to simplify the Fock term in {Fock_second_quantized_symbol} by reducing the momentum inside the expected value {expected_value}.
The expected value {expected_value} is only nonzero when the two momenta k_i, k_j are the same, namely, {expected_value_nonzero}.
You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i.
Once you reduce one momentum inside the expected value $\langle\ldots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term.
Return the final simplified Fock term {Fock_second_quantized_symbol}.
Excerpt:

$$\Sigma_H = \frac{1}{S}\sum_{\substack{bb'\\ss'}}\sum_{\substack{nn'n''\\kk'}} V_{bb'}((n'-n)\boldsymbol{Q})$$

$$\times \rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k'})\,a_{bsn'\boldsymbol{k}}^{\dagger}a_{bsn\boldsymbol{k}},$$

where the density matrix ρ is defined relative to the density matrix with valence bands filled and conduction bands empty:

$$\rho_{b's'n'}^{bsn}(\boldsymbol{k}) = \langle a_{b's'n'\boldsymbol{k}}^{\dagger} a_{bsn\boldsymbol{k}} \rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}.$$

For $n' = n$, the Hartree term accounts for the electrostatic potential energy difference $4\pi e^2 n_x d/\epsilon$ between the electron and hole layers, where

$$n_x = \frac{1}{S}\sum_{sn\boldsymbol{k}} \rho_{csn}^{csn}(\boldsymbol{k})$$

$$= -\frac{1}{S}\sum_{sn\boldsymbol{k}} \rho_{vsn}^{vsn}(\boldsymbol{k})$$

is the exciton density. The Fock term

$$\Sigma_F = -\frac{1}{S}\sum_{\substack{bb'\\ss'}}\sum_{\substack{nn'n''\\\boldsymbol{k}\boldsymbol{k}'}} V_{bb'}((n''-n)\boldsymbol{Q} + \boldsymbol{k}' - \boldsymbol{k})$$
$$\times \rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')a_{b's'n'\boldsymbol{k}}^{\dagger}a_{bsn\boldsymbol{k}}.$$

accounts for the exchange interaction. Together, the system is described by the mean-field Hamiltonian

$$H_{\mathrm{MF}} = H_{\mathrm{BHZ}} + \Sigma_H + \Sigma_F.$$

Completion
Template:
You will be instructed to simplify the Fock term in Σ_F by reducing the momentum inside the expected value $\rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$.
The expected value $\rho_{bs\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}$.
You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i.
Once you reduce one momentum inside the expected value $\langle \ldots \rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term. Return the final simplified Fock term Σ_F.

10 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:

$$\Sigma_H = \frac{1}{S}\sum_{\substack{bb'\\ss'}}\sum_{\substack{nn'n''\\\boldsymbol{k}\boldsymbol{k}'}} V_{bb'}((n'-n)\boldsymbol{Q})$$
$$\times \rho_{b's'\,n''}^{b's'\,n''+n'-n}(\boldsymbol{k}')\,a_{bsn'\boldsymbol{k}}^{\dagger}a_{bsn\boldsymbol{k}},$$

where the density matrix ρ is defined relative to the density matrix with valence bands filled and conduction bands empty:

$$\rho^{bsn}_{b's'n'}(\mathbf{k}) = \langle a^\dagger_{b's'n'\mathbf{k}} a_{bsn\mathbf{k}} \rangle - \delta_{bb'}\delta_{bv}\delta_{ss'}\delta_{nn'}.$$

For $n' = n$, the Hartree term accounts for the electrostatic potential energy difference $4\pi e^2 n_x d/\epsilon$ between the electron and hole layers, where

$$n_x = \frac{1}{S}\sum_{sn\mathbf{k}} \rho^{csn}_{csn}(\mathbf{k})$$

$$= -\frac{1}{S}\sum_{sn\mathbf{k}} \rho^{vsn}_{vsn}(\mathbf{k})$$

is the exciton density. The Fock term

$$\Sigma_F = -\frac{1}{S}\sum_{\substack{bb'\\ss'}}\sum_{\substack{nn'n''\\ \mathbf{k}\mathbf{k}'}} V_{bb'}((n''-n)\mathbf{Q} + \mathbf{k}' - \mathbf{k})$$

$$\times \rho^{b's'\,n''+n'-n}_{bs\,n''}(\mathbf{k}')a^\dagger_{b's'n'\mathbf{k}}a_{bsn\mathbf{k}}.$$

accounts for the exchange interaction. Together, the system is described by the mean-field Hamiltonian

$$H_{\mathrm{MF}} = H_{\mathrm{BHZ}} + \Sigma_H + \Sigma_F.$$

Completion

You will now be instructed to combine the Hartree term \Sigma*H and the Fock term \Sigma*F.
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.