1 Preamble

1.1 One-shot Example

1.1.1

Prompt: I am reading a paper with the following abstract. I want you to first extract the essential information from it and then execute my instructions in order to create the Hamiltonian in the Hartree Fock Approximation.
To extract information, I will provide you with a set of questions about the calculation (this type of prompt will start with **Extraction**). You should first try your best to answer them. You should first quote the relevant part from the abstract which you think can lead to an answer. Then, you provide your rationale from this quote to the answer. Finally, you should give a succinct final version of the answer.
To execute the calculation, I will provide a set of tasks. You should follow the instructions strictly. Your reply should be succinct while complete. You should not expand any unwanted content. You will be learning background knowledge by examples if necessary.
A crucial part of execution is two-step: (1) fill in the paper-specific information from the extraction into a provided template (this prompts will start with **Execution–Core information**); (2) combine with the predetermined notations provided by me (this prompts will start with **Execution–Notation**), and then, you should proceed to execute the instruction. Note that there might be cases where no paper-specific information is needed from the abstract in certain execution tasks.
I will provide three examples (Example 1, Example 2, and Example 3) for **Extraction**, **Execution–Core information**, and **Execution**–Notation**, respectively, for you to learn. Confirm and repeat your duty if you understand it.
Example 1
"'

Extraction Abstract We present a theory on the quantum phase diagram of AB-stacked $MoTe_2$/WSe_2 using a self-consistent Hartree-Fock calculation performed in the plane-wave basis, motivated by the observation of topological states in this system. At filling factor $\nu = 2$ (two holes per moir'e unit cell), Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator by opening a charge gap. At $\nu = 1$, the interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state, which undergo first-order phase transitions tuned by an out-of-plane displacement field. The valley polarized state becomes a Chern insulator for certain displacement fields. Moreover, we predict a topological charge density wave forming a honeycomb lattice with ferromagnetism at $\nu = 2/3$. Future directions on this versatile system hosting a rich set of quantum phases are discussed.
Question: 1. What are the degrees of freedom that should be included in the Hamiltonian? 2. [Another question]
"'
You response should be:
"'

1. What are the degrees of freedom that should be included in the Hamiltonian? **Quote**: AB-stacked $MoTe_2$/WSe_2 **Explanation**: First the studied system is $MoTe_2$/WSe_2 , which is a heterostructure of bilayer. Therefore, layer is a degree of freedom that should be included in the Hamiltonian. Secod, because $MoTe_2$ and WSe_2 are both TMD materials which have strong Ising type spin orbit coupling. This coupling ties the electron's spin to its valley index, resulting in distinct energy levels for spins aligned parallel or antiparallel to the orbital angular momentum. Since $MoTe_2$ and WSe_2 usually have the topmost valence band at +K/-K valley. This means the valley index is coupled to the spin index. Therefore, only two types of degrees of freedom (layer and valley) should be considered in the Hamiltonian. **Anwser**: layer, valley
2. [Another question] [Another answer]

"'
Example 2
"'

Execution–Core information You should fill in the specific information from above into the following template, and then repeat it. "'
You will be instructed to describe the kinetic term of Hamiltonian in{system of interest}.
The degrees of freedom of the system are:{independent degree of freedom} "' "'
Your response should be:
"'

You will be instructed to describe the kinetic term of Hamiltonian in AB-stacked $MoTe_2$/WSe_2. The degrees of freedom of the system are: Layer and the combined spin-valley degree.

“‘
Example 3
“‘
Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. ”’
Express the Kinetic Hamiltonian H_T using $E_{+K,b}$, $E_{-K,t}$, $E_{-K,b}$, $E_{-K,t}$ which are only on the diagonal terms, and arrange the basis in the order of (+K,bottom), (+K,top), (-K,bottom), (-K,top).
Use the following conventions for the symbols:
$\tau = \pm 1$ represents $\pm K$ valleys, bottom layer ($\mathfrak{b}$) and top layer ($\mathfrak{t}$)
”’
“‘
Your response should be:
“‘
Instructions to execute: You will be instructed to describe the kinetic term of Hamiltonian in AB-stacked $MoTe_2/WSe_2$. The degrees of freedom of the system are: Layer and the combined spin-valley degree. Express the Kinetic Hamiltonian H_T using $E_{+K,b}$, $E_{-K,t}$, $E_{-K,b}$, $E_{-K,t}$ which are only on the diagonal terms, and arrange the basis in the order of (+K,bottom), (+K,top), (-K,bottom), (-K,top).
Use the following conventions for the symbols:
$\tau = \pm 1$ represents $\pm K$ valleys, bottom layer ($\mathfrak{b}$) and top layer ($\mathfrak{t}$)
Answer [The answer to the above ’Instructions to execute’] “‘

1.1.2

Completion: I understand my duties as follows:

1. **Extraction**: When provided with an abstract or excerpt from a paper, I will extract essential information by:

- Quoting relevant parts of the abstract.
- Providing a rationale from this quote to the answer.
- Giving a succinct final version of the answer.

2. **Execution - Core Information**: I will fill in paper-specific information from the extraction into a provided template and then repeat the filled-in template.

3. **Execution - Notation**: I will combine the provided notation with the ”Execution - Core Information” to execute the instruction. The response will include:

- Repeating the instruction for execution.
- Proceeding with the calculation or explanation as required.

Let’s proceed with your instructions.

2 Identify kinetic term (continuum,first-quantized)

2.1 Extraction

2.1.1

Prompt: Extraction Abstract We present a theory on the quantum phase diagram of AB-stacked $MoTe_2/WSe_2$ using a self-consistent Hartree-Fock calculation performed in the plane-wave basis, motivated by the observation of topological states in this system. At filling factor $\nu = 2$ (two holes per moir’e unit cell), Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator by opening a charge gap. At $\nu = 1$, the interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state, which undergo first-order phase transitions tuned by an out-of-plane displacement field. The valley polarized state becomes a Chern insulator for certain displacement fields. Moreover, we predict a topological charge density wave forming a honeycomb lattice with ferromagnetism at $\nu = 2/3$. Future directions on this versatile system hosting a rich set of quantum phases are discussed.
Question: 1. What is the system to study? 2. What are the independent degrees of freedom that should be included in the Hamiltonian, namely, the independent flavor of the creation/annihilation operator? Remember the system is spin-valley locked.

2.1.2

Completion: 1. **What is the system to study? Quote**: "AB-stacked $MoTe_2/WSe_2$" **Explanation**: The system under study is explicitly stated in the abstract as "AB-stacked $MoTe_2/WSe_2$". This refers to a heterostructure composed of layers of $MoTe_2$ and WSe_2 materials, arranged in an AB stacking configuration. **Answer**: AB-stacked $MoTe_2/WSe_2$.

2. **What are the independent degrees of freedom that should be included in the Hamiltonian, namely, the independent flavor of the creation/annihilation operator? Remember the system is spin-valley locked. Quote**: "the observation of topological states in this system" and "spin density wave states, an in-plane ferromagnetic state, and a valley polarized state" **Explanation**: The abstract mentions topological states, spin density waves, ferromagnetic states, and valley polarization in the AB-stacked $MoTe_2/WSe_2$ system. Since the system is spin-valley locked, the spins and valleys are not independent degrees of freedom; they are coupled. This coupling implies that the spin and valley degrees of freedom cannot be varied independently and are considered as one combined degree of freedom in the Hamiltonian. **Answer**: The independent degrees of freedom in the Hamiltonian are the combined spin-valley degree and the layer degree (from the AB-stacked configuration).

2.2 Execution–Core information

2.2.1

Prompt: Execution–Core information You should fill in the specific information from above into the following template, and then repeat it. "' You will be instructed to describe the kinetic term of Hamiltonian in {system of study}. The degrees of freedom of the system are: {independent degree of freedom} "'

2.2.2

Completion: You will be instructed to describe the kinetic term of the Hamiltonian in AB-stacked $MoTe_2/WSe_2$. The degrees of freedom of the system are: the combined spin-valley degree and the layer degree.

2.3 Execution: Notation:

2.3.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' Express the Kinetic Hamiltonian H_T using $E_{+K,b}$, $E_{-K,t}$, $E_{-K,b}$, $E_{-K,t}$ which are only on the diagonal terms, and arrange the basis in the order of (+K,bottom), (+K,top), (-K,bottom), (-K,top).
Use the following conventions for the symbols:
$\tau = \pm 1$ represents $\pm K$ valleys, bottom layer ($\mathfrak{b}$) and top layer ($\mathfrak{t}$) "'

2.3.2

Completion: Instructions to execute: You will be instructed to describe the kinetic term of the Hamiltonian in AB-stacked $MoTe_2/WSe_2$. The degrees of freedom of the system are: the combined spin-valley degree and the layer degree. Express the Kinetic Hamiltonian H_T using $E_{+K,b}$, $E_{-K,t}$, $E_{-K,b}$, $E_{-K,t}$, which are only on the diagonal terms, and arrange the basis in the order of (+K,bottom), (+K,top), (-K,bottom), (-K,top).
Use the following conventions for the symbols:
$\tau = \pm 1$ represents $\pm K$ valleys, bottom layer ($\mathfrak{b}$) and top layer ($\mathfrak{t}$).
Answer: The kinetic Hamiltonian H_T for the AB-stacked $MoTe_2/WSe_2$ system with the considered degrees of freedom can be expressed in a matrix form as follows:

$$H_T = \begin{pmatrix} E_{+K,b} & 0 & 0 & 0 \\ 0 & E_{+K,t} & 0 & 0 \\ 0 & 0 & E_{-K,b} & 0 \\ 0 & 0 & 0 & E_{-K,t} \end{pmatrix}$$

In this matrix: - The diagonal elements represent the energy levels for each state. - $E_{+K,b}$ and $E_{+K,t}$ are the energy levels at the +K valley for the bottom and top layers, respectively. - $E_{-K,b}$ and $E_{-K,t}$ are the energy levels at the -K valley for the bottom and top layers, respectively. - The off-diagonal elements are all zero, indicating no direct coupling between these states in the kinetic term of the Hamiltonian.

3 Define energy dispersion (continuum)

3.1 Extraction

3.1.1

Prompt: Extraction Extraction Abstract We present a theory on the quantum phase diagram of AB-stacked $MoTe_2/WSe_2$ using a self-consistent Hartree-Fock calculation performed in the plane-wave basis, motivated by the observation of topological states in this system. At filling factor $\nu = 2$ (two holes per moir'e unit cell), Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator by opening a charge gap. At $\nu = 1$, the interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state, which undergo first-order phase transitions tuned by an out-of-plane displacement field. The valley polarized state becomes a Chern insulator for certain displacement fields. Moreover, we predict a topological charge density wave forming a honeycomb lattice with ferromagnetism at $\nu = 2/3$. Future directions on this versatile system hosting a rich set of quantum phases are discussed.
Question: 1. What should the energy dispersion of the kinetic term be like in this system? Choose from parabolic, Dirac, or cos-like. 2. Does the dispersion characterize electrons or holes in this system?

3.1.2

Completion: 1. **What should the energy dispersion of the kinetic term be like in this system? Choose from parabolic, Dirac, or cos-like. Quote**: "using a self-consistent Hartree-Fock calculation performed in the plane-wave basis" **Explanation**: The mention of a plane-wave basis in the Hartree-Fock calculation suggests that the energy dispersion in this system is likely to be parabolic. In solid-state physics, a plane-wave basis is often used to describe free electrons, which have a parabolic energy dispersion. While the abstract does not explicitly describe the dispersion type, the use of a plane-wave basis is a strong indicator of parabolic dispersion, as it is a common approach for systems where electron behavior can be approximated as free particle-like. **Answer**: The energy dispersion of the kinetic term in this system should be parabolic.

2. **Does the dispersion characterize electrons or holes in this system? Quote**: "At filling factor $\nu = 2$ (two holes per moiré unit cell)" **Explanation**: The abstract specifically mentions "two holes per moiré unit cell" at a filling factor $\nu = 2$. This indicates that the dispersion characterizes holes rather than electrons in this system. In semiconductor physics, when discussing holes, it is often in the context of the absence of an electron in an otherwise filled band, which affects the electronic properties of the material. **Answer**: The dispersion characterizes holes in this system.

3.2 Execution-Core Information

3.2.1

Prompt: Execution–Core information You should fill in the specific information from above into the following template, and then repeat it. "' For all energy dispersions, they characterize the {energy dispersion}. dispersion for {electron or hole}. "'

3.2.2

Completion: For all energy dispersions, they characterize the parabolic dispersion for holes.

3.3 Execution-Notation

3.3.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for

execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to construct each term, namely $E_{+K,b}$, $E_{-K,t}$, $E_{-K,b}$, $E_{-K,t}$. In addition, a shift of $+\kappa$ and $-\kappa$ in the momentum $\boldsymbol{k}$ for $E_{t,+K}$ and $E_{t,-K}$, respectively.
You should follow the EXAMPLE below to obtain the 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.
You should recall that

$$H_T = \begin{pmatrix} E_{+K,b} & 0 & 0 & 0 \\ 0 & E_{+K,t} & 0 & 0 \\ 0 & 0 & E_{-K,b} & 0 \\ 0 & 0 & 0 & E_{-K,t} \end{pmatrix}$$

.
Return the expression for $E_{+K,b}$, $E_{-K,t}$, $E_{-K,b}$, $E_{-K,t}$ in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian H_T.
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):
$\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$ is at a corner of the moir'e Brillouin zone, $(m_{\mathfrak{b}}, m_{\mathfrak{t}}) = (0.65, 0.35)m_e$ (m_e is the rest electron mass)
===
EXAMPLE 1:
A parabolic dispersion for electron is $E_{\alpha} = \frac{\hbar^2 k^2}{2m_{\alpha}}$, where α indicates the type of electron. If there is a further shift of q in the momentum k, the dispersion will become $E_{\alpha} = \frac{\hbar^2 (k-q)^2}{2m_{\alpha}}$.
EXAMPLE 2: A cos dispersion is $E_{\alpha} = -\cos(ka/2)$, where α indicates the type of particle. If there is a further shift of q in the momentum k, the dispersion will become $E_{\alpha} = -\cos((k-q)a/2))$. However, there could be more prefactors before cos depending on the geometry of the lattice.
EXAMPLE 3:
A dirac dispersion for electron/hole is a 2 by 2 matrix, i.e., $h_{\theta}(k) = -\hbar v_D |k| \begin{pmatrix} 0 & e^{i(\theta_k - \theta)} \\ e^{-i(\theta_{\bar{k}} - \theta)} & 0 \end{pmatrix}$, where v_D is the Fermi velocity, θ is the twist angle, and θ_k indicates the azumith angle of k. If there is a further shift of K_{θ} in the momentum k, the dispersion will become $h_{\theta}(k) = -\hbar v_D |k - K_{\theta}| \begin{pmatrix} 0 & e^{i(\theta_{k-K_{\theta}} - \theta)} \\ e^{-i(\theta_{k-K_{\theta}} - \theta)} & 0 \end{pmatrix}$. "'

3.3.2

Completion: Instructions to execute: For all energy dispersions, they characterize the parabolic dispersion for holes. You will be instructed to construct each term, namely $E_{+K,b}$, $E_{-K,t}$, $E_{-K,b}$, $E_{-K,t}$, with a shift of $+\kappa$ and $-\kappa$ in the momentum $\boldsymbol{k}$ for $E_{t,+K}$ and $E_{t,-K}$, respectively. You should follow the parabolic dispersion for holes as in Example 1 to obtain the correct energy dispersion. In real space, the momentum $\boldsymbol{k} = -i\partial_{\boldsymbol{r}}$. Keep the form of $\boldsymbol{k}$ in the Hamiltonian for short notations but remember $\boldsymbol{k}$ is an operator. Recall that

$$H_T = \begin{pmatrix} E_{+K,b} & 0 & 0 & 0 \\ 0 & E_{+K,t} & 0 & 0 \\ 0 & 0 & E_{-K,b} & 0 \\ 0 & 0 & 0 & E_{-K,t} \end{pmatrix}.$$

Use the following conventions for the symbols: $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$ is at a corner of the moiré Brillouin zone, $(m_{\mathfrak{b}}, m_{\mathfrak{t}}) = (0.65, 0.35)m_e$ (m_e is the rest electron mass).
Answer: Since the system describes holes with a parabolic dispersion, the dispersion relation is the inverse of that for electrons. Therefore, for a hole, the energy dispersion is $E_{\alpha} = -\frac{\hbar^2 k^2}{2m_{\alpha}}$ (negative sign because we are dealing with holes).
Considering the shifts in momentum for top layer terms, the expressions for each energy term will be: - $E_{+K,b} = -\frac{\hbar^2 k^2}{2m_{\mathfrak{b}}}$ - $E_{+K,t} = -\frac{\hbar^2 (k+\boldsymbol{\kappa})^2}{2m_{\mathfrak{t}}}$ - $E_{-K,b} = -\frac{\hbar^2 k^2}{2m_{\mathfrak{b}}}$ - $E_{-K,t} = -\frac{\hbar^2 (k-\boldsymbol{\kappa})^2}{2m_{\mathfrak{t}}}$
Substituting these into the kinetic Hamiltonian H_T, we get:

$$H_T = \begin{pmatrix} -\frac{\hbar^2 k^2}{2m_{\mathfrak{b}}} & 0 & 0 & 0 \\ 0 & -\frac{\hbar^2 (k+\boldsymbol{\kappa})^2}{2m_{\mathfrak{t}}} & 0 & 0 \\ 0 & 0 & -\frac{\hbar^2 k^2}{2m_{\mathfrak{b}}} & 0 \\ 0 & 0 & 0 & -\frac{\hbar^2 (k-\boldsymbol{\kappa})^2}{2m_{\mathfrak{t}}} \end{pmatrix}$$

Here, $\boldsymbol{k}$ remains as an operator, and the energy terms account for the parabolic dispersion of holes with the given mass parameters and momentum shifts.

4 Identify potential term (continuum)

4.1 Extraction

4.1.1

Prompt: Extraction Abstract We present a theory on the quantum phase diagram of AB-stacked $MoTe_2/WSe_2$ using a self-consistent Hartree-Fock calculation performed in the plane-wave basis, motivated by the observation of topological states in this system. At filling factor $\nu = 2$ (two holes per moir'e unit cell), Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator by opening a charge gap. At $\nu = 1$, the interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state, which undergo first-order phase transitions tuned by an out-of-plane displacement field. The valley polarized state becomes a Chern insulator for certain displacement fields. Moreover, we predict a topological charge density wave forming a honeycomb lattice with ferromagnetism at $\nu = 2/3$. Future directions on this versatile system hosting a rich set of quantum phases are discussed.
Question: 1. When constructing the potential term for such system, which two components of flavor can mix? Namely, Is there a mixing between opposite valleys? Is there a mixing between opposite layers?

4.1.2

Completion: 1. **When constructing the potential term for such a system, which two components of flavor can mix? Namely, is there a mixing between opposite valleys? Is there a mixing between opposite layers? Quote**: "At $\nu = 1$, the interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state, which undergo first-order phase transitions tuned by an out-of-plane displacement field."
Explanation: The mention of "valley polarized state" suggests that there is distinct behavior associated with different valleys, indicating that the valleys are a significant factor in the system's physics. However, the absence of explicit mention of mixing between opposite valleys in the abstract suggests that such mixing might not be a primary focus in this system. On the other hand, the reference to phase transitions "tuned by an out-of-plane displacement field" implies that there could be interactions or effects that involve both layers, as an out-of-plane field would affect the system in a direction perpendicular to the layers. This could hint at possible mixing between layers, depending on the nature of these interactions. **Answer**: There is likely no significant mixing between opposite valleys as implied by the focus on valley polarization, but there could be mixing between opposite layers, as suggested by the influence of the out-of-plane displacement field.

4.2 Execution-Core Information

4.2.1

Prompt: Execution–Core information You should fill in the specific information from above into the following template, and then repeat it.
The off-diagonal terms are the coupling between Mixing between {flavors}.

4.2.2

Completion: The off-diagonal terms are the coupling between mixing between opposite layers.

4.3 Execution-Notation

4.3.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to describe the potential term of Hamiltonian H_V in the real space in the single-particle form.
The potential Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian.
The diagonal terms are $\Delta_t(r)$ and $\Delta_b(r)$.
The off-diagonal terms are $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r})$, which should be kept hermitian.
All other terms are zero. Express the potential Hamiltonian H_V using $\Delta_t(r)$ and $\Delta_b(r)$ and $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r})$.

"'

4.3.2

Completion: Instructions to execute: You will be instructed to describe the potential term of Hamiltonian H_V in the real space in the single-particle form. The potential Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian. The diagonal terms are $\Delta_t(r)$ and $\Delta_b(r)$. The off-diagonal terms are $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r})$, which should be kept hermitian. All other terms are zero. Express the potential Hamiltonian H_V using $\Delta_t(r)$ and $\Delta_b(r)$ and $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r})$. The off-diagonal terms are the coupling between mixing between opposite layers.
Answer: The potential Hamiltonian H_V in the real space for the AB-stacked $\mathrm{MoTe_2}$/$\mathrm{WSe_2}$ system, considering the specified degrees of freedom and the hermitian nature of the off-diagonal terms, can be expressed as:

$$H_V = \begin{pmatrix} \Delta_b(r) & \Delta_{\mathrm{T},\tau}(\boldsymbol{r}) & 0 & 0 \\ \Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r}) & \Delta_t(r) & 0 & 0 \\ 0 & 0 & \Delta_b(r) & \Delta_{\mathrm{T},\tau}(\boldsymbol{r}) \\ 0 & 0 & \Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r}) & \Delta_t(r) \end{pmatrix}$$

In this matrix: - $\Delta_b(r)$ and $\Delta_t(r)$ are the potential terms for the bottom and top layers respectively, which appear on the diagonal. - $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and its hermitian conjugate $\Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r})$ are the off-diagonal terms that represent the coupling between the opposite layers. - The zero terms represent no direct potential coupling between other combinations of degrees of freedom.

5 Define potential term (continuum)

5.1 Extraction

5.1.1

Prompt: Extraction Abstract We present a theory on the quantum phase diagram of AB-stacked $\mathrm{MoTe_2}$/$\mathrm{WSe_2}$ using a self-consistent Hartree-Fock calculation performed in the plane-wave basis, motivated by the observation of topological states in this system. At filling factor $\nu = 2$ (two holes per moir'e unit cell), Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator by opening a charge gap. At $\nu = 1$, the interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state, which undergo first-order phase transitions tuned by an out-of-plane displacement field. The valley polarized state becomes a Chern insulator for certain displacement fields. Moreover, we predict a topological charge density wave forming a honeycomb lattice with ferromagnetism at $\nu = 2/3$. Future directions on this versatile system hosting a rich set of quantum phases are discussed.
Question: 1. What is the mathematical formula of the diagonal terms in the noninteracting moire potential term written in real space? Combine with your a priori knowledge when necessary. 2. What is the mathematical formula of the off-diagonal terms (which mixes the top and bottom layers) in the moire potential term written in real space? Combine with your a priori knowledge when necessary.

5.1.2

Completion: 1. **What is the mathematical formula of the diagonal terms in the noninteracting moire potential term written in real space? Quote**: None directly relevant to the mathematical formula of the diagonal terms in the noninteracting moire potential term. **Explanation**: The abstract does not provide a specific formula for the diagonal terms of the moire potential. However, based on a priori knowledge about moire potentials in similar systems, the diagonal terms usually represent the potential energy landscape in each layer. For a system like AB-stacked $\mathrm{MoTe_2}$/$\mathrm{WSe_2}$, the moire potential is typically a periodic function reflecting the moire superlattice structure. It can be represented mathematically as a sum of cosines corresponding to the periodicity of the moire pattern. **Answer**: A typical form for the diagonal terms in the moire potential, written in real space, could be:

$$\Delta_\alpha(r) = V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i \cdot \boldsymbol{r} + \phi_\alpha)$$

where α is either the top or bottom layer, V_0 is the potential strength, $\boldsymbol{G}_i$ are the reciprocal lattice vectors of the moire pattern, $\boldsymbol{r}$ is the position vector, and ϕ_α is a phase shift that may differ between layers.

2. **What is the mathematical formula of the off-diagonal terms (which mixes the top and bottom layers) in the moire potential term written in real space? Quote**: None directly relevant to the mathematical formula of the off-diagonal terms. **Explanation**: Similar to the diagonal terms, the abstract does not provide explicit information about the mathematical form of the off-diagonal terms of the moire potential. However, the off-diagonal terms in a moire potential usually represent tunneling or coupling between layers. These terms are often modeled as a spatially varying function that depends on the alignment and the periodicity of the layers. **Answer**: A typical form for the off-diagonal terms in the moire potential, which mix the top and bottom layers and are written in real space, could be modeled as:

$$\Delta_{\mathrm{T},\tau}(\boldsymbol{r}) = T_0 \sum_{i=1}^{3} e^{i\boldsymbol{G}_i\cdot\boldsymbol{r}}$$

where T_0 is the tunneling strength, and $\boldsymbol{G}_i$ are the reciprocal lattice vectors of the moire pattern. This term allows for spatially dependent coupling between the layers.

5.2 Execution-Core Information

5.2.1

Prompt: Execution–Core information You should fill in the specific information from above into the following template, and then repeat it. "' The expression for diagonal terms are: {diagonal terms} The expression for off-diagonal terms are: {offdiagonal terms} "'

5.2.2

Completion: The expression for diagonal terms are:

$$\Delta_\alpha(r) = V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i\cdot\boldsymbol{r}+\phi_\alpha)$$

The expression for off-diagonal terms are:

$$\Delta_{\mathrm{T},\tau}(\boldsymbol{r}) = T_0 \sum_{i=1}^{3} e^{i\boldsymbol{G}_i\cdot\boldsymbol{r}}$$

5.3 Execution-Notation

5.3.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to construct each term H_V, namely, $\Delta_t(r)$, $\Delta_b(r)$, $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta^\dagger_{\mathrm{T},\tau}(\boldsymbol{r})$.
You should recall that

$$H_V = \begin{pmatrix} \Delta_b(r) & \Delta_{\mathrm{T},+K}(\boldsymbol{r}) & 0 & 0 \\ \Delta^\dagger_{\mathrm{T},+K}(\boldsymbol{r}) & \Delta_t(r) & 0 & 0 \\ 0 & 0 & \Delta_b(r) & \Delta_{\mathrm{T},-K}(\boldsymbol{r}) \\ 0 & 0 & \Delta^\dagger_{\mathrm{T},-K}(\boldsymbol{r}) & \Delta_t(r) \end{pmatrix}$$

.Return the expressions for $\Delta_t(r)$, $\Delta_b(r)$, $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta^\dagger_{\mathrm{T},\tau}(\boldsymbol{r})$, and substitute it into the potential Hamiltonian H_V.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):the off diagonal terms describe the interlayer tunneling $\Delta_{\mathrm{T},\tau}$, intralayer potential $\Delta_{\mathfrak{b}/\mathfrak{t}}$ "'

5.3.2

Completion: Instructions to execute: You will be instructed to construct each term H_V, namely, $\Delta_t(r)$, $\Delta_b(r)$, $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r})$. Recall that

$$H_V = \begin{pmatrix} \Delta_b(r) & \Delta_{\mathrm{T},+K}(\boldsymbol{r}) & 0 & 0 \\ \Delta_{\mathrm{T},+K}^{\dagger}(\boldsymbol{r}) & \Delta_t(r) & 0 & 0 \\ 0 & 0 & \Delta_b(r) & \Delta_{\mathrm{T},-K}(\boldsymbol{r}) \\ 0 & 0 & \Delta_{\mathrm{T},-K}^{\dagger}(\boldsymbol{r}) & \Delta_t(r) \end{pmatrix}.$$

The expression for diagonal terms are: $\Delta_\alpha(r) = V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i \cdot \boldsymbol{r} + \phi_\alpha)$ The expression for off-diagonal terms are: $\Delta_{\mathrm{T},\tau}(\boldsymbol{r}) = T_0 \sum_{i=1}^{3} e^{i\boldsymbol{G}_i \cdot \boldsymbol{r}}$
Answer: The expressions for $\Delta_t(r)$, $\Delta_b(r)$, $\Delta_{\mathrm{T},\tau}(\boldsymbol{r})$ and $\Delta_{\mathrm{T},\tau}^{\dagger}(\boldsymbol{r})$ are as follows: - $\Delta_t(r) = V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i \cdot \boldsymbol{r} + \phi_t)$ - $\Delta_b(r) = V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i \cdot \boldsymbol{r} + \phi_b)$ - $\Delta_{\mathrm{T},+K}(\boldsymbol{r}) = T_0 \sum_{i=1}^{3} e^{i\boldsymbol{G}_i \cdot \boldsymbol{r}}$ - $\Delta_{\mathrm{T},-K}(\boldsymbol{r}) = T_0 \sum_{i=1}^{3} e^{-i\boldsymbol{G}_i \cdot \boldsymbol{r}}$
Substituting these into the potential Hamiltonian H_V, we get:

$$H_V = \begin{pmatrix} V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i \cdot \boldsymbol{r} + \phi_b) & T_0 \sum_{i=1}^{3} e^{i\boldsymbol{G}_i \cdot \boldsymbol{r}} & 0 & 0 \\ T_0 \sum_{i=1}^{3} e^{-i\boldsymbol{G}_i \cdot \boldsymbol{r}} & V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i \cdot \boldsymbol{r} + \phi_t) & 0 & 0 \\ 0 & 0 & V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i \cdot \boldsymbol{r} + \phi_b) & T_0 \sum_{i=1}^{3} e^{-i\boldsymbol{G}_i \cdot \boldsymbol{r}} \\ 0 & 0 & T_0 \sum_{i=1}^{3} e^{i\boldsymbol{G}_i \cdot \boldsymbol{r}} & V_0 \sum_{i=1}^{3} \cos(\boldsymbol{G}_i \cdot \boldsymbol{r} + \phi_t) \end{pmatrix}$$

Here, ϕ_t and ϕ_b are the phase shifts for the top and bottom layers respectively, and $\boldsymbol{G}_i$ are the reciprocal lattice vectors of the moiré pattern. The potential terms represent intralayer potentials and interlayer tunneling, consistent with the AB-stacked $MoTe_2/WSe_2$ system described.

6 Second-quantization (matrix)

6.1 Execution-Notation

6.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to construct the second quantized form of the total noninteracting Hamiltonian in the real space.The noninteracting Hamiltonian in the real space H_0 is the sum of Kinetic Hamiltonian H_T and Potential Hamiltonian H_V.To construct the second quantized form of a Hamiltonian. You should construct the creation and annihilation operators from the basis explicitly. You should follow the EXAMPLE below to convert a Hamiltonian from the single-particle form to second-quantized form.Finally by "total", it means you need to take a summation over the real space position r.Return the second quantized form of the total noninteracting Hamiltonian $\hat{H}^0$ Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):Note that the spin index of the fermion operators Ψ_τ is both layer and valley dependent.
===EXAMPLE:For a Hamiltonian H, where $H = \begin{pmatrix} H_{a,a} & H_{a,b} \\ H_{b,a} & H_{b,b} \end{pmatrix}$ and the order of basis is (a), (b), we can construct the creation operators $\psi_a^\dagger$ and $\psi_b^\dagger$, and the annihilation operator ψ_a and ψ_b.The corresponding second quantized form is $\hat{H} = \vec{\psi}^\dagger H \vec{\psi}$, where $\vec{\psi} = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$ and $\vec{\psi}^\dagger = \begin{pmatrix} \psi_a^\dagger & \psi_b^\dagger \end{pmatrix}$. "'

6.1.2

Completion: Instructions to execute: You will be instructed to construct the second quantized form of the total noninteracting Hamiltonian in the real space. The noninteracting Hamiltonian in the real space H_0 is the sum of Kinetic Hamiltonian H_T and Potential Hamiltonian H_V. To construct the second quantized form of a Hamiltonian, you should construct the creation and annihilation operators from the basis explicitly. Finally, by "total," it means you need to take a summation over the real space position r. Return the second quantized form of the total noninteracting Hamiltonian $\hat{H}^0$.

Answer: First, let's express the kinetic and potential Hamiltonians in the single-particle form: - Kinetic Hamiltonian H_T:

$$H_T = \begin{pmatrix} E_{+K,b} & 0 & 0 & 0 \\ 0 & E_{+K,t} & 0 & 0 \\ 0 & 0 & E_{-K,b} & 0 \\ 0 & 0 & 0 & E_{-K,t} \end{pmatrix}$$

- Potential Hamiltonian H_V:

$$H_V = \begin{pmatrix} \Delta_b(r) & \Delta_{\mathrm{T},+K}(\boldsymbol{r}) & 0 & 0 \\ \Delta^\dagger_{\mathrm{T},+K}(\boldsymbol{r}) & \Delta_t(r) & 0 & 0 \\ 0 & 0 & \Delta_b(r) & \Delta_{\mathrm{T},-K}(\boldsymbol{r}) \\ 0 & 0 & \Delta^\dagger_{\mathrm{T},-K}(\boldsymbol{r}) & \Delta_t(r) \end{pmatrix}$$

Now, to construct the second quantized form, let's define the creation ($\psi^\dagger$) and annihilation (ψ) operators for each of the basis states: (+K,bottom), (+K,top), (-K,bottom), and (-K,top). The basis order corresponds to the order of terms in the Hamiltonians.
The second quantized form of the total noninteracting Hamiltonian $\hat{H}^0$ is given by:

$$\hat{H}^0 = \int d\boldsymbol{r}\, \Psi^\dagger(\boldsymbol{r})\, (H_T + H_V)\, \Psi(\boldsymbol{r})$$

where $\Psi(\boldsymbol{r})$ is the column vector of annihilation operators and $\Psi^\dagger(\boldsymbol{r})$ is the row vector of creation operators, defined as:

$$\Psi(\boldsymbol{r}) = \begin{pmatrix} \psi_{+K,b}(\boldsymbol{r}) \\ \psi_{+K,t}(\boldsymbol{r}) \\ \psi_{-K,b}(\boldsymbol{r}) \\ \psi_{-K,t}(\boldsymbol{r}) \end{pmatrix}, \quad \Psi^\dagger(\boldsymbol{r})$$
$$= \begin{pmatrix} \psi^\dagger_{+K,b}(\boldsymbol{r}) & \psi^\dagger_{+K,t}(\boldsymbol{r}) & \psi^\dagger_{-K,b}(\boldsymbol{r}) & \psi^\dagger_{-K,t}(\boldsymbol{r}) \end{pmatrix}$$

The creation and annihilation operators correspond to different layers and valleys as indicated by their subscripts. The spin index of these fermion operators is both layer and valley dependent as per the conventions provided. The integration over $\boldsymbol{r}$ takes the sum over all space, accounting for the real space position in the Hamiltonian.

7 Second-quantization (summation)

7.1 Execution-Notation

7.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to expand the second-quantized form Hamiltonian $\hat{H}^0$ using H_τ and Ψ_τ. You should follow the EXAMPLE below to expand the Hamiltonian.You should use any previous knowledge to simplify it. For example, if any term of H_τ is zero, you should remove it from the summation. You should recall that $\hat{H}^0$ is

$$\hat{H}^0 = \int d\mathbf{r}\, \Psi^\dagger(\mathbf{r}) \begin{pmatrix} E_{+K,b} + V(\mathbf{r}) & T(\mathbf{r}) & 0 & 0 \\ T^\dagger(\mathbf{r}) & E_{+K,t} + V(\mathbf{r}) & 0 & 0 \\ 0 & 0 & E_{-K,b} + V(\mathbf{r}) & T(\mathbf{r}) \\ 0 & 0 & T^\dagger(\mathbf{r}) & E_{-K,t} + V(\mathbf{r}) \end{pmatrix} \Psi(\mathbf{r})$$

.Return the expanded form of $\hat{H}^0$ after simplification.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):$\hat{\mathcal{H}}_0$ is the second-quantized form Hamiltonian, H_τ is the matrix element, and Ψ_τ is the basis. $\tau = \pm$ represents $\pm K$ valleys. The spin index of the fermion operators Ψ_τ is both layer and valley dependent.
===EXAMPLE:For a $\hat{H} = \vec{\psi}^\dagger H \vec{\psi}$, where $\vec{\psi} = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}$ and $\vec{\psi}^\dagger = \begin{pmatrix} \psi_a^\dagger & \psi_b^\dagger \end{pmatrix}$, we can expand it as $\hat{H} = \sum_{i,j=\{a,b\}} \psi_i^\dagger H_{i,j} \psi_j$. "'

7.1.2

Completion: Instructions to execute: You will be instructed to expand the second-quantized form Hamiltonian $\hat{H}^0$ using H_τ and Ψ_τ. Recall that $\hat{H}^0$ is given by

$$\hat{H}^0 = \int d\mathbf{r}\, \Psi^\dagger(\mathbf{r}) \begin{pmatrix} E_{+K,b}+V(\mathbf{r}) & T(\mathbf{r}) & 0 & 0 \\ T^\dagger(\mathbf{r}) & E_{+K,t}+V(\mathbf{r}) & 0 & 0 \\ 0 & 0 & E_{-K,b}+V(\mathbf{r}) & T(\mathbf{r}) \\ 0 & 0 & T^\dagger(\mathbf{r}) & E_{-K,t}+V(\mathbf{r}) \end{pmatrix} \Psi(\mathbf{r})\,.$$

You should use any previous knowledge to simplify it, including removing any zero terms from the summation. The spin index of the fermion operators Ψ_τ is both layer and valley dependent.
Answer: Given the structure of $\hat{H}^0$, we can expand it as follows:

$$\hat{H}^0 \\ = \int d\mathbf{r}\, \Big[\Psi^\dagger_{+K,b}(\mathbf{r})\left(E_{+K,b}+V(\mathbf{r})\right)\Psi_{+K,b}(\mathbf{r}) + \Psi^\dagger_{+K,b}(\mathbf{r})T(\mathbf{r})\Psi_{+K,t}(\mathbf{r}) + \Psi^\dagger_{+K,t}(\mathbf{r})T^\dagger(\mathbf{r})\Psi_{+K,b}(\mathbf{r}) + \Psi^\dagger_{+K,t}(\mathbf{r})\left(E_{+K,t}+V(\mathbf{r})\right)\Psi_{+K}$$

$$+\Psi^\dagger_{-K,b}(\mathbf{r})\left(E_{-K,b}+V(\mathbf{r})\right)\Psi_{-K,b}(\mathbf{r}) + \Psi^\dagger_{-K,b}(\mathbf{r})T(\mathbf{r})\Psi_{-K,t}(\mathbf{r}) \\ + \Psi^\dagger_{-K,t}(\mathbf{r})T^\dagger(\mathbf{r})\Psi_{-K,b}(\mathbf{r}) + \Psi^\dagger_{-K,t}(\mathbf{r})\left(E_{-K,t}+V(\mathbf{r})\right)\Psi_{-K,t}(\mathbf{r})\Big]$$

In this expansion: - $\Psi^\dagger_{\tau,\alpha}(\mathbf{r})$ and $\Psi_{\tau,\alpha}(\mathbf{r})$ are the creation and annihilation operators for valley τ and layer α at position $\mathbf{r}$. - $E_{\tau,\alpha}$ represents the energy level for valley τ and layer α. - $V(\mathbf{r})$ is the potential at position $\mathbf{r}$. - $T(\mathbf{r})$ and $T^\dagger(\mathbf{r})$ are the tunneling terms between the layers.
The integration over $\mathbf{r}$ sums these contributions over all space. The expansion includes all the necessary terms while adhering to the conventions and structure provided.

8 Fourier transform noninteracting term to momentum space (continuum)

8.1 Execution-Notation

8.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to convert the total noninteracting Hamiltonian in the second quantized form from the basis in real space to the basis by momentum space.To do that, you should apply the Fourier transformation to $\psi^\dagger_{\tau,l}(r)$ in the real space to the $c^\dagger_{\tau,l}(k)$ in the momentum space, which is defined as $c^\dagger_{\tau,l}(k) = \frac{1}{\sqrt{V}}\int dr \psi^\dagger_{\tau,l}(r) e^{ik\cdot r}$, where $\boldsymbol{r}$ is integrated over the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation.Express the total noninteracting Hamiltonian $\hat{H}^0$ in terms of $c^\dagger_{\tau,l}(k)$. 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):$\tau = \pm$ represents $\pm K$ valleys, $\hbar\boldsymbol{k} = -i\hbar\partial_{\boldsymbol{r}}$ is the momentum operator, $\boldsymbol{\kappa} = \frac{4\pi}{3a_M}(1,0)$ is at a corner of the moir'e Brillouin zone, and a_M is the moir'e lattice constant. The spin index of the fermion operators Ψ_τ is both layer and valley dependent. $h^{(\tau)}$ is the Hamiltonian H_τ expanded in the plane-wave basis, and the momentum $\boldsymbol{k}$ is defined in the extended Brillouin zone that spans the full momentum space, i.e., $\boldsymbol{k}\in\mathbb{R}^2$. The subscripts α,β are index for momenta. Due to Bloch's theorem, $h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta}$ is nonzero only when $\boldsymbol{k}_\alpha - \boldsymbol{k}_\beta$ is equal to the linear combination of any multiples of one of the moir'e reciprocal lattice vectors (including the zero vector).
===EXAMPLE:Write a Hamiltonian $\hat{H}$ in the second quantized form, $\hat{H} = \int dr \psi(r)^\dagger H(r)\psi(r)$, where r is integrated over the entire real space.Define the Fourier transformation $c^\dagger(k) = \frac{1}{\sqrt{V}}\int \psi^\dagger(r) e^{ik\cdot r} dr$, where r is integrated over the entire real space, and V is the area of the unit cell in the real space.This leads to the inverse Fourier transformation $\psi^\dagger(r) = \frac{1}{\sqrt{V}}\sum_k c^\dagger(k) e^{-ik\cdot r}$, where k is summed over the extended Brillouin zone (i.e., the entire momentum space), Ω is the area of Brillouin zone

in the momentum space.Thus, substitute $\psi^\dagger(r)$ and $\psi(r)$ into $\hat{H}$, we get

$$\begin{aligned}\hat{H} &= \int dr \frac{1}{\sqrt{V}} \sum_{k_1} c^\dagger(k_1) e^{-ik_1\cdot r} H(r) \frac{1}{\sqrt{V}} \sum_{k_2} c(k_2) e^{ik_2\cdot r} \\ &= \sum_{k_1,k_2} c^\dagger(k_1) \frac{1}{V} \int dr e^{-i(k_1-k_2)\cdot r} H(r) c(k_2) \\ &= \sum_{k_1,k_2} c^\dagger(k_1) H(k_1,k_2) c(k_2)\end{aligned}$$

, where we define the Fourier transformation of $H(r)$ as $H(k_1,k_2) = \frac{1}{V}\int dr e^{-i(k_1-k_2)\cdot r} H(r)$. "'

8.1.2

Completion: Instructions to execute: You will be instructed to convert the total noninteracting Hamiltonian in the second quantized form from the basis in real space to the basis in momentum space. Apply the Fourier transformation to $\psi^\dagger_{\tau,l}(r)$ in the real space to $c^\dagger_{\tau,l}(k)$ in the momentum space. Express the total noninteracting Hamiltonian $\hat{H}^0$ in terms of $c^\dagger_{\tau,l}(k)$ and simplify any summation index if possible. Recall the conventions regarding the representation of valleys, momentum, reciprocal lattice vectors, and the relation of Hamiltonian matrix elements in the plane-wave basis.
Answer: First, let's define the Fourier transformation for the creation and annihilation operators:

$$c^\dagger_{\tau,l}(k) = \frac{1}{\sqrt{V}} \int dr\, \psi^\dagger_{\tau,l}(r) e^{ik\cdot r}$$

$$c_{\tau,l}(k) = \frac{1}{\sqrt{V}} \int dr\, \psi_{\tau,l}(r) e^{-ik\cdot r}$$

where V is the volume of the system.
The inverse Fourier transformation is then:

$$\psi^\dagger_{\tau,l}(r) = \frac{1}{\sqrt{V}} \sum_k c^\dagger_{\tau,l}(k) e^{-ik\cdot r}$$

$$\psi_{\tau,l}(r) = \frac{1}{\sqrt{V}} \sum_k c_{\tau,l}(k) e^{ik\cdot r}$$

Substituting these into $\hat{H}^0$, we get:

$$\hat{H}^0 = \int dr \frac{1}{\sqrt{V}} \sum_{k_1} c^\dagger_{\tau,l}(k_1) e^{-ik_1\cdot r} H(r) \frac{1}{\sqrt{V}} \sum_{k_2} c_{\tau,l}(k_2) e^{ik_2\cdot r}$$

$$= \sum_{k_1,k_2} c^\dagger_{\tau,l}(k_1) \frac{1}{V} \int dr\, e^{-i(k_1-k_2)\cdot r} H(r) c_{\tau,l}(k_2)$$

$$= \sum_{k_1,k_2} c^\dagger_{\tau,l}(k_1) H_\tau(k_1,k_2) c_{\tau,l}(k_2)$$

where $H_\tau(k_1,k_2)$ is the Fourier transform of the Hamiltonian $H(r)$ and is defined as:

$$H_\tau(k_1,k_2) = \frac{1}{V} \int dr\, e^{-i(k_1-k_2)\cdot r} H(r)$$

This represents the total noninteracting Hamiltonian $\hat{H}^0$ in the momentum space, with k_1 and k_2 being the momentum indices summed over the extended Brillouin zone. The Hamiltonian matrix elements are nonzero only when $\boldsymbol{k}_\alpha - \boldsymbol{k}_\beta$ equals a linear combination of moiré reciprocal lattice vectors (including the zero vector), according to Bloch's theorem.

9 Particle-hole transformation

9.1 Execution-Notation

9.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to perform a particle-hole transformation.Define a hole operator, $b_{\boldsymbol{k},l,\tau}$, which equals $c^\dagger_{\boldsymbol{k},l,\tau}$.You should replace $c^\dagger_{\boldsymbol{k},l,\tau}$ with $b_{\boldsymbol{k},l,\tau}$, and $c_{\boldsymbol{k},l,\tau}$ with $b^\dagger_{\boldsymbol{k},l,\tau}$. You should follow the EXAMPLE below to apply the particle-hole transformation.You should recall that $\hat{H}^0 = \sum_{\tau,k_\alpha,k_\beta} c^\dagger_{\tau,l}(k_\alpha) h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} c_{\tau,l}(k_\beta)$. Return the $\hat{H}^0$ in the hole operators.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):The hole operator is defined as $b_{\boldsymbol{k},l,\tau} = c^\dagger_{\boldsymbol{k},l,\tau}$. The Hamiltonian in the hole basis is represented as $\hat{\mathcal{H}}_0$.
===EXAMPLE:Give a Hamiltonian $\hat{H} = \sum_{k_1,k_2} c^\dagger(k_1) h(k_1,k_2) c(k_2)$, and the particle-hole transformation as $b(k) = c^\dagger(k)$. The transformed Hamiltonian is $\hat{H} = \sum_{k_1,k_2} b(k_1) h(k_1,k_2) b^\dagger(k_2)$ "'

9.1.2

Completion: Instructions to execute: You will be instructed to perform a particle-hole transformation. Define a hole operator, $b_{\boldsymbol{k},l,\tau}$, which equals $c^\dagger_{\boldsymbol{k},l,\tau}$. Replace $c^\dagger_{\boldsymbol{k},l,\tau}$ with $b_{\boldsymbol{k},l,\tau}$, and $c_{\boldsymbol{k},l,\tau}$ with $b^\dagger_{\boldsymbol{k},l,\tau}$. Recall that $\hat{H}^0 = \sum_{\tau,k_\alpha,k_\beta} c^\dagger_{\tau,l}(k_\alpha) h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} c_{\tau,l}(k_\beta)$. Return the $\hat{H}^0$ in the hole operators.
Answer: Given the definition of the hole operator $b_{\boldsymbol{k},l,\tau} = c^\dagger_{\boldsymbol{k},l,\tau}$ and the particle-hole transformation, the transformed Hamiltonian can be written as:

$$\hat{H}^0_{\text{hole}} = \sum_{\tau,k_\alpha,k_\beta} b_{\boldsymbol{k}_\alpha l_\alpha,\tau}(k_\alpha) h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} b^\dagger_{\boldsymbol{k}_\beta l_\beta,\tau}(k_\beta)$$

This expression represents the total noninteracting Hamiltonian $\hat{H}^0$ in terms of the hole operators $b_{\boldsymbol{k},l,\tau}$ and $b^\dagger_{\boldsymbol{k},l,\tau}$. The Hamiltonian matrix elements $h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta}$ remain unchanged, as they depend on the system's physical properties, which are independent of the chosen particle or hole representation. The transformation effectively switches the roles of filled and empty states in the system, which is a common technique in studying systems where the particle-like excitations are holes rather than electrons.

10 Simplify the Hamiltonian in the particle-hole basis

10.1 Execution-Notation

10.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to simplify the $\hat{H}^0$ in the hole basis.You should use canonical commutator relation for fermions to reorder the hole operator to the normal order. Normal order means that creation operators always appear before the annihilation operators. You should follow the EXAMPLE below to simplify it to the normal order.Express the $\hat{H}^0$ in the normal order of $b_{\boldsymbol{k},l,\tau}$ and also make $\boldsymbol{k}_\alpha$ always appear before $\boldsymbol{k}_\beta$ in the index of $b_{\boldsymbol{k},l,\tau}$ and $[h^{(\tau)}]^\intercal_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta}$.You should recall that $\hat{H}^0 = \sum_{\tau,k_\alpha,k_\beta} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau} h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau}$ 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):$b_{\boldsymbol{k},l,\tau} = c^\dagger_{\boldsymbol{k},l,\tau}$
=== EXAMPLE:For $\hat{H}^0 = \sum_{i,j} b_i H_{i,j} b^\dagger_j$, where b_i satisfies fermion statistics (anticommuting to its self-adjoint operator).This gives '$[b_i, b^\dagger_j]_+ = \delta_{i,j}$', which means $b_i b^\dagger_j = \delta_{i,j} - b^\dagger_j b_i$.Substitute it into $\hat{H}^0$, we have $\hat{H}^0 = \sum_{i,j} (\delta_{i,j} - b^\dagger_j b_i) H_{i,j} = \sum_{i,j} \delta_{i,j} H_{i,j} - \sum_{i,j} b^\dagger_j b_i H_{i,j} = \sum_i H_{i,i} - \sum_{i,j} b^\dagger_j b_i H_{i,j}$.The first term is simply $\sum_i H_{i,i}$ by summing over the index j due to $\delta_{i,j}$. The second term is $-\sum_{i,j} b^\dagger_j b_i H_{i,j}$.Relabeling the index of i and j by swapping them to make it consistent with the original order of index (namely, i appears before j in the index of b and H), it becomes $-\sum_{i,j} b^\dagger_i H_{j,i} b_j$. Finally, to fix the order of the index in

H such that i appears before j, we notice that '$H_{j,i} = (H_{i,j})^*$', where '*' means complex conjugate, because the Hamiltonian is Hermitian.Thus, we end up in $\hat{H}^0 = \sum_{i,j} b_i H_{i,j} b_j^\dagger = \sum_i H_{i,i} - \sum_{i,j} b_i^\dagger (H_{i,j})^* b_j$ "'

10.1.2

Completion: Instructions to execute: You will be instructed to simplify the $\hat{H}^0$ in the hole basis to normal order, where creation operators always appear before annihilation operators. Use the canonical commutator relation for fermions to reorder the hole operator. Express the $\hat{H}^0$ in the normal order of $b_{\boldsymbol{k},l,\tau}$ and ensure $\boldsymbol{k}_\alpha$ always appears before $\boldsymbol{k}_\beta$ in the index. Recall that $\hat{H}^0 = \sum_{\tau,k_\alpha,k_\beta} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau} h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau}$.
Answer: Starting from the given Hamiltonian in the hole basis:

$$\hat{H}^0 = \sum_{\tau,k_\alpha,k_\beta} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau} h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau}$$

We apply the fermionic anticommutation relations:

$$[b_{\boldsymbol{k}_\alpha,l_\alpha,\tau}, b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau}]_+ = \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\delta_{l_\alpha,l_\beta}\delta_{\tau,\tau}$$

which implies:

$$b_{\boldsymbol{k}_\alpha,l_\alpha,\tau} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau} = \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\delta_{l_\alpha,l_\beta}\delta_{\tau,\tau} - b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau}$$

Substituting this into $\hat{H}^0$:

$$\hat{H}^0 = \sum_{\tau,k_\alpha,k_\beta} (\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\delta_{l_\alpha,l_\beta}\delta_{\tau,\tau} - b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau}) h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta}$$

Simplifying and reordering the indices:

$$\hat{H}^0 = \sum_{\tau,k_\alpha,k_\beta} \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\delta_{l_\alpha,l_\beta}\delta_{\tau,\tau} h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} - \sum_{\tau,k_\alpha,k_\beta} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau} h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau}$$

Using the fact that $h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta}$ is Hermitian, and relabeling the indices:

$$\hat{H}^0 = \sum_{\tau,k} h^{(\tau)}_{\boldsymbol{k}l,\boldsymbol{k}l} - \sum_{\tau,k_\alpha,k_\beta} b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau} [h^{(\tau)}_{\boldsymbol{k}_\beta l_\beta,\boldsymbol{k}_\alpha l_\alpha}]^* b_{\boldsymbol{k}_\beta,l_\beta,\tau}$$

This is the Hamiltonian $\hat{H}^0$ in the normal order of $b_{\boldsymbol{k},l,\tau}$ operators, with $\boldsymbol{k}_\alpha$ always appearing before $\boldsymbol{k}_\beta$ in the indices, and the Hamiltonian matrix elements $h^{(\tau)}_{\boldsymbol{k}_\alpha l_\alpha,\boldsymbol{k}_\beta l_\beta}$ transposed and conjugated accordingly.

11 Identify interacting term (momentum space)

11.1 Extraction

11.1.1

Prompt: Extraction Abstract We present a theory on the quantum phase diagram of AB-stacked $MoTe_2/WSe_2$ using a self-consistent Hartree-Fock calculation performed in the plane-wave basis, motivated by the observation of topological states in this system. At filling factor $\nu = 2$ (two holes per moir'e unit cell), Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator by opening a charge gap. At $\nu = 1$, the interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state, which undergo first-order phase transitions tuned by an out-of-plane displacement field. The valley polarized state becomes a Chern insulator for certain displacement fields. Moreover, we predict a topological charge density wave forming a honeycomb lattice with ferromagnetism at $\nu = 2/3$. Future directions on this versatile system hosting a rich set of quantum phases are discussed.
Question: 1. What type of interaction should be used in the system? Remember the actual experimental device is usually dual-gated. 2. What is the mathematical formula for this interaction used in the Hamiltonian? You write it in the momentum space. Remember the interaction is a dual-gated screened Coulomb interaction (i.e., like a two-slab capacitor).

11.1.2

Completion: 1. **What type of interaction should be used in the system? Quote**: "Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator" and "interaction induces three classes of competing states" **Explanation**: The abstract explicitly mentions the role of Coulomb interaction in stabilizing various quantum states in the AB-stacked $MoTe_2/WSe_2$ system. Given that the actual experimental device is usually dual-gated, which typically influences the screening of interactions, the type of interaction to be used in the system is a screened Coulomb interaction. This type of interaction accounts for the screening effect due to the presence of gates, which can modify the strength and range of the Coulomb interaction between charged particles. **Answer**: The type of interaction to be used in the system should be a dual-gated screened Coulomb interaction.

2. **What is the mathematical formula for this interaction used in the Hamiltonian in the momentum space? Explanation**: The screened Coulomb interaction in a dual-gated system, such as a two-slab capacitor, is typically described by a formula that accounts for the screening effect of the gates. In momentum space, the screened Coulomb interaction can be represented as a function of the wave vector, which modifies the standard Coulomb potential due to the presence of the gates. **Answer**: The mathematical formula for the dual-gated screened Coulomb interaction in momentum space can be written as:

$$V(\boldsymbol{k}) = \frac{e^2}{2\epsilon_0\epsilon_r|\boldsymbol{k}|}\frac{\tanh(|\boldsymbol{k}|d)}{|\boldsymbol{k}|d}$$

Here, $V(\boldsymbol{k})$ is the potential in momentum space, $\boldsymbol{k}$ is the wave vector, e is the elementary charge, ϵ_0 is the vacuum permittivity, ϵ_r is the relative permittivity of the material, and d is the distance between the gates. The term $\tanh(|\boldsymbol{k}|d)/(|\boldsymbol{k}|d)$ represents the screening effect due to the dual-gate structure.

11.2 Execution-Core Information

11.2.1

Prompt: Execution–Core information You should fill in the specific information from above into the following template, and then repeat it. "' To obtain the interaction form. You should use type of interaction with mathematical expression of interaction, where q is the transferred total momentum between a creation operator and an annihilation operator with the same the valley index and layer index, namely $q = k_1 - k_4$.

11.2.2

Completion: To obtain the interaction form, you should use dual-gated screened Coulomb interaction with the mathematical expression $V(\boldsymbol{q}) = \frac{e^2}{2\epsilon_0\epsilon_r|\boldsymbol{q}|}\frac{\tanh(|\boldsymbol{q}|d)}{|\boldsymbol{q}|d}$, where $\boldsymbol{q}$ is the transferred total momentum between a creation operator and an annihilation operator with the same valley index and layer index, namely $\boldsymbol{q} = \boldsymbol{k}_1 - \boldsymbol{k}_4$.

11.3 Execution-Notation

11.3.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to construct the interaction part of the Hamiltonian $\hat{H}_{\text{int}}$ in the momentum space.

The interaction Hamiltonian is a product of the aforementioned interaction form and the following three 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 valley index and layer index, and $1, 2, 3, 4$ for the momentum. The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators.The last is the normalization factor, you should use $\frac{1}{2A}$ here. Finally, the summation should be running over all the valley index and layer index, and momentum Return the interaction term $\hat{H}_{\text{int}}$ in terms of $b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}$, $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}$, $b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$, $b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$ 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):$\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta$ are the momenta, l_α, l_β are the indices of operators, τ_α, τ_β are the spin indices, $V(\boldsymbol{k})$ is the dual-gate screened Coulomb interaction, d is the sample-to-gate distance, and ϵ is the dielectric constant. $\delta(..)$ is the Dirac delta function for momentum conservation. "'

11.3.2

Completion: Instructions to execute: You will be instructed to construct the interaction part of the Hamiltonian $\hat{H}_{\text{int}}$ in the momentum space. The interaction Hamiltonian involves the dual-gated screened Coulomb interaction, a product of four fermionic operators in normal order (creation operators before annihilation operators), momentum conservation, and a normalization factor. The momentum conservation ensures the total momentum of all creation operators equals that of all annihilation operators. The normalization factor is $\frac{1}{2A}$. Sum over all valley indices, layer indices, and momenta. Return the interaction term $\hat{H}_{\text{int}}$ using $b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}$, $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}$, $b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$, $b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$ and $V(q)$, with q expressed in terms of momentum.
Answer: The interaction Hamiltonian $\hat{H}_{\text{int}}$ in momentum space is given by:

$$\hat{H}_{\text{int}} = \frac{1}{2A} \sum_{\substack{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta \\ l_\alpha,l_\beta \\ \tau_\alpha,\tau_\beta}} V(\boldsymbol{q})\delta(\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta - \boldsymbol{k}_\gamma - \boldsymbol{k}_\delta) b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$$

where

$$V(\boldsymbol{q}) = \frac{e^2}{2\epsilon_0\epsilon_r|\boldsymbol{q}|}\frac{\tanh(|\boldsymbol{q}|d)}{|\boldsymbol{q}|d}$$

and

$$\boldsymbol{q} = \boldsymbol{k}_\alpha - \boldsymbol{k}_\delta$$

In this Hamiltonian: - $b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}$ and $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}$ are creation operators. - $b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$ and $b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$ are annihilation operators. - $V(\boldsymbol{q})$ is the dual-gated screened Coulomb interaction potential. - The delta function $\delta(\boldsymbol{k}_\alpha + \boldsymbol{k}_\beta - \boldsymbol{k}_\gamma - \boldsymbol{k}_\delta)$ enforces momentum conservation. - The normalization factor is $\frac{1}{2A}$, where A is the area of the system.
This Hamiltonian describes the interaction between particles (holes in this case) in the AB-stacked $MoTe_2/WSe_2$ system, taking into account the screening effect due to the dual-gated setup and momentum conservation.

12 Wick's theorem expansion

12.1 Execution-Notation

12.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $\hat{H}_{\text{int}}$.You should use Wick's theorem to expand the four-fermion term in $\hat{H}_{\text{int}}$ 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.You should recall that $\hat{H}_{\text{int}}$ is $\hat{H}_{\text{int}} = \frac{1}{2A}\sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$.Return the expanded interaction term after Hartree-Fock approximation as $\hat{H}^{\text{HF}}$.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):$\hat{H}^{\text{HF}}$ is the Hartree-Fock Hamiltonian, $\hat{H}^{\text{HF}}_{\text{int}}$ is the interaction term in the Hartree-Fock Hamiltonian, $\boldsymbol{k}_\alpha, \boldsymbol{k}_\beta, \boldsymbol{k}_\gamma, \boldsymbol{k}_\delta$ are the momentum vectors, l_α, l_β are the orbital quantum numbers, τ_α, τ_β are the spin quantum numbers, $V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$ is the interaction potential, $b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}$ and $b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$ are the creation and annihilation operators, and $\langle ... \rangle$ denotes the expectation value.
===EXAMPLE 1:For a four-fermion term $a_1^\dagger a_2^\dagger a_3 a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a_1^\dagger a_2^\dagger a_3 a_4 = \langle a_1^\dagger a_4 \rangle a_2^\dagger a_3 + \langle a_2^\dagger a_3 \rangle a_1^\dagger a_4 - \langle a_1^\dagger a_4 \rangle \langle a_2^\dagger a_3 \rangle - \langle a_1^\dagger a_3 \rangle a_2^\dagger a_4 - \langle a_2^\dagger a_4 \rangle a_1^\dagger a_3 + \langle a_1^\dagger a_3 \rangle \langle a_2^\dagger a_4 \rangle$Be cautious about the order of the index and sign before each term here.

EXAMPLE 2:For a four-fermion term $a_1^\dagger a_2 a_3^\dagger a_4$, using Wick's theorem and preserving only the normal terms. this is expanded as $a_1^\dagger a_2 a_3^\dagger a_4 = \langle a_1^\dagger a_2\rangle a_3^\dagger a_4 + \langle a_3^\dagger a_4\rangle a_1^\dagger a_2 - \langle a_1^\dagger a_2\rangle\langle a_3^\dagger a_4\rangle - \langle a_1^\dagger a_4\rangle a_3^\dagger a_2 - \langle a_3^\dagger a_2\rangle a_1^\dagger a_4 + \langle a_1^\dagger a_4\rangle\langle a_3^\dagger a_2\rangle$Be cautious about the order of the index and sign before each term here. "'

12.1.2

Completion: Instructions to execute: You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, $\hat{H}_{\text{int}}$, using Wick's theorem. The expansion should be carried out for the four-fermion term in $\hat{H}_{\text{int}}$ into quadratic terms, preserving only the normal terms (product of a creation operator and an annihilation operator). The interaction term $\hat{H}_{\text{int}}$ is given as $\hat{H}_{\text{int}} = \frac{1}{2A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$. Return the expanded interaction term after the Hartree-Fock approximation as $\hat{H}^{\text{HF}}$.
Answer: Using Wick's theorem and preserving only the normal terms, the interaction term $\hat{H}_{\text{int}}$ can be expanded. The order of the product is $1^\dagger, 2^\dagger, 3, 4$, so following Example 1:

$$\hat{H}_{\text{int}} = \frac{1}{2A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta}\Big(\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$$

$$+\langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$$

$$-\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle\langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle$$

$$-\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} - \langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\Big)$$

$$+\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle\langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

This expansion of $\hat{H}_{\text{int}}$ yields $\hat{H}^{\text{HF}}$, the Hartree-Fock Hamiltonian, where each term is the product of a creation operator and an annihilation operator (normal terms), and expectation values represent average occupations in the system. The terms involve sums over all possible combinations of momenta, layers, and spins, and include the interaction potential $V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta)$, ensuring momentum conservation.

13 Drop constant terms

13.1 Execution-Notation

13.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to extract the quadratic terms in the $\hat{H}^{\text{HF}}$.The quadratic terms mean terms that are proportional to $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$ and $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$, which excludes terms that are solely expectations or products of expectations.You should only preserve the quadratic terms in $\hat{H}^{\text{HF}}$, denoted as $\hat{H}^{\text{HF}}_{\text{int}}$.You should recall that $\hat{H}^{\text{HF}}$ is

$$\hat{H}^{\text{HF}} = \frac{1}{2A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta}\Bigg(\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$$

$$+\langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} - \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle\langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle$$

$$-\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} - \langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$$

$$+\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle\langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle\Bigg) V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

.Return $\hat{H}^{\text{HF}}_{\text{int}}$. "'

13.1.2

Completion: Instructions to execute: You will be instructed to extract the quadratic terms from the Hartree-Fock Hamiltonian, $\hat{H}^{\text{HF}}$. The quadratic terms are those proportional to $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$ and $b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$, excluding terms that are solely expectations or products of expectations. Preserve only the quadratic terms in $\hat{H}^{\text{HF}}$, denoted as $\hat{H}^{\text{HF}}_{\text{int}}$. Recall the expression for $\hat{H}^{\text{HF}}$ as provided.
Answer: From the Hartree-Fock Hamiltonian $\hat{H}^{\text{HF}}$, the quadratic terms can be extracted as $\hat{H}^{\text{HF}}_{\text{int}}$:

$$\hat{H}^{\text{HF}}_{\text{int}} = \frac{1}{2A} \sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \Bigg(\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$$

$$+\langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$$

$$-\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$$

$$-\langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \rangle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \Bigg) V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

This expression for $\hat{H}^{\text{HF}}_{\text{int}}$ includes only the quadratic terms from the Hartree-Fock Hamiltonian. Each term involves a product of a creation operator and an annihilation operator, weighted by the expectation values of the corresponding operator pairs. The interaction potential $V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)$ is included, and momentum conservation is enforced by the delta function $\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$. This Hamiltonian represents the effective interaction between particles (holes) in the system after applying the Hartree-Fock approximation.

14 Combine Hartree/Fock terms

14.1 Extraction

14.1.1

Prompt: Extraction Abstract We present a theory on the quantum phase diagram of AB-stacked $MoTe_2/WSe_2$ using a self-consistent Hartree-Fock calculation performed in the plane-wave basis, motivated by the observation of topological states in this system. At filling factor $\nu = 2$ (two holes per moir'e unit cell), Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator by opening a charge gap. At $\nu = 1$, the interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state, which undergo first-order phase transitions tuned by an out-of-plane displacement field. The valley polarized state becomes a Chern insulator for certain displacement fields. Moreover, we predict a topological charge density wave forming a honeycomb lattice with ferromagnetism at $\nu = 2/3$. Future directions on this versatile system hosting a rich set of quantum phases are discussed.
Question: 1. Do you need to keep both Hartree term and fock term in order to solve the problem in this paper?

14.1.2

Completion: 1. **Do you need to keep both Hartree term and Fock term in order to solve the problem in this paper? Quote**: ”Coulomb interaction can stabilize a $\mathbb{Z}_2$ topological insulator” and ”interaction induces three classes of competing states, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state” **Explanation**: The abstract indicates the importance of Coulomb interactions in stabilizing various states in the system, including a $\mathbb{Z}_2$ topological insulator, spin density wave states, an in-plane ferromagnetic state, and a valley polarized state. The Hartree and Fock terms represent different aspects of electron-electron interactions in the Hartree-Fock approximation. The Hartree term accounts for the average field effect due to electron-electron interactions, while the Fock term incorporates the exchange interaction, which is crucial for capturing the quantum mechanical nature of electrons, especially in systems showing topological and magnetic properties.
Given the complexity and variety of states mentioned, including those influenced by topological aspects and phase transitions, both Hartree and Fock terms seem necessary. The Hartree term

would contribute to understanding the general field effects due to electron-electron interactions, while the Fock term is essential for capturing the exchange effects that can lead to phenomena like spin density waves and other magnetic states.
Answer: Yes, both the Hartree term and the Fock term should be retained to solve the problem in this paper, as they collectively capture the critical aspects of electron-electron interactions necessary for understanding the various complex states mentioned, including topological insulators, spin density wave states, ferromagnetic states, and valley polarized states.

14.2 Execution-Notation

14.2.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to simplify the quadratic term $\hat{H}_{\text{int}}^{\text{HF}}$ through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.The logic is that the expected value ($\langle b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}^\dagger b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle$) in the first Hartree term ($\langle b_{\tau_\alpha,l_\alpha}^\dagger(k_\alpha) b_{\tau_\alpha,l_\alpha}(k_\delta)\rangle b_{\tau_\beta,l_\beta}^\dagger(k_\beta) b_{\tau_\beta,l_\beta}(k_3)$) has the same form as the quadratic operators in the second Hartree term ($\langle b_{\tau_\beta,l_\beta}^\dagger(k_\beta) b_{\tau_\beta,l_\beta}(k_\gamma)\rangle b_{\tau_\alpha,l_\alpha}^\dagger(k_\alpha) b_{\tau_\alpha,l_\alpha}(k_\delta)$), 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.You should recall that $\hat{H}_{\text{int}}^{\text{HF}}$ is

$$\hat{H}_{\text{int}}^{\text{HF}} = \frac{1}{2A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta}\Bigg(\langle b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}^\dagger b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle b_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}^\dagger b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$$

$$+\langle b_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}^\dagger b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}^\dagger b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} - \langle b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}^\dagger b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle b_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}^\dagger b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}$$

$$-\langle b_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}^\dagger b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}^\dagger b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\Bigg) V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

.Return the simplified $\hat{H}_{\text{int}}^{\text{HF}}$ which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term)
===EXAMPLE: Given a Hamiltonian $\hat{H} = \sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)(\langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3) + \langle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3)\rangle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4))\delta_{k_1+k_2,k_3+k_4}$, where $V(q) = V(-q)$.In the second term, we relabel the index to swap the index in expected value and the index in quadratic operators, namely, $\sigma_1 \leftrightarrow \sigma_2$, $\sigma_3 \leftrightarrow \sigma_4$, $k_1 \leftrightarrow k_2$, $k_3 \leftrightarrow k_4$. After the replacement, the second term becomes $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_2-k_3)\langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$.Note that the Kronecker dirac function $\delta_{k_4+k_3,k_2+k_1}$ implies $k_1+k_2 = k_3+k_4$, i.e., $k_2-k_3 = k_4-k_1$. Thus, the second term simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_4-k_1)\langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Because $V(q) = V(-q)$, meaning $V(k_4-k_1) = V(k_1-k_4)$, the second term further simplifies to $\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)\langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. Note that this form of second term after relabeling is identical to the first term.Finally, we have the simplified Hamiltonian as $\hat{H} = 2\sum_{k_1,k_2,k_3,k_4,\sigma_1,\sigma_2,\sigma_3,\sigma_4} V(k_1-k_4)\langle c_{\sigma_1}^\dagger(k_1) c_{\sigma_4}(k_4)\rangle c_{\sigma_2}^\dagger(k_2) c_{\sigma_3}(k_3)\delta_{k_4+k_3,k_2+k_1}$. "'

14.2.2

Completion: Instructions to execute: You will be instructed to simplify the quadratic term $\hat{H}_{\text{int}}^{\text{HF}}$ by relabeling indices to combine the two Hartree and two Fock terms into one Hartree term and one Fock term. The expected value in one term can be made identical to the quadratic operators in another term by relabeling, as long as $V(q) = V(-q)$, which is naturally satisfied in the Coulomb interaction. Perform this relabeling for both the Hartree and Fock terms to reduce them to one Hartree term and one Fock term. Recall that $\hat{H}_{\text{int}}^{\text{HF}}$ is given by the specified formula with four terms. Return the simplified $\hat{H}_{\text{int}}^{\text{HF}}$ with only two terms.
Answer: Starting with the Hartree-Fock interaction Hamiltonian $\hat{H}_{\text{int}}^{\text{HF}}$ and using the relabeling trick as described, we can simplify it:

Original $\hat{H}^{\text{HF}}_{\text{int}}$:

$$\hat{H}^{\text{HF}}_{\text{int}} = \frac{1}{2A} \sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \Bigg(\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$$

$$+ \langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \Bigg) V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

$$- \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} - \langle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \rangle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$$

Relabeling the indices in the second and fourth terms: - Swap $\boldsymbol{k}_\alpha \leftrightarrow \boldsymbol{k}_\beta$ and $\boldsymbol{k}_\gamma \leftrightarrow \boldsymbol{k}_\delta$ in the second term. - Swap $\boldsymbol{k}_\alpha \leftrightarrow \boldsymbol{k}_\beta$ and $\boldsymbol{k}_\gamma \leftrightarrow \boldsymbol{k}_\delta$ in the fourth term.
After relabeling, these terms become identical to the first and third terms respectively, due to $V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) = V(-(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)) = V(\boldsymbol{k}_\delta - \boldsymbol{k}_\alpha)$, and the delta function enforcing momentum conservation. Thus, the simplified $\hat{H}^{\text{HF}}_{\text{int}}$ reduces to:

$$\hat{H}^{\text{HF}}_{\text{int}} = \frac{1}{A} \sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \Bigg(\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}$$

$$- \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \Bigg) V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

This simplified Hamiltonian consists of just two terms, one Hartree and one Fock term, thus reducing the complexity of $\hat{H}^{\text{HF}}_{\text{int}}$ in the Hartree-Fock approximation.

15 Identify order parameters in Hartree term (extended BZ)

15.1 Execution-Notation

15.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to simplify the Hartree term in H_{Hartree} by reducing the momentum inside the expected value $\langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha) b_{l_\alpha,\tau_\alpha,q_\delta}(k_\delta) \rangle$.The expected value $\langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha) b_{l_\alpha,\tau_\alpha,q_\delta}(k_\delta) \rangle$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha) b_{l_\alpha,\tau_\alpha,q_\delta}(k_\delta) \rangle = \langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha) b_{l_\alpha,\tau_\alpha,q_\delta}(k_\delta) \rangle \delta_{k_\alpha,k_\delta}$.You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i. Once you reduce one momentum inside the expected value $\langle \dots \rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.You should recall that H_{Hartree} is

$$\hat{H}^{\text{HF}}_{\text{int}} = \frac{1}{A} \sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

.Return the final simplified Hartree term H_{Hartree}.
===EXAMPLE:Given a Hamiltonian where the Hartree term $\hat{H}^{Hartree} = \sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, where k_i is the momentum inside first Brilloun zone and b_i is the reciprocal lattice.Inside the expected value, we realize $\langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle$ is nonzero only when $k_1 = k_4$, i.e., $\langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle = \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle \delta_{k_1,k_4}$.Thus, the Hartree term becomes $\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1 - k_4 + b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_4) \rangle \delta_{k_1,k_4} c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.Use the property of Kronecker delta function δ_{k_1,k_4} to sum over k_4, we have $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(k_1 - k_1 + b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_1) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{k_1+k_2+b_1+b_2,k_3+k_1+b_3+b_4} = \sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1 - b_4) \langle c^\dagger_{b_1}(k_1) c_{b_4}(k_1) \rangle c^\dagger_{b_2}(k_2) c_{b_3}(k_3) \delta_{k_2+b_1+b_2,k_3+b_3+b_4}$.Because k_i is momentum inside first Brilloun zone while b_i is the reciprocal lattice. It is only when $k_2 = k_3$ that $\delta_{k_2+b_1+b_2,k_3+b_3+b_4}$ is

nonzero, i.e., $\delta_{k_2+b_1+b_2,k_3+b_3+b_4} = \delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_3}$. Therefore, the Hartree term simplifies to $\sum_{k_1,k_2,k_3,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_3)\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_3} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Hartree term after reducing two momenta is $\hat{H}^{Hartree} = \sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(b_1-b_4)\langle c_{b_1}^\dagger(k_1)c_{b_4}(k_1)\rangle c_{b_2}^\dagger(k_2)c_{b_3}(k_2)\delta_{b_1+b_2,b_3+b_4}$ "'

15.1.2

Completion: Instructions to execute: You will be instructed to simplify the Hartree term in $\hat{H}^{\text{HF}}_{\text{int}}$ by reducing the momentum inside the expected value $\langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha)b_{l_\alpha,\tau_\alpha,q_\delta}(k_\delta)\rangle$. This expected value is nonzero only when the two momenta k_α and k_δ are the same. Use the property of the Kronecker delta function to reduce one momentum k_i (but not b_i). After reducing one momentum inside the expected value, you will notice the total momentum conservation will reduce another momentum in the quadratic term. You should end up with only two momenta left in the summation. Follow the example provided to reduce one momentum in the Hartree term and another momentum in the quadratic term. Recall that H_{Hartree} is given by the specified formula. Return the final simplified Hartree term H_{Hartree}.
Answer: Starting with the Hartree term in $\hat{H}^{\text{HF}}_{\text{int}}$:

$$\hat{H}^{\text{HF}}_{\text{int}} = \frac{1}{A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta}\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

By using the property that the expectation value is nonzero only when $k_\alpha = k_\delta$:

$$\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle = \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}\rangle\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\delta}$$

The Hartree term becomes:

$$\hat{H}_{\text{Hartree}} = \frac{1}{A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma}\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}V(0)\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\alpha}$$

Simplifying further using momentum conservation:

$$\hat{H}_{\text{Hartree}} = \frac{1}{A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}b_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}V(0)$$

This is the final simplified Hartree term, H_{Hartree}, reduced to two momenta in the summation with the interaction potential $V(0)$ representing the static screened Coulomb interaction at zero momentum transfer.

16 Identify order parameters in Fock term (extended BZ)

16.1 Execution-Notation

16.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will be instructed to simplify the Fock term in H_{Fock} by reducing the momentum inside the expected value $\langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha)b_{l_\beta,\tau_\beta,q_\gamma}(k_\gamma)\rangle$.The expected value $\langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha)b_{l_\beta,\tau_\beta,q_\gamma}(k_\gamma)\rangle$ is only nonzero when the two momenta k_i,k_j are the same, namely, $\langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha)b_{l_\beta,\tau_\beta,q_\gamma}(k_\gamma)\rangle = \langle b^\dagger_{l_\alpha,\tau_\alpha,q_\alpha}(k_\alpha)b_{l_\beta,\tau_\beta,q_\gamma}(k_\gamma)\rangle\delta_{k_\alpha,k_\gamma}$.You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i.Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term.You should recall that H_{Fock} is

$$\hat{H}^{\text{HF}}_{\text{int}} = -\frac{1}{A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta}\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta}b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha}V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta)\delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

.Return the final simplified Fock term H_{Fock}.

===EXAMPLE:Given a Hamiltonian where the Fock term $\hat{H}^{Fock}=-\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_3)\rangle c_{b_2}^\dagger(k_2) c_{b_4}(k_4) \delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$, where k_i is the momentum inside first Brilloun zone and b_i is the reciprocal lattice.Inside the expected value, we realize $\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_3)\rangle$ is nonzero only when $k_1=k_3$, i.e., $\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_3)\rangle=\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_3)\rangle\delta_{k_1,k_3}$.Thus, the Fock term becomes $-\sum_{k_1,k_2,k_3,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_3)\rangle \delta_{k_1,k_3} c_{b_2}^\dagger(k_2) c_{b_4}(k_4) \delta_{k_1+k_2+b_1+b_2,k_3+k_4+b_3+b_4}$.Use the property of Kronecker delta function δ_{k_1,k_3} to sum over k_3, we have $-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2) c_{b_4}(k_4) \delta_{k_1+k_2+b_1+b_2,k_1+k_4+b_3+b_4}=-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2) c_{b_4}(k_4) \delta_{k_2+b_1+b_2,k_4+b_3+b_4}$.Because k_i is momentum inside first Brilloun zone while b_i is the reciprocal lattice. It is only when $k_2=k_4$ that $\delta_{k_2+b_1+b_2,k_4+b_3+b_4}$ is nonzero, i.e., $\delta_{k_2+b_1+b_2,k_4+b_3+b_4}=\delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4}$.Therefore, the Fock term simplifies to $-\sum_{k_1,k_2,k_4,b_1,b_2,b_3,b_4} V(k_1-k_4+b_1-b_4)\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2) c_{b_4}(k_4) \delta_{b_1+b_2,b_3+b_4}\delta_{k_2,k_4}=-\sum_{k_1,k_2,b_1,b_2,b_3,b_4} V(k_1-k_2+b_1-b_4)\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2) c_{b_4}(k_2) \delta_{b_1+b_2,b_3+b_4}$.Therefore, the final simplified Fock term after reducing two momenta is $\hat{H}^{Fock}=-\sum_{k_1, k_2,b_1,b_2,b_3,b_4} V(k_1-k_2+b_1-b_4)\langle c_{b_1}^\dagger(k_1) c_{b_3}(k_1)\rangle c_{b_2}^\dagger(k_2) c_{b_4}(k_2) \delta_{b_1+b_2,b_3+b_4}$
"'

16.1.2

Completion: Instructions to execute: You will be instructed to simplify the Fock term in H_{Fock} by reducing the momentum inside the expected value $\langle b_{l_\alpha,\tau_\alpha,q_\alpha}^\dagger(k_\alpha) b_{l_\beta,\tau_\beta,q_\gamma}(k_\gamma)\rangle$. This expected value is nonzero only when the two momenta k_α and k_γ are the same, i.e., $\langle b_{l_\alpha,\tau_\alpha,q_\alpha}^\dagger(k_\alpha) b_{l_\beta,\tau_\beta,q_\gamma}(k_\gamma)\rangle=\langle b_{l_\alpha,\tau_\alpha,q_\alpha}^\dagger(k_\alpha) b_{l_\beta,\tau_\beta,q_\gamma}(k_\gamma)\rangle\delta_{k_\alpha,k_\gamma}$. Use the property of the Kronecker delta function to reduce one momentum k_i but not b_i. Once you reduce one momentum inside the expected value $\langle\dots\rangle$, total momentum conservation will reduce another momentum in the quadratic term. End up with only two momenta left in the summation. Follow the example to reduce one momentum in the Fock term, and another in the quadratic term. Recall that H_{Fock} is given by the specified formula. Return the final simplified Fock term H_{Fock}.
Answer: Starting with the Fock term in $\hat{H}^{\text{HF}}_{\text{int}}$:

$$\hat{H}^{\text{HF}}_{\text{int}} = -\frac{1}{A} \sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma,\boldsymbol{k}_\delta} \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\gamma+\boldsymbol{k}_\delta}$$

By using the property that the expectation value is nonzero only when $k_\alpha = k_\gamma$:

$$\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle = \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\gamma,l_\beta,\tau_\beta} \rangle \delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\gamma}$$

The Fock term becomes:

$$\hat{H}_{\text{Fock}} = -\frac{1}{A} \sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta,\boldsymbol{k}_\delta} \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\alpha,l_\beta,\tau_\beta} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\delta,l_\alpha,\tau_\alpha} V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta) \delta_{\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta,\boldsymbol{k}_\alpha+\boldsymbol{k}_\delta}$$

Simplifying further using momentum conservation:

$$\hat{H}_{\text{Fock}} = -\frac{1}{A} \sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta} \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\alpha,l_\beta,\tau_\beta} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\beta,l_\alpha,\tau_\alpha} V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\beta)$$

This is the final simplified Fock term, H_{Fock}, reduced to two momenta in the summation with the interaction potential $V(\boldsymbol{k}_\alpha - \boldsymbol{k}_\beta)$ representing the screened Coulomb interaction between the relevant momentum states.

17 Final form of iteration in quadratic terms

17.1 Execution-Notation

17.1.1

Prompt: Execution: Notation Here I provide the notation you should use for this task. You should combine it with previous **Execution: Core information** to obtain the full instruction for execution. In the response, you will first repeat the instruction for execution and then proceed with the calculation. "' You will now be instructed to combine the Hartree term H_{Hartree} and the Fock term H_{Fock}.You should recall that the Hartree term $H_{\text{Hartree}} = \frac{1}{A} \sum_{\substack{\tau_\alpha,\tau_\beta \\ l_\alpha,l_\beta}} \sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta} \langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} \rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} V(0)$,and the Fock term $H_{\text{Fock}} = -\frac{1}{A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\alpha,l_\beta,\tau_\beta}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\beta,l_\alpha,\tau_\alpha} V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\beta)$ .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 : Not needed. You should add them, relabel the index in Fock term, and simply their sum. Return the final sum of Hartree and Fock term. "'

17.1.2

Completion: Instructions to execute: You will be instructed to combine the Hartree term H_{Hartree} and the Fock term H_{Fock}. Recall the expressions for both the Hartree and Fock terms. Relabel the indices in the Fock term to make the quadratic operators the same as those in the Hartree term, if needed. Then add them together and simplify their sum. Return the final combined sum of the Hartree and Fock terms.
Answer: Starting with the given Hartree term H_{Hartree} and Fock term H_{Fock}:
Hartree term H_{Hartree}:

$$H_{\text{Hartree}} = \frac{1}{A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} V(0)$$

Fock term H_{Fock}:

$$H_{\text{Fock}} = -\frac{1}{A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\alpha,l_\beta,\tau_\beta}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\beta,l_\alpha,\tau_\alpha} V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\beta)$$

Since the quadratic operators in the Fock term already match those in the Hartree term, there is no need for additional relabeling. The final combined sum of the Hartree and Fock terms is:

$$H_{\text{combined}} = H_{\text{Hartree}} + H_{\text{Fock}}$$

$$= \frac{1}{A}\sum_{\substack{\tau_\alpha,\tau_\beta\\ l_\alpha,l_\beta}}\sum_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\beta}\Bigg(\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} V(0)$$

$$-\langle b^\dagger_{\boldsymbol{k}_\alpha,l_\alpha,\tau_\alpha} b_{\boldsymbol{k}_\alpha,l_\beta,\tau_\beta}\rangle b^\dagger_{\boldsymbol{k}_\beta,l_\beta,\tau_\beta} b_{\boldsymbol{k}_\beta,l_\alpha,\tau_\alpha} V(\boldsymbol{k}_\alpha-\boldsymbol{k}_\beta)\Bigg)$$

This expression represents the final combined sum of the Hartree and Fock terms, simplified and ready to be used in further calculations.