1 Identify kinetic term (continuum,second-quantized)

Prompt

I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
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'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to describe the kinetic term of Hamiltonian in {system} in the {real|momentum} space in the {single-particle|second-quantized} form.
The degrees of freedom of the system are: {degrees_of_freedom}.
Express the Kinetic Hamiltonian {kinetic_symbol} using {dispersion_symbol}, {annihilation_op}, and {creation_op}, where the summation of $k|r$ should be running over the {entire_space|first_Brillouin_zone}.
Use the following conventions for the symbols:
{definition_of_variables}
Excerpt:
that is insensitive to commensurability between the moir'e pattern and the underlying lattice. Stimulated by the recent experimental realization \cite{kim2017tunable,cao2018correlated,cao2018unconventional} of magic angle physics in twisted bilayer graphene, expeimental attention has expanded to include other graphene based multilayers with twists \cite{Yankowitz1059,lu2019superconductors,sharpe2019emergent,Serlin2020IntrinsicQA,cao2020tunable,shen2020correlated,chen2019evidence,chen2019signatures}, and also
twisted transition metal dichalcogenide bilayers \cite{tang2020tTMD,regan2020mott,wang2020correlated,xu2020correlated,jin2021stripe,li2021charge,li2021imaging,fractionTMD2020,mak2021continuousMIT,dean2021quantumcritical,li2021quantum}.
The valence bands of TMD heterobilayers and Γ-valley homobilayers \cite{mattia2020gammaValley} are described by emergent models in which interacting spin-$1/2$ electrons experience an external potential with triangular lattice periodicity, and therefore map directly to models of electrons on triangular or honeycomb lattices.
This paper is devoted to a study of the properties of triangular lattice moir'e materials and focuses on the case of one-hole per moir'e period, where correlations are strongest.
We examine the crossover from the narrow-band regime at small twist angles, where the system maps to a one-band Hubbard model with dominant on-site interactions, to the regime closer to the metal-insulator phase transition where important differences appear.
\begin{figure}[t] \centering \includegraphics[width=0.45\textwidth]{phaseSche.pdf} \caption{Hartree-Fock phase diagram for triangular lattice moir'e materials with one hole per unit cell. The two dimensionless control parameters (see main text) are the interaction strength r_s^* and α^2 - a parameter that is inversely related to the moir'e potential strength. First order and second order phase transitions are marked by solid and dashed black lines, respectively. States close to the top-left corner of the phase diagram (hashed) are metallic. States at the bottom right of the phase diagram are insulating. A narrow semi-metallic state (labelled SDW - spin density wave) that shares spatial symmetries with the three-sublattice non-collinear insulating state hugs the metallic side of the metal-insulator transition. An unexpected phase transition into an insulating ferromagnetic (blue) state at strong interaction strengths is interrupted by a narrow collinear antiferromagneric stripe state (orange). This phase diagram was calculated for moir'e modulation phase (see main text) $\phi = 26\,^\circ$. The lines in this figure follow approximate phase boundary expressions explained in the main text. } \label{fig:phaseD} \end{figure}
Our discussion is based mainly on a mean-field Hartree-Fock approximation used to address the interplay between periodic modulation and Coulomb interactions that controls the hybridization between orbitals centered on different sites, and therefore exchange interactions of spins on the system's triangular lattice.
Because it is a mean-field approach, the Hartree-Fock approximation cannot account for dynamic fluctuations in spin-configuration, but can accurately describe the energy of particular spin-configurations.
Importantly for the present application, the Hartree-Fock approximation has the advantage over spin-density-functional theory \cite{liangfuCTI} that it correctly accounts for the absence of self-interaction \cite{selfInt81} when electrons are localized near lattice sites. We expect the Hartree-

Fock approximation to overestimate the stability of insulating states relative to metallic states. (Indeed this expectation is confirmed by comparisoin with separate exact-diagonalization calculations for the same model \cite{nicolas2020ed}.) Our calculations can therefore provide a lower bound on the moir'e modulation strength that drives the system from a metallic to an insulating state at a given interaction strength. Unlike exact-diagonalization calcualations, Hartree-Fock calculations can be accurately converged with respect to system size.

Our goal in this manuscript is to identify differences between moir'e material physics and single-band Hubbard model physics, with particular emphasis on the prospects for tuning the system into exotic spin liquid states. Fig.~\ref{fig:phaseD} shows the phase diagram in a space defined by dimensionless modulation strength $\alpha^2(V_M, \phi, a_M)$ and interaction strength $r_s^*(\epsilon, a_M)$ parameters. The full phase space of the problem is actually 3-dimensional since the phase (ϕ - see below) of moir'e potential Fourier amplitude also plays a role. (a_M is the moir'e material lattice constant.) The lowest energy hole band is spectrally isolated for $\alpha \lesssim 0.1$, the range covered in Fig.~\ref{fig:phaseD}, unless ϕ is very close to a honeycomb value. (See below.) We find that the three sublattice antiferromagnetism expected~ \cite{JolicoeurPhysRevB1990} in the insulating state transform to stripe magnetism and finally to ferromagnetism with increasing r_s^*, and that a semimetallic state with three sublattice order occurs on the metallic side of the metal-insulator phase transition.

The transition to ferromagnetic insulating states at strong interactions opens up new opportunities to engineer strongly frustrated quantum magnetism. Given the possiblity of {\em in situ} tuning between different spin states, these findings demonstrate that moir'e materials are an exceptionally promising new system for the exploration of two-dimensional quantum magnetism.

The rest of the paper is organized as follows: In Sec.~\ref{sec:hf} we review the moir'e material model, discuss expected properties, and introduce the mean-field formalism. In Sec.~\ref{sec:results}, we discuss our results for spin-interactions in insulating moir'e materials. We comment specifically on necessary conditions for non-zero Hall conductance, concluding that though non-trivial band topology is unlikely, applying a magnetic field might induce a non-zero Hall conductance in doped insulators. Finally in Sec.~\ref{sec:outlook} we summarize our results and highlight important directions for future research.

\section{\label{sec:hf}Interacting continuum model} The low energy physics of TMD moir'e materials, like that of twisted bilayer graphene, is most conveniently captured by a continuum model \cite{fengchengHubbard}. Since TMDs are generally good insulators with strong spin-orbit coupling from the transition metal atoms, only the topmost valence band needs to be included in the low energy model - yielding one state for each valley. Because of spin-valley locking, we can equivalently choose to identify these states by their spins or by their valleys.

The type-II band alignment of TMD heterojunctions means that only one layer is active at low energy. Hence the fermion field operators $\psi_\alpha^{(\dagger)}(\mathbf{r})$ in this model carry only one label, representing locked spin/valley, while the effect of the other layer is integrated out, appearing only only as a contribution to the moir'e potential \cite{fengchengDelta,fengchengHubbard}, $\Delta(\boldsymbol{r})$. When the Fourier expansion of Δ is truncated at the first shell of moir'e reciprocal lattice vectors $\mathbf{b}_j$,

$$\Delta(\mathbf{r}) = \sum_{j=1}^{6} V_j \exp\left[i \mathbf{b}_j \cdot \mathbf{r}\right],$$

where $V_j = V_M \exp\left[(-1)^{j-1} i\phi\right]$. V_j and ϕ are material-dependent parameters, with V_M characterizing the moir'e modulation strength and ϕ its shape. The single-particle Hamiltonian of the moir'e continuum model

$$H_0 = T + \Delta(\mathbf{r}),$$

where T is the single-particle kinetic energy operator for electrons with effective mass m^*, is spin-independent. In a plane-wave representation

$$H_{0\mathbf{b},\mathbf{b}'}(\mathbf{k}) = -\frac{\hbar^2}{2m^*}\left(\mathbf{k}+\mathbf{b}\right)^2 \delta_{\mathbf{b},\mathbf{b}'} + \sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j,\mathbf{b}-\mathbf{b}'},$$

where momentum $\mathbf{k}$ is in the first moir'e Brillouin zone and the $\mathbf{b}$'s are moir'e reciprocal lattice vectors.

Completion

You will be instructed to describe the kinetic term of Hamiltonian in TMD moiré materials in the real space in the single-particle form.

The degrees of freedom of the system are: spin/valley.

Express the Kinetic Hamiltonian T using $\hbar$, m^*, $\mathbf{k}$, and $\mathbf{b}$, where the summation of $\mathbf{k}$ should be running over the first Brillouin zone.

Use the following conventions for the symbols:

- $\hbar$ is the reduced Planck constant
- m^* is the effective mass of the electrons
- $\mathbf{k}$ is the momentum in the first moiré Brillouin zone
- $\mathbf{b}$'s are moiré reciprocal lattice vectors.

2 Define energy dispersion (continuum)

Prompt
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Template:
You will be instructed to construct each term, namely {Energy_dispersion}.
For all energy dispersions, {Energy_dispersion}, it characterizes the {parabolic|Dirac|cos} dispersion for {electrons|holes}.
[In addition, a shift of {momentum_shift} in the momentum k_symbol for {shifted_Ek}, respectively.]
You should follow the EXAMPLE below to obtain correct energy dispersion, select the correct EXAMPLE by noticing the type of dispersion.
Finally, in the real space, the momentum $k\_symbol = -i\partial_{r\_symbol}$. You should keep the form of k_symbol in the Hamiltonian for short notations but should remember k_symbol is an operator.
Return the expression for {Energy_dispersion} in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian {kinetic_symbol}.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{definition_of_variables}
Excerpt:
that is insensitive to commensurability between the moir'e pattern and the underlying lattice. Stimulated by the recent experimental realization \cite{kim2017tunable,cao2018correlated,cao2018unconventional} of magic angle physics in twisted bilayer graphene, expeimental attention has expanded to include other graphene based multilayers with twists \cite{Yankowitz1059,lu2019superconductors,sharpe2019emergent,Serlin2020IntrinsicQA,cao2020tunable,shen2020correlated,chen2019evidence,chen2019signatures}, and also
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moir'e modulation phase (see main text) $\phi = 26^\circ$. The lines in this figure follow approximate phase boundary expressions explained in the main text. } \label{fig:phaseD} \end{figure}

Our discussion is based mainly on a mean-field Hartree-Fock approximation used to address the interplay between periodic modulation and Coulomb interactions that controls the hybridization between orbitals centered on different sites, and therefore exchange interactions of spins on the system's triangular lattice.

Because it is a mean-field approach, the Hartree-Fock approximation cannot account for dynamic fluctuations in spin-configuration, but can accurately describe the energy of particular spin-configurations.

Importantly for the present application, the Hartree-Fock approximation has the advantage over spin-density-functional theory \cite{liangfuCTI} that it correctly accounts for the absence of self-interaction \cite{selfInt81} when electrons are localized near lattice sites. We expect the Hartree-Fock approximation to overestimate the stability of insulating states relative to metallic states. (Indeed this expectation is confirmed by comparisoin with separate exact-diagonalization calculations for the same model \cite{nicolas2020ed}.) Our calculations can therefore provide a lower bound on the moir'e modulation strength that drives the system from a metallic to an insulating state at a given interaction strength. Unlike exact-diagonalization calcualations, Hartree-Fock calculations can be accurately converged with respect to system size.

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The transition to ferromagnetic insulating states at strong interactions opens up new opportunities to engineer strongly frustrated quantum magnetism. Given the possiblity of {\em in situ} tuning between different spin states, these findings demonstrate that moir'e materials are an exceptionally promising new system for the exploration of two-dimensional quantum magnetism.

The rest of the paper is organized as follows: In Sec.~\ref{sec:hf} we review the moir'e material model, discuss expected properties, and introduce the mean-field formalism. In Sec.~\ref{sec:results}, we discuss our results for spin-interactions in insulating moir'e materials. We comment specifically on necessary conditions for non-zero Hall conductance, concluding that though non-trivial band topology is unlikely, applying a magnetic field might induce a non-zero Hall conductance in doped insulators. Finally in Sec.~\ref{sec:outlook} we summarize our results and highlight important directions for future research.

\section{\label{sec:hf}Interacting continuum model} The low energy physics of TMD moir'e materials, like that of twisted bilayer graphene, is most conveniently captured by a continuum model \cite{fengchengHubbard}. Since TMDs are generally good insulators with strong spin-orbit coupling from the transition metal atoms, only the topmost valence band needs to be included in the low energy model - yielding one state for each valley. Because of spin-valley locking, we can equivalently choose to identify these states by their spins or by their valleys.

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$$\Delta(\mathbf{r}) = \sum_{j=1}^{6} V_j \exp\left[i\mathbf{b}_j \cdot \mathbf{r}\right],$$

where $V_j = V_M \exp\left[(-1)^{j-1} i\phi\right]$. V_j and ϕ are material-dependent parameters, with V_M characterizing the moir'e modulation strength and ϕ its shape. The single-particle Hamiltonian of the moir'e continuum model

$$H_0 = T + \Delta(\mathbf{r}),$$

where T is the single-particle kinetic energy operator for electrons with effective mass m^*, is spin-independent. In a plane-wave representation

$$H_{0\mathbf{b},\mathbf{b}'}(\mathbf{k}) = -\frac{\hbar^2}{2m^*}\left(\mathbf{k}+\mathbf{b}\right)^2 \delta_{\mathbf{b},\mathbf{b}'} + \sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j,\mathbf{b}-\mathbf{b}'},$$

where momentum $\mathbf{k}$ is in the first moir'e Brillouin zone and the $\mathbf{b}$'s are moir'e reciprocal lattice vectors.
Completion
Template:
You will be instructed to construct each term, namely $H_{0\mathbf{b},\mathbf{b}'}(\mathbf{k})$.
For all energy dispersions, $H_{0\mathbf{b},\mathbf{b}'}(\mathbf{k})$, it characterizes the parabolic dispersion for electrons.
In addition, a shift of b in the momentum k for $H_{0\mathbf{b},\mathbf{b}'}(\mathbf{k})$, respectively.
You should follow the EXAMPLE below to obtain correct energy dispersion, select the correct EXAMPLE by noticing the type of dispersion.
Finally, in the real space, the momentum $k=-i\partial_r$. You should keep the form of k in the Hamiltonian for short notations but should remember k is an operator.
Return the expression for $H_{0\mathbf{b},\mathbf{b}'}(\mathbf{k})$ in the Kinetic Hamiltonian, and substitute it into the Kinetic Hamiltonian H_0.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{b: moir'e reciprocal lattice vectors, k: momentum, H_0: single-particle Hamiltonian, m^*: effective mass of electrons, V_j: material-dependent parameters, V_M: moir'e modulation strength, ϕ: shape of moir'e modulation, Delta: moir'e potential, r: position vector, $\psi_\alpha^{(\dagger)}(\mathbf{r})$: fermion field operators, α: label representing locked spin/valley}

3 Identify potential term (continuum)

Prompt
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Template:
You will be instructed to describe the potential term of Hamiltonian {potential_symbol} in the {real|momentum} space in the {single-particle|second-quantized} form.
The potential Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian.
The diagonal terms are {diagonal_potential}.
The off-diagonal terms are the coupling between {interaction_degrees_of_freedom}, {offdiagonal_potential}, which should be kept hermitian.
All others terms are zero. Express the potential Hamiltonian {potential_symbol} using {diagonal_potential} and {offdiagonal_potential}.
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):
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Excerpt:
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bution to the moir'e potential \cite{fengchengDelta,fengchengHubbard}, $\Delta(r)$. When the Fourier expansion of Δ is truncated at the first shell of moir'e reciprocal lattice vectors $\mathbf{b}_j$,

$$\Delta(\mathbf{r}) = \sum_{j=1}^{6} V_j \exp\left[i\mathbf{b}_j \cdot \mathbf{r}\right],$$

where $V_j = V_M \exp\left[(-1)^{j-1} i\phi\right]$. V_j and ϕ are material-dependent parameters, with V_M characterizing the moir'e modulation strength and ϕ its shape. The single-particle Hamiltonian of the moir'e continuum model

$$H_0 = T + \Delta(\mathbf{r}),$$

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where momentum $\mathbf{k}$ is in the first moir'e Brillouin zone and the $\mathbf{b}$'s are moir'e reciprocal lattice vectors.

Completion

Template:
You will be instructed to describe the potential term of Hamiltonian H_0 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 $-\frac{\hbar^2}{2m^*}\left(\mathbf{k}+\mathbf{b}\right)^2 \delta_{\mathbf{b},\mathbf{b}'}$.
The off-diagonal terms are the coupling between {orbitals centered on different sites}, $\sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j,\mathbf{b}-\mathbf{b}'}$, which should be kept hermitian.
All others terms are zero. Express the potential Hamiltonian H_0 using $-\frac{\hbar^2}{2m^*}\left(\mathbf{k}+\mathbf{b}\right)^2 \delta_{\mathbf{b},\mathbf{b}'}$ and $\sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j,\mathbf{b}-\mathbf{b}'}$.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{H_0 is the single-particle Hamiltonian of the moir'e continuum model, T is the single-particle kinetic energy operator for electrons with effective mass m^*, $\Delta(\mathbf{r})$ is the moir'e potential, $V_j = V_M \exp\left[(-1)^{j-1} i\phi\right]$ where V_M characterizes the moir'e modulation strength and \phi its shape, $\mathbf{k}$ is in the first moir'e Brillouin zone and the $\mathbf{b}$'s are moir'e reciprocal lattice vectors.}

4 Define potential term (continuum)

Prompt

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Template:
You will be instructed to construct each term {potential_symbol}, namely, {Potential_variables}.
The expression for diagonal terms are: {expression_diag}.
The expression for off-diagonal terms are: {expression_offdiag}.
Return the expressions for {Potential_variables}, and substitute it into the potential Hamiltonian {potential_symbol}.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or have conflicts in the conventions, you should stop and let me know):
{definition_of_variables}
Excerpt:
that is insensitive to commensurability between the moir'e pattern and the underlying lattice. Stimulated by the recent experimental realization \cite{kim2017tunable,cao2018correlated,cao2018unconventional} of magic angle physics in twisted bilayer graphene, expeimental attention has

expanded to include other graphene based multilayers with twists \cite{Yankowitz1059,lu2019superconductors,sharpe2019emergent,Serlin2020IntrinsicQA,cao2020tunable,shen2020correlated,chen2019evidence,chen2019signatures}, and also
twisted transition metal dichalcogenide bilayers \cite{tang2020tTMD,regan2020mott,wang2020correlated,xu2020correlated,jin2021stripe,li2021charge,li2021imaging,fractionTMD2020,mak2021continuousMIT,dean2021quantumcritical,li2021quantum}.
The valence bands of TMD heterobilayers and Γ-valley homobilayers \cite{mattia2020gammaValley} are described by emergent models in which interacting spin-$1/2$ electrons experience an external potential with triangular lattice periodicity, and therefore map directly to models of electrons on triangular or honeycomb lattices.
This paper is devoted to a study of the properties of triangular lattice moir'e materials and focuses on the case of one-hole per moir'e period, where correlations are strongest.
We examine the crossover from the narrow-band regime at small twist angles, where the system maps to a one-band Hubbard model with dominant on-site interactions, to the regime closer to the metal-insulator phase transition where important differences appear.
\begin{figure}[t] \centering \includegraphics[width=0.45\textwidth]{phaseSche.pdf} \caption{Hartree-Fock phase diagram for triangular lattice moir'e materials with one hole per unit cell. The two dimensionless control parameters (see main text) are the interaction strength r_s^* and α^2 - a parameter that is inversely related to the moir'e potential strength. First order and second order phase transitions are marked by solid and dashed black lines, respectively. States close to the top-left corner of the phase diagram (hashed) are metallic. States at the bottom right of the phase diagram are insulating. A narrow semi-metallic state (labelled SDW - spin density wave) that shares spatial symmetries with the three-sublattice non-collinear insulating state hugs the metallic side of the metal-insulator transition. An unexpected phase transition into an insulating ferromagnetic (blue) state at strong interaction strengths is interrupted by a narrow collinear antiferromagneric stripe state (orange). This phase diagram was calculated for moir'e modulation phase (see main text) $\phi = 26\,^\circ$. The lines in this figure follow approximate phase boundary expressions explained in the main text. } \label{fig:phaseD} \end{figure}
Our discussion is based mainly on a mean-field Hartree-Fock approximation used to address the interplay between periodic modulation and Coulomb interactions that controls the hybridization between orbitals centered on different sites, and therefore exchange interactions of spins on the system's triangular lattice.
Because it is a mean-field approach, the Hartree-Fock approximation cannot account for dynamic fluctuations in spin-configuration, but can accurately describe the energy of particular spin-configurations.
Importantly for the present application, the Hartree-Fock approximation has the advantage over spin-density-functional theory \cite{liangfuCTI} that it correctly accounts for the absence of self-interaction \cite{selfInt81} when electrons are localized near lattice sites. We expect the Hartree-Fock approximation to overestimate the stability of insulating states relative to metallic states. (Indeed this expectation is confirmed by comparisoin with separate exact-diagonalization calculations for the same model \cite{nicolas2020ed}.) Our calculations can therefore provide a lower bound on the moir'e modulation strength that drives the system from a metallic to an insulating state at a given interaction strength. Unlike exact-diagonalization calcualations, Hartree-Fock calculations can be accurately converged with respect to system size.
Our goal in this manuscript is to identify differences between moir'e material physics and single-band Hubbard model physics, with particular emphasis on the prospects for tuning the system into exotic spin liquid states. Fig.~\ref{fig:phaseD} shows the phase diagram in a space defined by dimensionless modulation strength $\alpha^2(V_M,\phi,a_M)$ and interaction strength $r_s^*(\epsilon,a_M)$ parameters. The full phase space of the problem is actually 3-dimensional since the phase (ϕ - see below) of moir'e potential Fourier amplitude also plays a role. (a_M is the moir'e material lattice constant.) The lowest energy hole band is spectrally isolated for $\alpha \lesssim 0.1$, the range covered in Fig.~\ref{fig:phaseD}, unless ϕ is very close to a honeycomb value. (See below.) We find that the three sublattice antiferromagnetism expected~ \cite{JolicoeurPhysRevB1990} in the insulating state transform to stripe magnetism and finally to ferromagnetism with increasing r_s^*, and that a semimetallic state with three sublattice order occurs on the metallic side of the metal-insulator phase transition.
The transition to ferromagnetic insulating states at strong interactions opens up new opportunities to engineer strongly frustrated quantum magnetism. Given the possiblity of {\em in situ} tuning between different spin states, these findings demonstrate that moir'e materials are an exceptionally promising new system for the exploration of two-dimensional quantum magnetism.
The rest of the paper is organized as follows: In Sec.~\ref{sec:hf} we review the moir'e material model, discuss expected properties, and introduce the mean-field formalism. In Sec.~\ref{sec:results}, we discuss our results for spin-interactions in insulating moir'e materials. We comment specifically on necessary conditions for non-zero Hall conductance, concluding that though non-trivial band topology is unlikely, applying a magnetic field might induce a non-zero Hall conductance

in doped insulators. Finally in Sec.~\ref{sec:outlook} we summarize our results and highlight important directions for future research.
\section{\label{sec:hf}Interacting continuum model} The low energy physics of TMD moir'e materials, like that of twisted bilayer graphene, is most conveniently captured by a continuum model \cite{fengchengHubbard}. Since TMDs are generally good insulators with strong spin-orbit coupling from the transition metal atoms, only the topmost valence band needs to be included in the low energy model - yielding one state for each valley. Because of spin-valley locking, we can equivalently choose to identify these states by their spins or by their valleys.
The type-II band alignment of TMD heterojunctions means that only one layer is active at low energy. Hence the fermion field operators $\psi_{\alpha}^{(\dagger)}(\mathbf{r})$ in this model carry only one label, representing locked spin/valley, while the effect of the other layer is integrated out, appearing only only as a contribution to the moir'e potential \cite{fengchengDelta,fengchengHubbard}, $\Delta(\boldsymbol{r})$. When the Fourier expansion of Δ is truncated at the first shell of moir'e reciprocal lattice vectors $\mathbf{b}_j$,

$$\Delta(\mathbf{r}) = \sum_{j=1}^{6} V_j \exp\left[i\mathbf{b}_j \cdot \mathbf{r}\right],$$

where $V_j = V_M \exp\left[(-1)^{j-1} i\phi\right]$. V_j and ϕ are material-dependent parameters, with V_M characterizing the moir'e modulation strength and ϕ its shape. The single-particle Hamiltonian of the moir'e continuum model

$$H_0 = T + \Delta(\mathbf{r}),$$

where T is the single-particle kinetic energy operator for electrons with effective mass m^*, is spin-independent. In a plane-wave representation

$$H_{0\mathbf{b},\mathbf{b}'}(\mathbf{k}) = -\frac{\hbar^2}{2m^*}\left(\mathbf{k}+\mathbf{b}\right)^2 \delta_{\mathbf{b},\mathbf{b}'} + \sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j,\mathbf{b}-\mathbf{b}'},$$

where momentum $\mathbf{k}$ is in the first moir'e Brillouin zone and the $\mathbf{b}$'s are moir'e reciprocal lattice vectors.
Completion
You will be instructed to construct each term $\Delta(\mathbf{r})$, namely, V_j and ϕ.
The expression for diagonal terms are: $-\frac{\hbar^2}{2m^*}\left(\mathbf{k}+\mathbf{b}\right)^2 \delta_{\mathbf{b},\mathbf{b}'}$.
The expression for off-diagonal terms are: $\sum_{j=1}^{6} V_j \delta_{\mathbf{b}_j,\mathbf{b}-\mathbf{b}'}$.
Return the expressions for V_j and ϕ, and substitute it into the potential Hamiltonian $\Delta(\mathbf{r})$.
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 have conflicts in the conventions, you should stop and let me know):
$V_j = V_M \exp\left[(-1)^{j-1} i\phi\right]$ where V_M characterizes the moir'e modulation strength and ϕ its shape. The fermion field operators $\psi_{\alpha}^{(\dagger)}(\mathbf{r})$ in this model carry only one label, representing locked spin/valley. The single-particle Hamiltonian of the moir'e continuum model $H_0 = T + \Delta(\mathbf{r})$, where T is the single-particle kinetic energy operator for electrons with effective mass m^*.

5 Identify interacting term (momentum space)

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to construct the interaction part of the Hamiltonian {second_int_symbol} in the momentum space.
The interaction Hamiltonian is a product of four parts. The first part is the product of four operators with two creation and two annihilation operators following the normal order, namely, creation operators are before annihilation operators. You should follow the order of $1,2,2,1$ for the {index_of_operator}, and $1,2,3,4$ for the {momentum}. The second part is the constraint of total momentum

conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators. [For each operator, the total momentum is the sum of moire reciprocal lattice b_i and momentum with in the first BZ k_i]
The third part is the interaction form. You should use {interaction} with $V(q) = int\_form$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same {index_of_operator}, namely $q = k_1 - k_4$.
The fourth part is the normalization factor, you should use {normalization_factor} here. Finally, the summation should be running over all {index_of_operator}, and {momentum} Return the interaction term {second_int_symbol} in terms of {op} and $V(q)$ (with q expressed in terms of {momentum}).
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{definition_of_variables}
Excerpt:
is that the lowest energy hole band is isolated and has a bandwidth W that decreases exponentially with moir'e period a_M. One physical intuition for this behavior is based on the observation that the model can be approximated, in the large-a_M limit, as a lattice of weakly coupled harmonically confined electrons. Ignoring the "remote-band" holes for the moment, we can readily see that the largest effect of Coulomb interactions is to impose an energy penalty U on doubly occupied sites, which is the essence of Hubbard model physics. But in contrast to simplest nearest-neighbor Hubbard model, the ratio of second nearest-neighbor hopping to the nearest-neighbor hopping can be increased by decreasing the modulation strength, a property easily explained in the harmonic oscillator approximation, increasing the magnetic frustration of insulating states.
Completion
Template:
You will be instructed to construct the interaction part of the Hamiltonian {second_int_symbol} in the momentum space.
The interaction Hamiltonian is a product of four parts. The first part is the product of four operators with two creation and two annihilation operators following the normal order, namely, creation operators are before annihilation operators. You should follow the order of $1, 2, 2, 1$ for the {index_of_operator}, and $1, 2, 3, 4$ for the {momentum}. The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators. [For each operator, the total momentum is the sum of moire reciprocal lattice b_i and momentum with in the first BZ k_i]
The third part is the interaction form. You should use {interaction} with $V(q) = int\_form$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same {index_of_operator}, namely $q = k_1 - k_4$.
The fourth part is the normalization factor, you should use {normalization_factor} here. Finally, the summation should be running over all {index_of_operator}, and {momentum} Return the interaction term {second_int_symbol} in terms of {op} and $V(q)$ (with q expressed in terms of {momentum}).
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{definition_of_variables}

6 Wick's theorem expansion

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
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{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, {second_int_symbol}.

You should use Wick's theorem to expand the four-fermion term in {second_int_symbol} into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without †, and be extremely cautious about the order of the index and sign before each term.
You should only preserve the normal terms. Here, the normal terms mean the product of a creation operator and an annihilation operator.
Return the expanded interaction term after Hartree-Fock approximation as {Hartree_Fock_symbol}.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{definition_of_variables}
Excerpt:
single Slater determinant ground state. Minimizing the energy functional with respect to single-particle wave-functions yields a mean-field Hamiltonian that adds an interaction self-energy Σ^{HF} to the single-particle Hamiltonian which can be expressed in terms of the single-particle density matrix $\rho=\sum_n \left|\psi_n\right\rangle\left\langle\psi_n\right|$, where the sum is over occupied moir'e-band Bloch wavefunctions. The mean-field electronic structure of moir'e superlattices is best evaluated using a plane-wave representation in which the Hartree-Fock self energy Σ^{HF} at each $\mathbf{k}$ in the Brillouin-zone is a matrix in reciprocal lattice vectors $\mathbf{b}$: \begin{widetext}

$$\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})=\frac{\delta_{\alpha,\beta}}{A}\sum_{\alpha'}V_{\alpha'\alpha}(\mathbf{b}'-\mathbf{b})\sum_{\mathbf{k}',\mathbf{b}''}\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')-\frac{1}{A}\sum_{\mathbf{b}'',k'}V_{\alpha\beta}(\mathbf{b}''+\mathbf{k}'-\mathbf{k})\rho_{\alpha,\mathbf{b}+\mathbf{b}'';\beta,\mathbf{b}'+\mathbf{b}''}(\mathbf{k}').$$

\end{widetext} In Eq.~\ref{eq:self-energy} Greek letters label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$ is the self-consistently determined momentum-space density matrix. Starting with a physically plausible density matrix ρ_0, we minimize the energy by performing self-consistent iterations. Because the many-body interaction is invariant under both translations and spin-rotations, if we start from a density matrix ρ_0 which satisfies a symmetry $\hat{O}$ of H_0 ($[\rho_0,\hat{O}]=0$, $[H_0,\hat{O}]=0$) then the symmetry survives under iteration.
That is to say that H^{HF} commutes with $\hat{O}$ at every iteration step. In many-cases the minimum energy Hartree-Fock state breaks symmetries of H_0 and these solutions are found under iteration only by starting with a broken-symmetry density-matrix. As argued in Sec.~\ref{sec:lim}, the phase diagram contains paramagnetic states that do not break any symmetries, ferromagnetic states with spontaneous collinear spin-polarization that do not break lattice translational symmetries, stripe states with collinear order and a doubled unit cell area, and 120° N'eel states with both a tripled unit cell area and and non-collinear spin-order. We obtain solutions of the first two kinds by appropriate choices of the initial density ρ_0. Each possible type of reduced translational symmetry implies a different reciprocal lattice, and therefore has to be encoded explicitly in the recriprocal lattice employed and considered separately. Solutions can be classified as insulating with a gap between occupied and empty states, or metallic with Fermi surfaces in the Brillouin-zone on which occupation numbers change.
At one electron per moir'e period, the paramagnetic state must be metallic, but all other states we consider can be insulating. We show typical Hartree-Fock self-consistent band structures for insulating and metallic magnetic ordered sates in Fig.~\ref{fig:hfbands}.
Completion
You will be instructed to perform a Hartree-Fock approximation to expand the interaction term, Σ^{HF}.
You should use Wick's theorem to expand the four-fermion term in Σ^{HF} into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without †, and be extremely cautious about the order of the index and sign before each term.
You should only preserve the normal terms. Here, the normal terms mean the product of a creation operator and an annihilation operator.
Return the expanded interaction term after Hartree-Fock approximation as Σ^{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):
Σ^{HF} is the Hartree-Fock self-energy, ρ is the single-particle density matrix, $\mathbf{k}$ is the Brillouin-zone, $\mathbf{b}$ is the reciprocal lattice vectors, α and β label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$ is the self-consistently determined momentum-space density matrix.

7 Drop constant terms

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to extract the quadratic terms in the {Hartree_Fock_term_symbol}.
The quadratic terms mean terms that are proportional to {bilinear_op}, which excludes terms that are solely expectations or products of expectations.
You should only preserve the quadratic terms in {Hartree_Fock_term_symbol}, denoted as {Hartree_Fock_second_quantized_symbol}.
Return {Hartree_Fock_second_quantized_symbol}.
Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
{definition_of_variables}
Excerpt:
single Slater determinant ground state. Minimizing the energy functional with respect to single-particle wave-functions yields a mean-field Hamiltonian that adds an interaction self-energy Σ^{HF} to the single-particle Hamiltonian which can be expressed in terms of the single-particle density matrix $\rho=\sum_n |\psi_n\rangle\langle\psi_n|$, where the sum is over occupied moir'e-band Bloch wavefunctions. The mean-field electronic structure of moir'e superlattices is best evaluated using a plane-wave representation in which the Hartree-Fock self energy Σ^{HF} at each $\mathbf{k}$ in the Brillouin-zone is a matrix in reciprocal lattice vectors $\mathbf{b}$: \begin{widetext}

$$\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})=\frac{\delta_{\alpha,\beta}}{A}\sum_{\alpha'}V_{\alpha'\alpha}(\mathbf{b}'-\mathbf{b})\sum_{\mathbf{k}',\mathbf{b}''}\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')-\frac{1}{A}\sum_{\mathbf{b}'',k'}V_{\alpha\beta}(\mathbf{b}''+\mathbf{k}'-\mathbf{k})\rho_{\alpha,\mathbf{b}+\mathbf{b}'';\beta,\mathbf{b}'+\mathbf{b}''}(\mathbf{k}').$$

\end{widetext} In Eq.~\ref{eq:self-energy} Greek letters label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$ is the self-consistently determined momentum-space density matrix. Starting with a physically plausible density matrix ρ_0, we minimize the energy by performing self-consistent iterations. Because the many-body interaction is invariant under both translations and spin-rotations, if we start from a density matrix ρ_0 which satisfies a symmetry $\hat{O}$ of H_0 ($[\rho_0,\hat{O}]=0$, $[H_0,\hat{O}]=0$) then the symmetry survives under iteration.
That is to say that H^{HF} commutes with $\hat{O}$ at every iteration step. In many-cases the minimum energy Hartree-Fock state breaks symmetries of H_0 and these solutions are found under iteration only by starting with a broken-symmetry density-matrix. As argued in Sec.~\ref{sec:lim}, the phase diagram contains paramagnetic states that do not break any symmetries, ferromagnetic states with spontaneous collinear spin-polarization that do not break lattice translational symmetries, stripe states with collinear order and a doubled unit cell area, and 120° N'eel states with both a tripled unit cell area and and non-collinear spin-order. We obtain solutions of the first two kinds by appropriate choices of the initial density ρ_0. Each possible type of reduced translational symmetry implies a different reciprocal lattice, and therefore has to be encoded explicitly in the recriprocal lattice employed and considered separately. Solutions can be classified as insulating with a gap between occupied and empty states, or metallic with Fermi surfaces in the Brillouin-zone on which occupation numbers change.
At one electron per moir'e period, the paramagnetic state must be metallic, but all other states we consider can be insulating. We show typical Hartree-Fock self-consistent band structures for insulating and metallic magnetic ordered sates in Fig.~\ref{fig:hfbands}.
Completion
You will be instructed to extract the quadratic terms in the Σ^{HF} term.
The quadratic terms mean terms that are proportional to $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$, which excludes terms that are solely expectations or products of expectations.
You should only preserve the quadratic terms in Σ^{HF}, denoted as $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$.
Return $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know):
In $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$, Greek letters label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$ is the self-consistently determined momentum-space density matrix.

8 Identify momentum transfer in interaction

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
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{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to expand interaction term $V(q)$ in the MF quadratic term {Hartree_Fock_second_quantized_symbol}. If you find the $V(q)$ in {Hartree_Fock_second_quantized_symbol} does not contain any momentum that is not in the summation sign. The interaction term is already expanded. No action to perform on interaction term. Otherwise, you will expand $V(q)$ by replacing q with the momentum {momentum}. Return {Hartree_Fock_second_quantized_symbol} with expanded interaction.
Excerpt:
single Slater determinant ground state. Minimizing the energy functional with respect to single-particle wave-functions yields a mean-field Hamiltonian that adds an interaction self-energy Σ^{HF} to the single-particle Hamiltonian which can be expressed in terms of the single-particle density matrix $\rho=\sum_n |\psi_n\rangle\langle\psi_n|$, where the sum is over occupied moir'e-band Bloch wavefunctions. The mean-field electronic structure of moir'e superlattices is best evaluated using a plane-wave representation in which the Hartree-Fock self energy Σ^{HF} at each $\mathbf{k}$ in the Brillouin-zone is a matrix in reciprocal lattice vectors $\mathbf{b}$: \begin{widetext}

$$\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})=\frac{\delta_{\alpha,\beta}}{A}\sum_{\alpha'}V_{\alpha'\alpha}(\mathbf{b}'-\mathbf{b})\sum_{\mathbf{k}',\mathbf{b}''}\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')-\frac{1}{A}\sum_{\mathbf{b}'',k'}V_{\alpha\beta}(\mathbf{b}''+\mathbf{k}'-\mathbf{k})\rho_{\alpha,\mathbf{b}+\mathbf{b}'';\beta,\mathbf{b}'+\mathbf{b}''}(\mathbf{k}').$$

\end{widetext} In Eq.~\ref{eq:self-energy} Greek letters label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$ is the self-consistently determined momentum-space density matrix. Starting with a physically plausible density matrix ρ_0, we minimize the energy by performing self-consistent iterations. Because the many-body interaction is invariant under both translations and spin-rotations, if we start from a density matrix ρ_0 which satisfies a symmetry $\hat{O}$ of H_0 ($[\rho_0,\hat{O}]=0$, $[H_0,\hat{O}]=0$) then the symmetry survives under iteration.
That is to say that H^{HF} commutes with $\hat{O}$ at every iteration step. In many-cases the minimum energy Hartree-Fock state breaks symmetries of H_0 and these solutions are found under iteration only by starting with a broken-symmetry density-matrix. As argued in Sec.~\ref{sec:lim}, the phase diagram contains paramagnetic states that do not break any symmetries, ferromagnetic states with spontaneous collinear spin-polarization that do not break lattice translational symmetries, stripe states with collinear order and a doubled unit cell area, and 120° N'eel states with both a tripled unit cell area and and non-collinear spin-order. We obtain solutions of the first two kinds by appropriate choices of the initial density ρ_0. Each possible type of reduced translational symmetry implies a different reciprocal lattice, and therefore has to be encoded explicitly in the recriprocal lattice employed and considered separately. Solutions can be classified as insulating with a gap between occupied and empty states, or metallic with Fermi surfaces in the Brillouin-zone on which occupation numbers change.
At one electron per moir'e period, the paramagnetic state must be metallic, but all other states we consider can be insulating. We show typical Hartree-Fock self-consistent band structures for insulating and metallic magnetic ordered sates in Fig.~\ref{fig:hfbands}.
Completion
You will be instructed to expand interaction term $V(q)$ in the MF quadratic term $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})$. If you find the $V(q)$ in $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})$ does not contain any momentum that is not in the summation sign. The interaction term is already expanded. No action to perform on interaction term. Otherwise, you will expand $V(q)$ by replacing q with the momentum $\mathbf{k}$. Return $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})$ with expanded interaction.

9 Combine Hartree/Fock terms

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
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'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to simplify the quadratic term {Hartree_Fock_second_quantized_symbol} through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.
The logic is that the expected value ({expected_value}) in the first Hartree term ({expression_Hartree_1}) has the same form as the quadratic operators in the second Hartree term ({expression_Hartree_2}), and vice versa. The same applies to the Fock term.
This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree term, you can make the second Hartree term look identical to the first Hartree term, as long as $V(q) = V(-q)$, which is naturally satisfied in Coulomb interaction. You should follow the EXAMPLE below to simplify it through relabeling the index.
You should perform this trick of "relabeling the index" for both two Hartree terms and two Fock terms to reduce them to one Hartree term, and one Fock term.
Return the simplified {Hartree_Fock_second_quantized_symbol} which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term)
Excerpt:
single Slater determinant ground state. Minimizing the energy functional with respect to single-particle wave-functions yields a mean-field Hamiltonian that adds an interaction self-energy Σ^{HF} to the single-particle Hamiltonian which can be expressed in terms of the single-particle density matrix $\rho = \sum_n |\psi_n\rangle\langle\psi_n|$, where the sum is over occupied moir'e-band Bloch wavefunctions. The mean-field electronic structure of moir'e superlattices is best evaluated using a plane-wave representation in which the Hartree-Fock self energy Σ^{HF} at each $\mathbf{k}$ in the Brillouin-zone is a matrix in reciprocal lattice vectors $\mathbf{b}$: \begin{widetext}

$$\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k}) = \frac{\delta_{\alpha,\beta}}{A}\sum_{\alpha'} V_{\alpha'\alpha}(\mathbf{b}'-\mathbf{b})\sum_{\mathbf{k}',\mathbf{b}''}\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}') - \frac{1}{A}\sum_{\mathbf{b}'',k'} V_{\alpha\beta}(\mathbf{b}''+\mathbf{k}'-\mathbf{k})\rho_{\alpha,\mathbf{b}+\mathbf{b}'';\beta,\mathbf{b}'+\mathbf{b}''}(\mathbf{k}').$$

\end{widetext} In Eq.~\ref{eq:self-energy} Greek letters label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$ is the self-consistently determined momentum-space density matrix. Starting with a physically plausible density matrix ρ_0, we minimize the energy by performing self-consistent iterations. Because the many-body interaction is invariant under both translations and spin-rotations, if we start from a density matrix ρ_0 which satisfies a symmetry $\hat{O}$ of H_0 ($[\rho_0, \hat{O}] = 0$, $[H_0, \hat{O}] = 0$) then the symmetry survives under iteration.
That is to say that H^{HF} commutes with $\hat{O}$ at every iteration step. In many-cases the minimum energy Hartree-Fock state breaks symmetries of H_0 and these solutions are found under iteration only by starting with a broken-symmetry density-matrix. As argued in Sec.~\ref{sec:lim}, the phase diagram contains paramagnetic states that do not break any symmetries, ferromagnetic states with spontaneous collinear spin-polarization that do not break lattice translational symmetries, stripe states with collinear order and a doubled unit cell area, and 120° N'eel states with both a tripled unit cell area and and non-collinear spin-order. We obtain solutions of the first two kinds by appropriate choices of the initial density ρ_0. Each possible type of reduced translational symmetry implies a different reciprocal lattice, and therefore has to be encoded explicitly in the recriprocal lattice employed and considered separately. Solutions can be classified as insulating with a gap between occupied and empty states, or metallic with Fermi surfaces in the Brillouin-zone on which occupation numbers change.
At one electron per moir'e period, the paramagnetic state must be metallic, but all other states we consider can be insulating. We show typical Hartree-Fock self-consistent band structures for insulating and metallic magnetic ordered sates in Fig.~\ref{fig:hfbands}.
Completion
You will be instructed to simplify the quadratic term Σ^{HF} through relabeling the index to combine the two Hartree/Fock term into one Hartree/Fock term.

The logic is that the expected value ($\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')$ and $\rho_{\alpha,\mathbf{b}+\mathbf{b}'';\beta,\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')$) in the first Hartree term ($\frac{\delta_{\alpha,\beta}}{A}\sum_{\alpha'}V_{\alpha'\alpha}(\mathbf{b}'-\mathbf{b})\sum_{\mathbf{k}',\mathbf{b}''}$) has the same form as the quadratic operators in the second Hartree term ($-\frac{1}{A}\sum_{\mathbf{b}'',k'}V_{\alpha\beta}(\mathbf{b}''+\mathbf{k}'-\mathbf{k})$), and vice versa. The same applies to the Fock term.
This means, if you relabel the index by swapping the index in the "expected value" and "quadratic operators" in the second Hartree term, you can make the second Hartree term look identical to the first Hartree term, as long as $V(q)=V(-q)$, which is naturally satisfied in Coulomb interaction. You should follow the EXAMPLE below to simplify it through relabeling the index.
You should perform this trick of "relabeling the index" for both two Hartree terms and two Fock terms to reduce them to one Hartree term, and one Fock term.
Return the simplified Σ^{HF} which reduces from four terms (two Hartree and two Fock terms) to only two terms (one Hartree and one Fock term).

10 Identify order parameters in Hartree term (extended BZ)

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to simplify the Hartree term in {Hartree_second_quantized_symbol} by reducing the momentum inside the expected value {expected_value}.
The expected value {expected_value} is only nonzero when the two momenta k_i,k_j are the same, namely, {expected_value_nonzero}.
You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i. Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.
You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.
Return the final simplified Hartree term {Hartree_second_quantized_symbol}.
Excerpt:
single Slater determinant ground state. Minimizing the energy functional with respect to single-particle wave-functions yields a mean-field Hamiltonian that adds an interaction self-energy Σ^{HF} to the single-particle Hamiltonian which can be expressed in terms of the single-particle density matrix $\rho=\sum_n |\psi_n\rangle\langle\psi_n|$, where the sum is over occupied moir'e-band Bloch wavefunctions. The mean-field electronic structure of moir'e superlattices is best evaluated using a plane-wave representation in which the Hartree-Fock self energy Σ^{HF} at each $\mathbf{k}$ in the Brillouin-zone is a matrix in reciprocal lattice vectors $\mathbf{b}$: \begin{widetext}

$$\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})=\frac{\delta_{\alpha,\beta}}{A}\sum_{\alpha'}V_{\alpha'\alpha}(\mathbf{b}'-\mathbf{b})\sum_{\mathbf{k}',\mathbf{b}''}\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')-\frac{1}{A}\sum_{\mathbf{b}'',k'}V_{\alpha\beta}(\mathbf{b}''+\mathbf{k}'-\mathbf{k})\rho_{\alpha,\mathbf{b}+\mathbf{b}'';\beta,\mathbf{b}'+\mathbf{b}''}(\mathbf{k}').$$

\end{widetext} In Eq.~\ref{eq:self-energy} Greek letters label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$ is the self-consistently determined momentum-space density matrix. Starting with a physically plausible density matrix ρ_0, we minimize the energy by performing self-consistent iterations. Because the many-body interaction is invariant under both translations and spin-rotations, if we start from a density matrix ρ_0 which satisfies a symmetry $\hat{O}$ of H_0 ($[\rho_0,\hat{O}]=0$, $[H_0,\hat{O}]=0$) then the symmetry survives under iteration.
That is to say that H^{HF} commutes with $\hat{O}$ at every iteration step. In many-cases the minimum energy Hartree-Fock state breaks symmetries of H_0 and these solutions are found under iteration only by starting with a broken-symmetry density-matrix. As argued in Sec.~\ref{sec:lim}, the phase diagram contains paramagnetic states that do not break any symmetries, ferromagnetic states with spontaneous collinear spin-polarization that do not break lattice translational symmetries, stripe states with collinear order and a doubled unit cell area, and 120° N'eel states with both a tripled unit cell area and and non-collinear spin-order. We obtain solutions of the first two kinds by appropriate choices of the initial density ρ_0. Each possible type of reduced translational symmetry implies a different reciprocal lattice, and therefore has to be encoded explicitly in the recriprocal lattice

employed and considered separately. Solutions can be classified as insulating with a gap between occupied and empty states, or metallic with Fermi surfaces in the Brillouin-zone on which occupation numbers change.
At one electron per moir'e period, the paramagnetic state must be metallic, but all other states we consider can be insulating. We show typical Hartree-Fock self-consistent band structures for insulating and metallic magnetic ordered sates in Fig.~\ref{fig:hfbands}.
Completion
You will be instructed to simplify the Hartree term in $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})$ by reducing the momentum inside the expected value $\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')$.
The expected value $\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\delta_{\alpha,\beta}$.
You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i. Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation.
You should follow the EXAMPLE below to reduce one momentum in the Hartree term, and another momentum in the quadratic term.
Return the final simplified Hartree term $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})$.

11 Identify order parameters in Fock term (extended BZ)

Prompt
I will provide you a Excerpt of physics paper, and a Template. You will need to fill the placeholders in the template using the correct information from the excerpt. Here are conventions:
{..} means a placeholder which you need to fill by extracting information from the excerpt.
{A|B} means you need to make a choice between A and B
[..] means optional sentence. You should decide whether to use it depending on the excerpt.
{{..}} DOES NOT mean a placeholder. You should not change the content inside double curly braces {{..}}.
'You should recall that {..}.' : this sentence should be kept as is.
Finally, if you cannot figure out the placeholder, you should leave it as is.
Template:
You will be instructed to simplify the Fock term in {Fock_second_quantized_symbol} by reducing the momentum inside the expected value {expected_value}.
The expected value {expected_value} is only nonzero when the two momenta k_i, k_j are the same, namely, {expected_value_nonzero}.
You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i.
Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term.
Return the final simplified Fock term {Fock_second_quantized_symbol}.
Excerpt:
single Slater determinant ground state. Minimizing the energy functional with respect to single-particle wave-functions yields a mean-field Hamiltonian that adds an interaction self-energy Σ^{HF} to the single-particle Hamiltonian which can be expressed in terms of the single-particle density matrix $\rho=\sum_n |\psi_n\rangle\langle\psi_n|$, where the sum is over occupied moir'e-band Bloch wavefunctions. The mean-field electronic structure of moir'e superlattices is best evaluated using a plane-wave representation in which the Hartree-Fock self energy Σ^{HF} at each $\mathbf{k}$ in the Brillouin-zone is a matrix in reciprocal lattice vectors $\mathbf{b}$: \begin{widetext}

$$\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k}) = \frac{\delta_{\alpha,\beta}}{A}\sum_{\alpha'} V_{\alpha'\alpha}(\mathbf{b}'-\mathbf{b})\sum_{\mathbf{k}',\mathbf{b}''}\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}') - \frac{1}{A}\sum_{\mathbf{b}'',\mathbf{k}'} V_{\alpha\beta}(\mathbf{b}''+\mathbf{k}'-\mathbf{k})\rho_{\alpha,\mathbf{b}+\mathbf{b}'';\beta,\mathbf{b}'+\mathbf{b}''}(\mathbf{k}').$$

\end{widetext} In Eq.~\ref{eq:self-energy} Greek letters label spin, A is the finite sample area corresponding to a discrete Brillouin-zone mesh, and $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$ is the self-consistently determined momentum-space density matrix. Starting with a physically plausible density matrix ρ_0, we minimize the energy by performing self-consistent iterations. Because the many-body interaction is invariant under both translations and spin-rotations, if we start from a density matrix ρ_0 which satisfies a symmetry $\hat{O}$ of H_0 ($[\rho_0,\hat{O}]=0$, $[H_0,\hat{O}]=0$) then the symmetry survives under iteration.
That is to say that H^{HF} commutes with $\hat{O}$ at every iteration step. In many-cases the minimum energy Hartree-Fock state breaks symmetries of H_0 and these solutions are found under iteration

only by starting with a broken-symmetry density-matrix. As argued in Sec.~\ref{sec:lim}, the phase diagram contains paramagnetic states that do not break any symmetries, ferromagnetic states with spontaneous collinear spin-polarization that do not break lattice translational symmetries, stripe states with collinear order and a doubled unit cell area, and 120° N'eel states with both a tripled unit cell area and and non-collinear spin-order. We obtain solutions of the first two kinds by appropriate choices of the initial density ρ_0. Each possible type of reduced translational symmetry implies a different reciprocal lattice, and therefore has to be encoded explicitly in the recriprocal lattice employed and considered separately. Solutions can be classified as insulating with a gap between occupied and empty states, or metallic with Fermi surfaces in the Brillouin-zone on which occupation numbers change.

At one electron per moir'e period, the paramagnetic state must be metallic, but all other states we consider can be insulating. We show typical Hartree-Fock self-consistent band structures for insulating and metallic magnetic ordered sates in Fig.~\ref{fig:hfbands}.

Completion

You will be instructed to simplify the Fock term in $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})$ by reducing the momentum inside the expected value $\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')$.

The expected value $\rho_{\alpha',\mathbf{b}+\mathbf{b}'';\alpha',\mathbf{b}'+\mathbf{b}''}(\mathbf{k}')$ is only nonzero when the two momenta k_i, k_j are the same, namely, $\rho_{\alpha,\mathbf{b};\beta,\mathbf{b}'}$.

You should use the property of Kronecker delta function δ_{k_i,k_j} to reduce one momentum k_i but not b_i.

Once you reduce one momentum inside the expected value $\langle\dots\rangle$. You will also notice the total momentum conservation will reduce another momentum in the quadratic term. Therefore, you should end up with only two momenta left in the summation. You should follow the EXAMPLE below to reduce one momentum in the Fock term, and another momentum in the quadratic term.

Return the final simplified Fock term $\Sigma^{HF}_{\alpha,\mathbf{b};\beta,\mathbf{b}'}(\mathbf{k})$.