1 Identify kinetic term (lattice)

Excerpt: We introduce a simple but realistic effective model for $BiNiO_3$, and clarify the ground-state and finite-T phase diagrams within the mean-field (MF) approximation. \begin{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}{i \sigma} a{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}{i \sigma} b{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}{i \sigma} b{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \uparrow} n^{\rm N}{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}{i} n^{\rm B}{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}{i} n^{\rm B}{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$. In Eq.~(\ref{eq:hamil}), the first and second lines represent the electron hopping on the Ni-Ni, Bi-Bi, and Bi-Ni bonds.

Completion
Template: You will be instructed to describe the kinetic term of Hamiltonian in $BiNiO_3$ in the real space in the second-quantized form.
The degrees of freedom of the system are: Ni-Ni, Bi-Bi, and Bi-Ni bonds.
The kinetic term is a tight-binding model composed of the following hopping process: Ni-Ni bonds with the amplitude t{\rm N}, Bi-Bi bonds with the amplitude t{\rm B}, and Bi-Ni bonds with the amplitude t_{\rm BN}. You should ensure the hermiticity of the Hamiltonian. The summation should be taken over all Ni-Ni, Bi-Bi, and Bi-Ni bonds and all real space positions.
Return the Kinetic Hamiltonian $\mathcal{H}$.
Use the following conventions for the symbols:
$a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$.

2 Identify interacting term (real space)

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: We introduce a simple but realistic effective model for BiNiO$_3$, and clarify the ground-state and finite-T phase diagrams within the mean-field (MF) approximation. \begin{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}{i \sigma} a{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}{i \sigma} b{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}{i \sigma} b{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \uparrow} n^{\rm N}{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}{i} n^{\rm B}{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}{i} n^{\rm B}{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$. The fourth line represents the intersite Coulomb interactions on the Bi-Bi and Bi-Ni bonds.

Completion

You will be instructed to construct the interaction part of the Hamiltonian, $\Delta \sum_{i\sigma}^{\rm Ni} n_{i\sigma}^{\rm N} + U_{\rm N} \sum_{i\sigma}^{\rm Ni} n_{i\uparrow}^{\rm N} n_{i\downarrow}^{\rm N} + U_{\rm B} \sum_{i\sigma}^{\rm Bi} n_{i\uparrow}^{\rm B} n_{i\downarrow}^{\rm B} + V_{\rm B} \sum_{\langle ij \rangle}^{\rm Bi-Bi} n_i^{\rm B} n_j^{\rm B} + V_{\rm BN} \sum_{\langle ij \rangle}^{\rm Bi-Ni} n_i^{\rm N} n_j^{\rm B}$ in the real space in the second-quantized form.

The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian $t_{\rm N} \sum_{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a_{i\sigma}^{\dagger} a_{j\sigma} + {\rm H.c.} \right) + t_{\rm B} \sum_{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b_{i\sigma}^{\dagger} b_{j\sigma} + {\rm H.c.} \right) + t_{\rm BN} \sum_{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a_{i\sigma}^{\dagger} b_{j\sigma} + {\rm H.c.} \right)$.

The interaction is a density-density interaction composed of the following process: Bi-Bi and Bi-Ni sites with the interaction strength $V_{\rm B}$ and $V_{\rm BN}$ respectively. The summation should be taken over all spins and all real space positions.

Return the interaction term $\Delta \sum_{i\sigma}^{\rm Ni} n_{i\sigma}^{\rm N} + U_{\rm N} \sum_{i\sigma}^{\rm Ni} n_{i\uparrow}^{\rm N} n_{i\downarrow}^{\rm N} + U_{\rm B} \sum_{i\sigma}^{\rm Bi} n_{i\uparrow}^{\rm B} n_{i\downarrow}^{\rm B} + V_{\rm B} \sum_{\langle ij \rangle}^{\rm Bi-Bi} n_i^{\rm B} n_j^{\rm B} + V_{\rm BN} \sum_{\langle ij \rangle}^{\rm Bi-Ni} n_i^{\rm N} n_j^{\rm B}$ in terms of $n_{i\sigma}^{\rm N}$ and $n_{i\sigma}^{\rm B}$.

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): $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$.

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 transform 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 transform. [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): {definitionofvariables}

Excerpt: \begin{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}{i \sigma} a{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}{i \sigma} b{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}{i \sigma} b{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \uparrow} n^{\rm N}{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}{i} n^{\rm B}{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}{i} n^{\rm B}{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger}a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger}b_{i\sigma}$. In Eq.~(\ref{eq:hamil}), the first and second lines represent the electron hopping on the Ni-Ni, Bi-Bi, and Bi-Ni bonds.

Completion

You will be instructed to convert the noninteracting Hamiltonian $\mathcal{H}$ in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transform to $a_{i\sigma}^{\dagger}$ and $b_{i\sigma}^{\dagger}$ in the real space to the {momentum$creationop$} in the momentum space, which is defined as {definitionofFourier$Transformation$}, where i is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transform. [Note that hopping have no position dependence now.] Express the total noninteracting Hamiltonian $\mathcal{H}$ 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): $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger}a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger}b_{i\sigma}$.

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, {secondintsymbol}, 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 transform to {real$creationop$} in the real space to the {momentum$creationop$} in the momentum space, which is defined as {definitionofFourier$Transformation$}, 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 transform. [Note that interaction have no position dependence now]

Express {secondintsymbol} in terms of {momentum$creationop$}. Simplify any summation index if possible.

Excerpt: \begin{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}{i \sigma} a{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}{i \sigma} b{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}{i \sigma} b{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \uparrow} n^{\rm N}{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}{i} n^{\rm B}{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}{i} n^{\rm B}{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th

unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$. The fourth line represents the intersite Coulomb interactions on the Bi-Bi and Bi-Ni bonds.

Completion
You will be instructed to convert the interacting Hamiltonian, $\mathcal{H}$, in the second-quantized form the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transform to $a_{i\sigma}$ and $b_{i\sigma}$ in the real space to the {momentum*creation*op} in the momentum space, which is defined as {definition*of*Fourier*Transformation}, where i 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 transform. [Note that interaction have no position dependence now]
Express $\mathcal{H}$ in terms of {momentum*creation*op}. 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{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}{i \sigma} a{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}{i \sigma} b{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}{i \sigma} b{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \uparrow} n^{\rm N}{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}{i} n^{\rm B}{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}{i} n^{\rm B}{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$. In Eq.~(\ref{eq:hamil}), the first and second lines represent the electron hopping on the Ni-Ni, Bi-Bi, and Bi-Ni bonds. In the third line, the first term is the energy difference between the Bi-$6s$ and Ni-$3d$ levels, the second term is the on-site Coulomb interactions on the Ni sites, and the third term is the effective interaction that describes the valence skipping nature of Bi~\cite{Varma, Anderson, Hase}; we consider not only positive but also negative values for $U_{\rm B}$. The fourth line represents the intersite Coulomb interactions on the Bi-Bi and Bi-Ni bonds. We take the unit cell that includes four Bi and four Ni sites, as shown in Fig.~\ref{fig:vst}(d). By investigating several sets of parameters and varying them, we find that $U_{\rm B}$ and Δ are most relevant to the valence transition; hence, below we show the results by varying these two parameters while fixing the others at $t_{\rm N} = t_{\rm B} = 1$, $t_{\rm BN} = 0.5$, $U_{\rm N} = 3$, $V_{\rm B} = 0.65$, $V_{\rm BN} = 1$. We have confirmed that the detailed changes of the parameters do not alter the following results qualitatively.

Completion
You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $\mathcal{H}$.

You should use Wick's theorem to expand the four-fermion term in $\mathcal{H}$ 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):

$a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^\dagger a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^\dagger b_{i\sigma}$.

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: \begin{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}*{i \sigma} a*{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}*{i \sigma} b*{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}*{i \sigma} b*{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}*{i \uparrow} n^{\rm N}*{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}*{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}*{i} n^{\rm B}*{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}*{i} n^{\rm B}*{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^\dagger a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^\dagger b_{i\sigma}$. In Eq.~(\ref{eq:hamil}), the first and second lines represent the electron hopping on the Ni-Ni, Bi-Bi, and Bi-Ni bonds. In the third line, the first term is the energy difference between the Bi-$6s$ and Ni-$3d$ levels, the second term is the on-site Coulomb interactions on the Ni sites, and the third term is the effective interaction that describes the valence skipping nature of Bi~\cite{Varma, Anderson, Hase}; we consider not only positive but also negative values for $U_{\rm B}$. The fourth line represents the intersite Coulomb interactions on the Bi-Bi and Bi-Ni bonds. We take the unit cell that includes four Bi and four Ni sites, as shown in Fig.~\ref{fig:vst}(d). By investigating several sets of parameters and varying them, we find that $U_{\rm B}$ and Δ are most relevant to the valence transition; hence, below we show the results by varying these two parameters while fixing the others at $t_{\rm N} = t_{\rm B} = 1$, $t_{\rm BN} = 0.5$, $U_{\rm N} = 3$, $V_{\rm B} = 0.65$, $V_{\rm BN} = 1$. We have confirmed that the detailed changes of the parameters do not alter the following results qualitatively.

Completion
You will be instructed to extract the quadratic terms in the $\mathcal{H}$.

The quadratic terms mean terms that are proportional to $a_{i\sigma}^\dagger a_{j\sigma}$, $b_{i\sigma}^\dagger b_{j\sigma}$, and $a_{i\sigma}^\dagger b_{j\sigma}$, which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in $\mathcal{H}$, denoted as $\mathcal{H}_{\rm quad}$.

Return $\mathcal{H}_{\rm quad}$.

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):

$a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$.

7 Keep 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 keep only the Hartree term in {Hartree*Fock*second*quantized*symbol}.

Here, Hartree term only means that only the expected value in the form {expected*value*Hartree} (Note that the two indices are the same) should be the preserved. All other expected value terms should be dropped. Return the simplified Hamiltonian with {Hartree*second*quantized_symbol}.

Excerpt: \begin{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}{i \sigma} a{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}{i \sigma} b{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}{i \sigma} b{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \uparrow} n^{\rm N}{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}{i} n^{\rm B}{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}{i} n^{\rm B}{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$. In Eq.~(\ref{eq:hamil}), the first and second lines represent the electron hopping on the Ni-Ni, Bi-Bi, and Bi-Ni bonds. In the third line, the first term is the energy difference between the Bi-$6s$ and Ni-$3d$ levels, the second term is the on-site Coulomb interactions on the Ni sites, and the third term is the effective interaction that describes the valence skipping nature of Bi~\cite{Varma, Anderson, Hase}; we consider not only positive but also negative values for $U_{\rm B}$. The fourth line represents the intersite Coulomb interactions on the Bi-Bi and Bi-Ni bonds. We take the unit cell that includes four Bi and four Ni sites, as shown in Fig.~\ref{fig:vst}(d). By investigating several sets of parameters and varying them, we find that $U_{\rm B}$ and Δ are most relevant to the valence transition; hence, below we show the results by varying these two parameters while fixing the others at $t_{\rm N} = t_{\rm B} = 1$, $t_{\rm BN} = 0.5$, $U_{\rm N} = 3$, $V_{\rm B} = 0.65$, $V_{\rm BN} = 1$. We have confirmed that the detailed changes of the parameters do not alter the following results qualitatively.

Completion

You will be instructed to keep only the Hartree term in $\mathcal{H}$.

Here, Hartree term only means that only the expected value in the form $U_{\rm N} \sum_{i\sigma}^{\rm Ni} n_{i\uparrow}^{\rm N} n_{i\downarrow}^{\rm N}$ and $U_{\rm B} \sum_{i\sigma}^{\rm Bi} n_{i\uparrow}^{\rm B} n_{i\downarrow}^{\rm B}$ (Note that the two indices are the same) should be the preserved. All other expected value terms should be dropped. Return the simplified Hamiltonian with $\mathcal{H} = U_{\rm N} \sum_{i\sigma}^{\rm Ni} n_{i\uparrow}^{\rm N} n_{i\downarrow}^{\rm N} + U_{\rm B} \sum_{i\sigma}^{\rm Bi} n_{i\uparrow}^{\rm B} n_{i\downarrow}^{\rm B}$.

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 {HartreeFocksecondquantizedsymbol} through relabeling the index.

The logic is that the expected value ({expectedvalue}) in the first Hartree term ({expressionHartree1}) has the same form as the quadratic operators in the second Hartree term ({expressionHartree_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 {HartreeFocksecondquantizedsymbol}.

Excerpt: \begin{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}{i \sigma} a{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}{i \sigma} b{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}{i \sigma} b{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \uparrow} n^{\rm N}{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}{i} n^{\rm B}{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}{i} n^{\rm B}{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$. In Eq.~(\ref{eq:hamil}), the first and second lines represent the electron hopping on the Ni-Ni, Bi-Bi, and Bi-Ni bonds. In the third line, the first term is the energy difference between the Bi-$6s$ and Ni-$3d$ levels, the second term is the on-site Coulomb interactions on the Ni sites, and the third term is the effective interaction that describes the valence skipping nature of Bi~\cite{Varma, Anderson, Hase}; we consider not only positive but also negative values for $U_{\rm B}$. The fourth line represents the intersite Coulomb interactions on the Bi-Bi and Bi-Ni bonds. We take the unit cell that includes four Bi and four Ni sites, as shown in Fig.~\ref{fig:vst}(d). By investigating several sets of parameters and varying them, we find that $U_{\rm B}$ and Δ are most relevant to the valence transition; hence, below we show the results by varying these two parameters while fixing the others at $t_{\rm N} = t_{\rm B} = 1$, $t_{\rm BN} = 0.5$, $U_{\rm N} = 3$, $V_{\rm B} = 0.65$, $V_{\rm BN} = 1$. We have confirmed that the detailed changes of the parameters do not alter the following results qualitatively.

Completion

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

The logic is that the expected value ($n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$) in the first Hartree term ($t_{\rm N} \sum_{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a_{i\sigma}^{\dagger} a_{j\sigma} + {\rm H.c.} \right)$) has the same form as the quadratic operators in the second Hartree term ($t_{\rm B} \sum_{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b_{i\sigma}^{\dagger} b_{j\sigma} + {\rm H.c.} \right)$), 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 $\mathcal{H}$.

9 Identify order parameters in Hartree term

Prompt

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

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

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

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

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

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

Template: You will be instructed to simplify the Hartree term, *{Hartreesecondquantizedsymbol}*, *by reducing the momentum inside the expected value {expectedvalue}*.

The expected value *{expectedvalue} is only nonzero when the two momenta* k_i, k_j *are the same, namely, {expectedvalue_nonzero}*.

You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i. Once you reduce one momentum inside the expected value $\langle \ldots \rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.

You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.

Return the final simplified Hartree term {Hartreesecondquantized_symbol}.

Excerpt: \begin{align} {\cal H} &= t{\rm N} \sum{\langle ij \rangle \sigma}^{\rm Ni-Ni} \left(a^{\dagger}{i \sigma} a{j \sigma} + {\rm H.c.} \right) + t{\rm B} \sum{\langle ij \rangle \sigma}^{\rm Bi-Bi} \left(b^{\dagger}{i \sigma} b{j \sigma}+ {\rm H.c.} \right) \notag \ &+ t{\rm BN} \sum{\langle ij \rangle \sigma}^{\rm Bi-Ni} \left(a^{\dagger}{i \sigma} b{j \sigma} + {\rm H.c.} \right) \notag \ &+ {\Delta} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \sigma} + U{\rm N} \sum{i \sigma}^{\rm Ni} n^{\rm N}{i \uparrow} n^{\rm N}{i \downarrow} + U{\rm B} \sum{i \sigma}^{\rm Bi} n^{\rm B}{i \uparrow} n^{\rm B}{i \downarrow} \notag \ &+ V{\rm B} \sum{\langle ij \rangle}^{\rm Bi-Bi} n^{\rm B}{i} n^{\rm B}{j} + V{\rm BN} \sum{\langle ij \rangle}^{\rm Bi-Ni} n^{\rm N}{i} n^{\rm B}{j}, \label{eq:hamil} \end{align} where $a_{i\sigma}$ and $b_{i\sigma}$ represent the annihilation operators of electron with the spin $\sigma(=\uparrow,\downarrow)$ at the Ni and Bi sites of i-th unit cell, respectively; $n_{i\sigma}^{\rm N} = a_{i\sigma}^{\dagger} a_{i\sigma}$ and $n_{i\sigma}^{\rm B} = b_{i\sigma}^{\dagger} b_{i\sigma}$. In Eq.~(\ref{eq:hamil}), the first and second lines represent the electron hopping on the Ni-Ni, Bi-Bi, and Bi-Ni bonds. In the third line, the first term is the energy difference between the Bi-$6s$ and Ni-$3d$ levels, the second term is the on-site Coulomb interactions on the Ni sites, and the third term is the effective interaction that describes the valence skipping nature of Bi~\cite{Varma, Anderson, Hase}; we consider not only positive but also negative values for $U_{\rm B}$. The fourth line represents the intersite Coulomb interactions on the Bi-Bi and Bi-Ni bonds. We take the unit cell that includes four Bi and four Ni sites, as shown in Fig.~\ref{fig:vst}(d). By investigating several sets of parameters and varying them, we find that $U_{\rm B}$ and Δ are most relevant to the valence transition; hence, below we show the results by varying these two parameters while fixing the others at $t_{\rm N} = t_{\rm B} = 1$, $t_{\rm BN} = 0.5$, $U_{\rm N} = 3$, $V_{\rm B} = 0.65$, $V_{\rm BN} = 1$. We have confirmed that the detailed changes of the parameters do not alter the following results qualitatively.

Completion

You will be instructed to simplify the Hartree term, $\mathcal{H}$, by reducing the momentum inside the expected value $\langle ij \rangle$.

The expected value $\langle ij \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle ij \rangle = \delta_{k_i,k_j}$.

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 $\langle ij \rangle$. 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 $\mathcal{H}$.