

1 Identify kinetic term (lattice)

Prompt

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

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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 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}

The kinetic term is a tight-binding model composed of the following hopping process: {site i and site
j with the amplitude hopping} [You should ensure the hermiticity of the Hamiltonian] The summation
should be taken over all {degrees_of_freedom} and all {real|momentum} space positions.

Return the Kinetic Hamiltonian {kinetic_symbol}.

Use the following conventions for the symbols:

{definition_of_variables}

Excerpt:

of holes in the CuO₂ plane is

$$\begin{aligned}\mathcal{H}_0 = & -t_{pd} \sum_{i,s} \sum_{\nu} (\hat{d}_{i,s}^{\dagger} \hat{p}_{i+\hat{\nu}/2,s} + \text{h.c.}) \\ & - t_{pp} \sum_{i,s} \sum_{\langle \nu, \nu' \rangle} (\hat{p}_{i+\hat{\nu}/2,s}^{\dagger} \hat{p}_{i+\hat{\nu}'/2,s} + \text{h.c.}) \\ & - \mu \sum_{i,s} \hat{n}_{i,s}^d - \frac{1}{2}(\mu - \Delta) \sum_{i,s} \sum_{\nu} \hat{n}_{i+\hat{\nu}/2,s}^p\end{aligned}$$

with t_{pd} and t_{pp} the Cu-O and O-O hopping integrals. Here, $\hat{d}_{i,s}^{\dagger}$ creates a hole in the copper $d_{x^2-y^2}$ orbital at site i with spin s , $\hat{p}_{i+\hat{\nu}/2,s}^{\dagger}$ creates a hole in the oxygen p_{ν} orbital at the site $i + \hat{\nu}/2$ for $\nu = x, y$, and $\hat{n}_{i,s}^d$, $\hat{n}_{i+\hat{\nu}/2,s}^p$ are the corresponding number operators. The Cu sites i form a square lattice with unit vectors \hat{x} and \hat{y} , and the total number of lattice sites is N . The chemical potential μ and the charge transfer energy Δ control the total and relative Cu/O hole densities, and $\langle \nu, \nu' \rangle$ point to neighboring oxygen sites.

Completion

You will be instructed to describe the kinetic term of Hamiltonian in the CuO₂ plane in the real space in the second-quantized form.

The degrees of freedom of the system are: spin s and site i

The kinetic term is a tight-binding model composed of the following hopping process: between copper $d_{x^2-y^2}$ orbital at site i and oxygen p_{ν} orbital at site $i + \hat{\nu}/2$ with the amplitude t_{pd} , and between neighboring oxygen sites with the amplitude t_{pp} . You should ensure the hermiticity of the Hamiltonian. The summation should be taken over all spin s and all real space positions.

Return the Kinetic Hamiltonian \mathcal{H}_0 .

Use the following conventions for the symbols:

$\hat{d}_{i,s}^{\dagger}$ creates a hole in the copper $d_{x^2-y^2}$ orbital at site i with spin s , $\hat{p}_{i+\hat{\nu}/2,s}^{\dagger}$ creates a hole in the oxygen p_{ν} orbital at the site $i + \hat{\nu}/2$ for $\nu = x, y$, and $\hat{n}_{i,s}^d$, $\hat{n}_{i+\hat{\nu}/2,s}^p$ are the corresponding number operators. The Cu sites i form a square lattice with unit vectors \hat{x} and \hat{y} , and the total number of lattice sites is N . The chemical potential μ and the charge transfer energy Δ control the total and relative Cu/O hole densities, and $\langle \nu, \nu' \rangle$ point to neighboring oxygen sites.

2 Identify interacting term (real space)

Prompt

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

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

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

Template:

You will be instructed to construct the interaction part of the Hamiltonian, {second_int_symbol} in the real space in the second-quantized form.

The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian {kinetic_symbol}.

The interaction is a density-density interaction composed of the following process: {site i and site j with the interaction strength} The summation should be taken over all {degrees_of_freedom} and all real space positions.

Return the interaction term {second_int_symbol} in terms of {density_symbol}.

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

Excerpt:

$$\begin{aligned}\mathcal{H}' = & U_d \sum_i \hat{n}_{i\uparrow}^d \hat{n}_{i\downarrow}^d + \frac{U_p}{2} \sum_{i,\nu} \hat{n}_{i+\hat{\nu}/2,\uparrow}^p \hat{n}_{i+\hat{\nu}/2,\downarrow}^p \\ & + V_{pd} \sum_{i,\nu} \sum_{s,s'} \hat{n}_{i,s}^d \hat{n}_{i+\hat{\nu}/2,s'}^p \\ & + V_{pp} \sum_i \sum_{\langle \nu,\nu' \rangle} \sum_{s,s'} \hat{n}_{i+\hat{\nu}/2,s}^p \hat{n}_{i+\hat{\nu}'/2',s'}^p.\end{aligned}$$

The different orbitals and parameters of the model are shown in Fig.~\ref{fig:unitcell}. Setting $t_{pd} = 1$, we fix the energy scale in the following.

Completion

You will be instructed to construct the interaction part of the Hamiltonian, \HH' in the real space in the second-quantized form.

The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian.

The interaction is a density-density interaction composed of the following processes: - Interaction between site i and itself with the interaction strength $U\{d\}$ - *Interaction between site i and its neighboring site $i+\hat{\nu}/2$ with the interaction strength $U\{p\}/2$* - Interaction between site i and its neighboring site $i+\hat{\nu}/2$ with the interaction strength $V\{pd\}$ - *Interaction between site i and its neighboring site $i+\hat{\nu}/2'$ with the interaction strength $V\{pp\}$* The summation should be taken over all spin states (s, s') and all real space positions.

Return the interaction term \HH' in terms of \hat{n}.

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): - \HH' is the interaction part of the Hamiltonian - $U\{d\}$, $U\{p\}$, $V\{pd\}$, and $V\{pp\}$ are the interaction strengths - \hat{n} is the density operator - i is the site index - \nu is the direction index - s and s' are the spin states - d and p denote different orbitals - $t_{pd}=1$ sets the energy scale.

3 Fourier transform noninteracting term to momentum space (lattice)

Prompt

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

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

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

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

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

Template:

You will be instructed to convert the noninteracting Hamiltonian {nonint_symbol} in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should

apply the Fourier transformation to $\{\text{real_creation_op}\}$ in the real space to the $\{\text{momentum_creation_op}\}$ in the momentum space, which is defined as $\{\text{definition_of_Fourier_Transformation}\}$, where $\{\text{real_variable}\}$ is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that hopping have no position dependence now.] Express the total noninteracting Hamiltonian $\{\text{nonint_symbol}\}$ in terms of $\{\text{momentum_creation_op}\}$. 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): $\{\text{definition_of_variables}\}$

Excerpt:

$$\mathcal{H}_{\text{MF}} = \sum_{\mathbf{k}, s} \hat{C}_{\mathbf{k}s}^\dagger \mathcal{H}_{\mathbf{k}s} \hat{C}_{\mathbf{k}s} + f(n^p, \eta)$$

with $\hat{C}_{\mathbf{k}s}^\dagger = (\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger)$,

$$\mathcal{H}_{\mathbf{k}s} = \begin{pmatrix} \xi_x & \gamma_2(\mathbf{k}) & \gamma_1(k_x) \\ \gamma_2(\mathbf{k}) & \xi_y & \gamma_1(k_y) \\ \gamma_1(k_x) & \gamma_1(k_y) & \xi_d \end{pmatrix}$$

and

$$\frac{f(n^p, \eta)}{N} = -\tilde{U}_p \frac{(n^p)^2}{8} + \tilde{V}_{pp} \frac{\eta^2}{8} - \tilde{U}_d \frac{(n - n^p)^2}{4}.$$

Here, n is the total density of holes, n^p is the total density of holes on the oxygen sites, i.e.,

$$n^p \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) + (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

and the nematic order parameter η is defined in Eq.\eqref{eq:eta}. The elements of the matrix~\eqref{eq:h0k} are given by

$$\begin{aligned} \gamma_1(k_i) &= -2t_{pd} \cos \frac{k_i}{2}, \\ \gamma_2(\mathbf{k}) &= -4t_{pp} \cos \frac{k_x}{2} \cos \frac{k_y}{2}, \end{aligned}$$

and

$$\begin{aligned} \xi_x &= \Delta + \tilde{U}_p \frac{n^p}{4} - \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_y &= \Delta + \tilde{U}_p \frac{n^p}{4} + \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_d &= \tilde{U}_d \frac{(n - n^p)}{2} - \mu, \end{aligned}$$

and also, we introduced the effective interaction parameters

$$\begin{aligned} \tilde{U}_p &= U_p + 8V_{pp} - 8V_{pd}, \\ \tilde{V}_{pp} &= 8V_{pp} - U_p, \\ \tilde{U}_d &= U_d - 4V_{pd}. \end{aligned}$$

In addition, we have put all the constant terms, i.e. $2V_{pd}n - V_{pd}n^2$, into the chemical potential μ . %%%%%%%%%%%%%%% The mean-field Hamiltonian~\eqref{eq:mhamiltonian} can be diagonalized to yield three bands each with mixed orbital character and dispersion $\xi_{\alpha\mathbf{k}s}$, where $\alpha = 1, 2, 3$ is the band index for the lowest lying and the two upper bands.

Completion

You will be instructed to convert the noninteracting Hamiltonian \mathcal{H}_{MF} in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to $\hat{C}_{\mathbf{k}s}^\dagger$ in the real space to the $\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger$ in the momentum space, which is defined as $\mathcal{H}_{\mathbf{k}s}$, where \mathbf{k} is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that hopping have no position dependence now.] Express the total noninteracting Hamiltonian \mathcal{H}_{MF} in terms of $\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger$. Simplify any summation index if possible.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): $\mathcal{H}_{\mathbf{k}s}$ is the Hamiltonian in momentum space, $\hat{C}_{\mathbf{k}s}^\dagger$ is the creation operator in real space, $\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger$ are the creation operators in momentum space, \mathbf{k} is the momentum, s is the spin index, n is the total density of holes, n^p is the total density of holes on the oxygen sites, η is the nematic order parameter, $\gamma_1(k_i)$ and $\gamma_2(\mathbf{k})$ are elements of the Hamiltonian matrix, ξ_x, ξ_y , and ξ_d are the diagonal elements of the Hamiltonian matrix, $\tilde{U}_p, \tilde{V}_{pp}$, and \tilde{U}_d are the effective interaction parameters, and μ is the chemical potential.

4 Fourier transform interacting term to momentum space (lattice)

Prompt

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

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

Template:

You will be instructed to convert the interacting Hamiltonian, {second_int_symbol}, in the {single-particle|second-quantized} form the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to {real_creation_op} in the real space to the {momentum_creation_op} in the momentum space, which is defined as {definition_of_Fourier_Transformation}, where {real_variable} is integrated over all sites in the entire real space, and {momentum_var} is defined within the first Brillouin zone. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that interaction have no position dependence now]

Express {second_int_symbol} in terms of {momentum_creation_op}. Simplify any summation index if possible.

Excerpt:

$$\mathcal{H}_{\text{MF}} = \sum_{\mathbf{k},s} \hat{C}_{\mathbf{k}s}^\dagger \mathcal{H}_{\mathbf{k}s} \hat{C}_{\mathbf{k}s} + f(n^p, \eta)$$

with $\hat{C}_{\mathbf{k}s}^\dagger = (\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger)$,

$$\mathcal{H}_{\mathbf{k}s} = \begin{pmatrix} \xi_x & \gamma_2(\mathbf{k}) & \gamma_1(k_x) \\ \gamma_2(\mathbf{k}) & \xi_y & \gamma_1(k_y) \\ \gamma_1(k_x) & \gamma_1(k_y) & \xi_d \end{pmatrix}$$

and

$$\frac{f(n^p, \eta)}{N} = -\tilde{U}_p \frac{(n^p)^2}{8} + \tilde{V}_{pp} \frac{\eta^2}{8} - \tilde{U}_d \frac{(n - n^p)^2}{4}.$$

Here, n is the total density of holes, n^p is the total density of holes on the oxygen sites, i.e.,

$$n^p \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) + (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

and the nematic order parameter η is defined in Eq.\eqref{eq:eta}. The elements of the matrix~\eqref{eq:h0k} are given by

$$\begin{aligned} \gamma_1(k_i) &= -2t_{pd} \cos \frac{k_i}{2}, \\ \gamma_2(\mathbf{k}) &= -4t_{pp} \cos \frac{k_x}{2} \cos \frac{k_y}{2}, \end{aligned}$$

and

$$\begin{aligned} \xi_x &= \Delta + \tilde{U}_p \frac{n^p}{4} - \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_y &= \Delta + \tilde{U}_p \frac{n^p}{4} + \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_d &= \tilde{U}_d \frac{(n - n^p)}{2} - \mu, \end{aligned}$$

and also, we introduced the effective interaction parameters

$$\begin{aligned} \tilde{U}_p &= U_p + 8V_{pp} - 8V_{pd}, \\ \tilde{V}_{pp} &= 8V_{pp} - U_p, \\ \tilde{U}_d &= U_d - 4V_{pd}. \end{aligned}$$

In addition, we have put all the constant terms, i.e. $2V_{pd}n - V_{pd}n^2$, into the chemical potential μ . %%%%%%%%%%%%%%% The mean-field Hamiltonian~\eqref{eq:mhamiltonian}

can be diagonalized to yield three bands each with mixed orbital character and dispersion $\xi_{\alpha\mathbf{k}s}$, where $\alpha = 1, 2, 3$ is the band index for the lowest lying and the two upper bands.

Completion

You will be instructed to convert the interacting Hamiltonian, \mathcal{H}_{MF} , in the second-quantized form the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to $\hat{C}_{\mathbf{k}s}^\dagger$ in the real space to the $\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger$ in the momentum space, which is defined as $\mathcal{H}_{\mathbf{k}s}$, where \mathbf{k} is integrated over all sites in the entire real space, and s is defined within the first Brillouin zone. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that interaction have no position dependence now] Express \mathcal{H}_{MF} in terms of $\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger$. Simplify any summation index if possible.

5 Wick's theorem expansion

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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:

$$\mathcal{H}_{\text{MF}} = \sum_{\mathbf{k},s} \hat{C}_{\mathbf{k}s}^\dagger \mathcal{H}_{\mathbf{k}s} \hat{C}_{\mathbf{k}s} + f(n^p, \eta)$$

with $\hat{C}_{\mathbf{k}s}^\dagger = (\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger)$,

$$\mathcal{H}_{\mathbf{k}s} = \begin{pmatrix} \xi_x & \gamma_2(\mathbf{k}) & \gamma_1(k_x) \\ \gamma_2(\mathbf{k}) & \xi_y & \gamma_1(k_y) \\ \gamma_1(k_x) & \gamma_1(k_y) & \xi_d \end{pmatrix}$$

and

$$\frac{f(n^p, \eta)}{N} = -\tilde{U}_p \frac{(n^p)^2}{8} + \tilde{V}_{pp} \frac{\eta^2}{8} - \tilde{U}_d \frac{(n - n^p)^2}{4}.$$

Here, n is the total density of holes, n^p is the total density of holes on the oxygen sites, i.e.,

$$n^p \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) + (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

and the nematic order parameter η is defined in Eq.\eqref{eq:eta}. The elements of the matrix~\eqref{eq:h0k} are given by

$$\begin{aligned} \gamma_1(k_i) &= -2t_{pd} \cos \frac{k_i}{2}, \\ \gamma_2(\mathbf{k}) &= -4t_{pp} \cos \frac{k_x}{2} \cos \frac{k_y}{2}, \end{aligned}$$

and

$$\begin{aligned}\xi_x &= \Delta + \tilde{U}_p \frac{n^p}{4} - \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_y &= \Delta + \tilde{U}_p \frac{n^p}{4} + \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_d &= \tilde{U}_d \frac{(n - n^p)}{2} - \mu,\end{aligned}$$

and also, we introduced the effective interaction parameters

$$\begin{aligned}\tilde{U}_p &= U_p + 8V_{pp} - 8V_{pd}, \\ \tilde{V}_{pp} &= 8V_{pp} - U_p, \\ \tilde{U}_d &= U_d - 4V_{pd}.\end{aligned}$$

In addition, we have put all the constant terms, i.e. $2V_{pd}n - V_{pd}n^2$, into the chemical potential μ . The mean-field Hamiltonian can be diagonalized to yield three bands each with mixed orbital character and dispersion $\xi_{\alpha\mathbf{k}s}$, where $\alpha = 1, 2, 3$ is the band index for the lowest lying and the two upper bands.

Completion

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

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

\mathcal{H}_{MF} is the mean-field Hamiltonian, $\hat{C}_{\mathbf{k}s}^\dagger$ is the creation operator, $\mathcal{H}_{\mathbf{k}s}$ is the Hamiltonian, $f(n^p, \eta)$ is a function of the total density of holes on the oxygen sites and the nematic order parameter, n is the total density of holes, n^p is the total density of holes on the oxygen sites, η is the nematic order parameter, $\gamma_1(k_i)$, $\gamma_2(\mathbf{k})$, ξ_x , ξ_y , and ξ_d are elements of the matrix, \tilde{U}_p , \tilde{V}_{pp} , and \tilde{U}_d are the effective interaction parameters, and μ is the chemical potential.

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:

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

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

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

Template:

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

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

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

Return {Hartree_Fock_second_quantized_symbol}.

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

{definition_of_variables}

Excerpt:

$$\mathcal{H}_{\text{MF}} = \sum_{\mathbf{k},s} \hat{C}_{\mathbf{k}s}^\dagger \mathcal{H}_{\mathbf{k}s} \hat{C}_{\mathbf{k}s} + f(n^p, \eta)$$

with $\hat{C}_{\mathbf{k}s}^\dagger = (\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger)$,

$$\mathcal{H}_{\mathbf{k}s} = \begin{pmatrix} \xi_x & \gamma_2(\mathbf{k}) & \gamma_1(k_x) \\ \gamma_2(\mathbf{k}) & \xi_y & \gamma_1(k_y) \\ \gamma_1(k_x) & \gamma_1(k_y) & \xi_d \end{pmatrix}$$

and

$$\frac{f(n^p, \eta)}{N} = -\tilde{U}_p \frac{(n^p)^2}{8} + \tilde{V}_{pp} \frac{\eta^2}{8} - \tilde{U}_d \frac{(n - n^p)^2}{4}.$$

Here, n is the total density of holes, n^p is the total density of holes on the oxygen sites, i.e.,

$$n^p \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) + (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

and the nematic order parameter η is defined in Eq.~\eqref{eq:eta}. The elements of the matrix~\eqref{eq:h0k} are given by

$$\begin{aligned} \gamma_1(k_i) &= -2t_{pd} \cos \frac{k_i}{2}, \\ \gamma_2(\mathbf{k}) &= -4t_{pp} \cos \frac{k_x}{2} \cos \frac{k_y}{2}, \end{aligned}$$

and

$$\begin{aligned} \xi_x &= \Delta + \tilde{U}_p \frac{n^p}{4} - \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_y &= \Delta + \tilde{U}_p \frac{n^p}{4} + \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_d &= \tilde{U}_d \frac{(n - n^p)}{2} - \mu, \end{aligned}$$

and also, we introduced the effective interaction parameters

$$\begin{aligned} \tilde{U}_p &= U_p + 8V_{pp} - 8V_{pd}, \\ \tilde{V}_{pp} &= 8V_{pp} - U_p, \\ \tilde{U}_d &= U_d - 4V_{pd}. \end{aligned}$$

In addition, we have put all the constant terms, i.e. $2V_{pd}n - V_{pd}n^2$, into the chemical potential μ . %%%%%%%%%%%%%%% The mean-field Hamiltonian~\eqref{eq:mhamiltonian} can be diagonalized to yield three bands each with mixed orbital character and dispersion $\xi_{\alpha\mathbf{k}s}$, where $\alpha = 1, 2, 3$ is the band index for the lowest lying and the two upper bands.

Completion

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

The quadratic terms mean terms that are proportional to $\hat{C}_{\mathbf{k}s}^\dagger \mathcal{H}_{\mathbf{k}s} \hat{C}_{\mathbf{k}s}$, which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in \mathcal{H}_{MF} , denoted as $\mathcal{H}_{\mathbf{k}s}$.

Return $\mathcal{H}_{\mathbf{k}s}$.

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

\mathcal{H}_{MF} is the mean-field Hamiltonian, $\hat{C}_{\mathbf{k}s}^\dagger$ is the creation operator, $\mathcal{H}_{\mathbf{k}s}$ is the Hamiltonian matrix, and $\hat{C}_{\mathbf{k}s}$ is the annihilation operator. The elements of the matrix $\mathcal{H}_{\mathbf{k}s}$ are given by $\gamma_1(k_i)$, $\gamma_2(\mathbf{k})$, ξ_x , ξ_y , and ξ_d . The effective interaction parameters are \tilde{U}_p , \tilde{V}_{pp} , and \tilde{U}_d . The total density of holes is denoted by n , the total density of holes on the oxygen sites is denoted by n^p , and the nematic order parameter is denoted by η .

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 $\{\text{Hartree_Fock_second_quantized_symbol}\}$. Here, Hartree term only means that only the expected value in the form $\{\text{expected_value_Hartree}\}$ (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 $\{\text{Hartree_second_quantized_symbol}\}$.

Excerpt:

with the hole densities on the oxygen sites $n_{\nu s}^p = \langle \hat{n}_{i+\hat{\nu}/2, s}^p \rangle$. In the absence of an overall magnetization on the oxygen sites, i.e.

$$\begin{aligned} m &\equiv (n_{x\uparrow}^p - n_{x\downarrow}^p) + (n_{y\uparrow}^p - n_{y\downarrow}^p) \\ &= 0, \end{aligned}$$

there are two distinct ways to break the lattice symmetry within each unit-cell, a nematic order and a nematic-spin nematic order. IUC nematic order in this model can be measured in terms of a spontaneous imbalance between the density of holes at the oxygen sites

$$\eta \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) - (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

while nematic-spin-nematic order corresponds to having equal, but opposite magnetization on the two oxygen sites,

$$\eta_s \equiv (n_{x\uparrow}^p - n_{x\downarrow}^p) - (n_{y\uparrow}^p - n_{y\downarrow}^p).$$

Fig.~\ref{fig:fs} shows the distorted Fermi surfaces associated with these ordering possibilities as well as for ferromagnetic ordering for contrast. \begin{figure}[tb] \begin{center} \includegraphics{fs} \end{center} \caption{Static Fermi surface instabilities analyzed in this work: (a) Nematic phase breaking C_4 symmetry, (b) nematic-spin-nematic and (c) ferromagnetic instability. In (b) and (c), the solid and dashed lines denote the up- and down-spin band. } \label{fig:fs} \end{figure}

We arrive in the following at the mean-field Hamiltonian for nematic or nematic-spin-nematic order by a standard decoupling of all the interaction terms in Eq.~\eqref{eq:interaction} in the Hartree channel. We seek self-consistent solution with $\eta \neq 0$ or $\eta_s \neq 0$, respectively, for nematic and nematic-spin-nematic order.

\subsubsection{Nematic order} The mean-field Hamiltonian can be written in momentum space as

$$\mathcal{H}_{\text{MF}} = \sum_{\mathbf{k}, s} \hat{C}_{\mathbf{k}s}^\dagger \mathcal{H}_{\mathbf{k}s} \hat{C}_{\mathbf{k}s} + f(n^p, \eta)$$

with $\hat{C}_{\mathbf{k}s}^\dagger = (\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger)$,

$$\mathcal{H}_{\mathbf{k}s} = \begin{pmatrix} \xi_x & \gamma_2(\mathbf{k}) & \gamma_1(k_x) \\ \gamma_2(\mathbf{k}) & \xi_y & \gamma_1(k_y) \\ \gamma_1(k_x) & \gamma_1(k_y) & \xi_d \end{pmatrix}$$

and

$$\frac{f(n^p, \eta)}{N} = -\tilde{U}_p \frac{(n^p)^2}{8} + \tilde{V}_{pp} \frac{\eta^2}{8} - \tilde{U}_d \frac{(n - n^p)^2}{4}.$$

Here, n is the total density of holes, n^p is the total density of holes on the oxygen sites, i.e.,

$$n^p \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) + (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

and the nematic order parameter η is defined in Eq.~\eqref{eq:eta}. The elements of the matrix~\eqref{eq:h0k} are given by

$$\begin{aligned} \gamma_1(k_i) &= -2t_{pd} \cos \frac{k_i}{2}, \\ \gamma_2(\mathbf{k}) &= -4t_{pp} \cos \frac{k_x}{2} \cos \frac{k_y}{2}, \end{aligned}$$

and

$$\begin{aligned} \xi_x &= \Delta + \tilde{U}_p \frac{n^p}{4} - \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_y &= \Delta + \tilde{U}_p \frac{n^p}{4} + \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_d &= \tilde{U}_d \frac{(n - n^p)}{2} - \mu, \end{aligned}$$

and also, we introduced the effective interaction parameters

$$\begin{aligned} \tilde{U}_p &= U_p + 8V_{pp} - 8V_{pd}, \\ \tilde{V}_{pp} &= 8V_{pp} - U_p, \\ \tilde{U}_d &= U_d - 4V_{pd}. \end{aligned}$$

In addition, we have put all the constant terms, i.e. $2V_{pd}n - V_{pd}n^2$, into the chemical potential μ . The mean-field Hamiltonian can be diagonalized to yield three bands each with mixed orbital character and dispersion $\xi_{\alpha\mathbf{k}s}$, where $\alpha = 1, 2, 3$ is the band index for the lowest lying and the two upper bands.

Completion

You will be instructed to keep only the Hartree term in Eq.~\eqref{eq:interaction}.

Here, Hartree term only means that only the expected value in the form $\langle \hat{n}_{i+\hat{\nu}/2,s}^p \rangle$ (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}_{MF} .

8 Relabel the index

Prompt

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

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

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

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

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

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

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

Template:

You will be instructed to simplify the quadratic term {Hartree_Fock_second_quantized_symbol} through relabeling the index.

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

Namely, a replacement of {relabel} is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes {Unsummed_Indices}.

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

Return the simplified {Hartree_Fock_second_quantized_symbol}.

Excerpt:

with the hole densities on the oxygen sites $n_{\nu s}^p = \langle \hat{n}_{i+\hat{\nu}/2,s}^p \rangle$. In the absence of an overall magnetization on the oxygen sites, i.e.

$$\begin{aligned} m &\equiv (n_{x\uparrow}^p - n_{x\downarrow}^p) + (n_{y\uparrow}^p - n_{y\downarrow}^p) \\ &= 0, \end{aligned}$$

there are two distinct ways to break the lattice symmetry within each unit-cell, a nematic order and a nematic-spin nematic order. IUC nematic order in this model can be measured in terms of a spontaneous imbalance between the density of holes at the oxygen sites

$$\eta \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) - (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

while nematic-spin-nematic order corresponds to having equal, but opposite magnetization on the two oxygen sites,

$$\eta_s \equiv (n_{x\uparrow}^p - n_{x\downarrow}^p) - (n_{y\uparrow}^p - n_{y\downarrow}^p).$$

Fig.~\ref{fig:fs} shows the distorted Fermi surfaces associated with these ordering possibilities as well as for ferromagnetic ordering for contrast. \begin{figure}[tb] \begin{center} \includegraphics{fs} \end{center} \caption{Static Fermi surface instabilities analyzed in this work: (a) Nematic phase breaking C_4 symmetry, (b) nematic-spin-nematic and (c) ferromagnetic instability. In (b) and (c), the solid and dashed lines denote the up- and down-spin band. } \label{fig:fs} \end{figure}

We arrive in the following at the mean-field Hamiltonian for nematic or nematic-spin-nematic order by a standard decoupling of all the interaction terms in Eq.~\eqref{eq:interaction} in the Hartree channel. We seek self-consistent solution with $\eta \neq 0$ or $\eta_s \neq 0$, respectively, for nematic and nematic-spin-nematic order.

\subsubsection{Nematic order} The mean-field Hamiltonian can be written in momentum space as

$$\mathcal{H}_{\text{MF}} = \sum_{\mathbf{k},s} \hat{C}_{\mathbf{k}s}^\dagger \mathcal{H}_{\mathbf{k}s} \hat{C}_{\mathbf{k}s} + f(n^p, \eta)$$

with $\hat{C}_{\mathbf{k}s}^\dagger = (\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger)$,

$$\mathcal{H}_{\mathbf{k}s} = \begin{pmatrix} \xi_x & \gamma_2(\mathbf{k}) & \gamma_1(k_x) \\ \gamma_2(\mathbf{k}) & \xi_y & \gamma_1(k_y) \\ \gamma_1(k_x) & \gamma_1(k_y) & \xi_d \end{pmatrix}$$

and

$$\frac{f(n^p, \eta)}{N} = -\tilde{U}_p \frac{(n^p)^2}{8} + \tilde{V}_{pp} \frac{\eta^2}{8} - \tilde{U}_d \frac{(n - n^p)^2}{4}.$$

Here, n is the total density of holes, n^p is the total density of holes on the oxygen sites, i.e.,

$$n^p \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) + (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

and the nematic order parameter η is defined in Eq.~\eqref{eq:eta}. The elements of the matrix~\eqref{eq:h0k} are given by

$$\begin{aligned} \gamma_1(k_i) &= -2t_{pd} \cos \frac{k_i}{2}, \\ \gamma_2(\mathbf{k}) &= -4t_{pp} \cos \frac{k_x}{2} \cos \frac{k_y}{2}, \end{aligned}$$

and

$$\begin{aligned} \xi_x &= \Delta + \tilde{U}_p \frac{n^p}{4} - \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_y &= \Delta + \tilde{U}_p \frac{n^p}{4} + \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_d &= \tilde{U}_d \frac{(n - n^p)}{2} - \mu, \end{aligned}$$

and also, we introduced the effective interaction parameters

$$\begin{aligned} \tilde{U}_p &= U_p + 8V_{pp} - 8V_{pd}, \\ \tilde{V}_{pp} &= 8V_{pp} - U_p, \\ \tilde{U}_d &= U_d - 4V_{pd}. \end{aligned}$$

In addition, we have put all the constant terms, i.e. $2V_{pd}n - V_{pd}n^2$, into the chemical potential μ . %%%%%%%%%%%%%%% The mean-field Hamiltonian~\eqref{eq:mhamiltonian} can be diagonalized to yield three bands each with mixed orbital character and dispersion $\xi_{\alpha\mathbf{k}s}$, where $\alpha = 1, 2, 3$ is the band index for the lowest lying and the two upper bands.

Completion

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

The logic is that the expected value ($n_{\nu s}^p$) in the first Hartree term ($\tilde{U}_p \frac{n^p}{4}$ and $\tilde{V}_{pp} \frac{\eta}{4}$) has the same form as the quadratic operators in the second Hartree term ($\tilde{U}_d \frac{(n - n^p)}{2}$), and vice versa. The same applies to the Fock term.

Namely, a replacement of n^p and η is applied to ONLY the second Hartree or Fock term. You should not swap any index that is not in the summation, which includes n , η , and μ .

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}_{MF} .

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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'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, $\{\text{Hartree_second_quantized_symbol}\}$, 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 . 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 $\{\text{Hartree_second_quantized_symbol}\}$.

Excerpt:

with the hole densities on the oxygen sites $n_{\nu s}^p = \langle \hat{n}_{i+\hat{\nu}/2, s}^p \rangle$. In the absence of an overall magnetization on the oxygen sites, i.e.

$$\begin{aligned} m &\equiv (n_{x\uparrow}^p - n_{x\downarrow}^p) + (n_{y\uparrow}^p - n_{y\downarrow}^p) \\ &= 0, \end{aligned}$$

there are two distinct ways to break the lattice symmetry within each unit-cell, a nematic order and a nematic-spin nematic order. IUC nematic order in this model can be measured in terms of a spontaneous imbalance between the density of holes at the oxygen sites

$$\eta \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) - (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

while nematic-spin-nematic order corresponds to having equal, but opposite magnetization on the two oxygen sites,

$$\eta_s \equiv (n_{x\uparrow}^p - n_{x\downarrow}^p) - (n_{y\uparrow}^p - n_{y\downarrow}^p).$$

Fig.~\ref{fig:fs} shows the distorted Fermi surfaces associated with these ordering possibilities as well as for ferromagnetic ordering for contrast. \begin{figure}[tb] \begin{center} \includegraphics{fs} \end{center} \caption{Static Fermi surface instabilities analyzed in this work: (a) Nematic phase breaking C_4 symmetry, (b) nematic-spin-nematic and (c) ferromagnetic instability. In (b) and (c), the solid and dashed lines denote the up- and down-spin band. } \label{fig:fs} \end{figure}

We arrive in the following at the mean-field Hamiltonian for nematic or nematic-spin-nematic order by a standard decoupling of all the interaction terms in Eq.~\eqref{eq:interaction} in the Hartree channel. We seek self-consistent solution with $\eta \neq 0$ or $\eta_s \neq 0$, respectively, for nematic and nematic-spin-nematic order.

\subsubsection{Nematic order} The mean-field Hamiltonian can be written in momentum space as

$$\mathcal{H}_{\text{MF}} = \sum_{\mathbf{k}, s} \hat{C}_{\mathbf{k}s}^\dagger \mathcal{H}_{\mathbf{k}s} \hat{C}_{\mathbf{k}s} + f(n^p, \eta)$$

with $\hat{C}_{\mathbf{k}s}^\dagger = (\hat{p}_{x\mathbf{k}s}^\dagger, \hat{p}_{y\mathbf{k}s}^\dagger, \hat{d}_{\mathbf{k}s}^\dagger)$,

$$\mathcal{H}_{\mathbf{k}s} = \begin{pmatrix} \xi_x & \gamma_2(\mathbf{k}) & \gamma_1(k_x) \\ \gamma_2(\mathbf{k}) & \xi_y & \gamma_1(k_y) \\ \gamma_1(k_x) & \gamma_1(k_y) & \xi_d \end{pmatrix}$$

and

$$\frac{f(n^p, \eta)}{N} = -\tilde{U}_p \frac{(n^p)^2}{8} + \tilde{V}_{pp} \frac{\eta^2}{8} - \tilde{U}_d \frac{(n - n^p)^2}{4}.$$

Here, n is the total density of holes, n^p is the total density of holes on the oxygen sites, i.e.,

$$n^p \equiv (n_{x\uparrow}^p + n_{x\downarrow}^p) + (n_{y\uparrow}^p + n_{y\downarrow}^p),$$

and the nematic order parameter η is defined in Eq.~\eqref{eq:eta}. The elements of the matrix~\eqref{eq:h0k} are given by

$$\begin{aligned} \gamma_1(k_i) &= -2t_{pd} \cos \frac{k_i}{2}, \\ \gamma_2(\mathbf{k}) &= -4t_{pp} \cos \frac{k_x}{2} \cos \frac{k_y}{2}, \end{aligned}$$

and

$$\begin{aligned} \xi_x &= \Delta + \tilde{U}_p \frac{n^p}{4} - \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_y &= \Delta + \tilde{U}_p \frac{n^p}{4} + \tilde{V}_{pp} \frac{\eta}{4} - \mu, \\ \xi_d &= \tilde{U}_d \frac{(n - n^p)}{2} - \mu, \end{aligned}$$

and also, we introduced the effective interaction parameters

$$\begin{aligned}\tilde{U}_p &= U_p + 8V_{pp} - 8V_{pd}, \\ \tilde{V}_{pp} &= 8V_{pp} - U_p, \\ \tilde{U}_d &= U_d - 4V_{pd}.\end{aligned}$$

In addition, we have put all the constant terms, i.e. $2V_{pd}n - V_{pd}n^2$, into the chemical potential μ . The mean-field Hamiltonian~\eqref{eq:mhamiltonian} can be diagonalized to yield three bands each with mixed orbital character and dispersion $\xi_{\alpha\mathbf{k}s}$, where $\alpha = 1, 2, 3$ is the band index for the lowest lying and the two upper bands.

Completion

You will be instructed to simplify the Hartree term, \mathcal{H}_{MF} , by reducing the momentum inside the expected value $n_{\nu s}^p$.

The expected value $n_{\nu s}^p$ is only nonzero when the two momenta k_i, k_j are the same, namely, $n_{i+\hat{\nu}/2, s}^p$.

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

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

Return the final simplified Hartree term \mathcal{H}_{MF} .