

1 Identify kinetic term (lattice)

Prompt

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

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

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

Template:

You will be instructed to describe the kinetic term of Hamiltonian in {system} in the {real|momen-
tum} space in the {single-particle|second-quantized} form.

The degrees of freedom of the system are: {degrees_of_freedom}

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

Return the Kinetic Hamiltonian {kinetic_symbol}.

Use the following conventions for the symbols:

{definition_of_variables}

Excerpt:

$$H_{\text{TB}} = \sum_s \sum_{i,j} t_s(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s},$$

where $s = \uparrow, \downarrow$ represents spin \uparrow and \downarrow states associated respectively with $+K$ and $-K$ valleys, \mathbf{R}_i represents a site in the triangular lattice, and $c_{j,s}$ ($c_{j,s}^\dagger$) is electron annihilation (creation) operator. $t_s(\mathbf{R}_i - \mathbf{R}_j)$ is the hopping parameter, which is constrained by the following relations. (1) Hermiticity of Hamiltonian~\eqref{eq:tb} requires that $t_s(\mathbf{R}) = t_s^*(-\mathbf{R})$; (2) threefold rotational symmetry (C_3) requires that $t_s(\mathbf{R}) = t_s(\hat{\mathcal{R}}(2\pi/3)\mathbf{R})$, where $\hat{\mathcal{R}}(2\pi/3)$ is a $2\pi/3$ rotation matrix; (3) time-reversal symmetry (\mathcal{T}) requires that $t_s(\mathbf{R}) = t_{-s}^*(\mathbf{R})$. In Fig.~\ref{fig:lattice}, we use $|t_n|$ and ϕ_n^\uparrow to denote the magnitude and phase for {it representative} hopping parameters between n -th nearest neighbors in the spin \uparrow channel. Since all the hopping terms within the n -th hopping shell are related by the aforementioned three relations, they can be determined once $|t_n|$ and ϕ_n^\uparrow are determined.

$$H = \sum_s \sum_{i,j} t_s(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where the repulsion $U(\mathbf{R}_i - \mathbf{R}_j)$ between sites i and j is calculated by projecting the Coulomb repulsion $\tilde{U}(\mathbf{r}) = e^2/(\epsilon r)$ onto the Wannier states. Here ϵ is the effective background dielectric constant that can be controlled by the three-dimensional dielectric environment. We take ϵ as a free parameter in our theory since its precise value is tunable (and not always precisely known). Numerical values of U_0 (on site repulsion) and U_n ($n = 1, 2, 3$ for repulsion between n -th nearest neighbors) are presented in Fig.~\ref{fig:hopping}(b). For a typical value of ϵ about 10, the on-site interaction U_0 can be at least one order-of-magnitude greater than the hopping parameters for twist angle θ below 5° . Therefore, tWSe₂ provides a platform to simulate the generalized Hubbard model on a triangular lattice. Moreover, the hopping parameters can be {it in situ} controlled by an external displacement field. The effective interacting model is a generalized Hubbard model since both interaction and hopping in Eq.~\eqref{eq:hubbard} are not necessarily restricted to being on-site or nearest-neighbor, respectively as the whole many-body Hamiltonian matrix of Eq.~\eqref{eq:hubbard} can be calculated from our moir'e band calculations for a given ϵ .

Completion

You will be instructed to describe the kinetic term of Hamiltonian in a system with a triangular lattice in the real space in the second-quantized form.

The degrees of freedom of the system are: spin states associated with $+K$ and $-K$ valleys

The kinetic term is a tight-binding model composed of the following hopping process: between site i and site j with the amplitude $t_s(\mathbf{R}_i - \mathbf{R}_j)$ You should ensure the hermiticity of the Hamiltonian The summation should be taken over all spin states and all real space positions.

Return the Kinetic Hamiltonian H_{TB} .

Use the following conventions for the symbols:

\uparrow, \downarrow represents spin \uparrow and \downarrow states associated respectively with $+K$ and $-K$ valleys, \mathbf{R}_i represents a site in the triangular lattice, and $c_{j,s}$ ($c_{j,s}^\dagger$) is electron annihilation (creation) operator. $t_s(\mathbf{R}_i - \mathbf{R}_j)$ is the hopping parameter.

2 Identify interacting term (real space)

Prompt

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$[..]$ 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, $\{\text{second_int_symbol}\}$ in the real space in the second-quantized form.

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

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

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

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

Excerpt:

$$H = \sum_s \sum_{i,j} t_s(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where the repulsion $U(\mathbf{R}_i - \mathbf{R}_j)$ between sites i and j is calculated by projecting the Coulomb repulsion $\tilde{U}(\mathbf{r}) = e^2/(\epsilon r)$ onto the Wannier states. Here ϵ is the effective background dielectric constant that can be controlled by the three-dimensional dielectric environment. We take ϵ as a free parameter in our theory since its precise value is tunable (and not always precisely known). Numerical values of U_0 (on site repulsion) and U_n ($n = 1, 2, 3$ for repulsion between n -th nearest neighbors) are presented in Fig.~\ref{fig:hopping}(b). For a typical value of ϵ about 10, the on-site interaction U_0 can be at least one order-of-magnitude greater than the hopping parameters for twist angle θ below 5° . Therefore, tWSe₂ provides a platform to simulate the generalized Hubbard model on a triangular lattice. Moreover, the hopping parameters can be *in situ* controlled by an external displacement field. The effective interacting model is a generalized Hubbard model since both interaction and hopping in Eq.~\eqref{eq:hubbard} are not necessarily restricted to being on-site or nearest-neighbor, respectively as the whole many-body Hamiltonian matrix of Eq.~\eqref{eq:hubbard} can be calculated from our moir'e band calculations for a given ϵ .

Completion

You will be instructed to construct the interaction part of the Hamiltonian, $U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s}$ in the real space in the second-quantized form.

The interacting Hamiltonian has the same degrees of freedom as the kinetic Hamiltonian $\sum_s \sum_{i,j} t_s(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s}$.

The interaction is a density-density interaction composed of the following process: between sites i and j with the interaction strength $U(\mathbf{R}_i - \mathbf{R}_j)$. The summation should be taken over all s, s' and all real space positions.

Return the interaction term $U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s}$ in terms of $c_{i,s}^\dagger, c_{j,s'}^\dagger, c_{j,s'}, c_{i,s}$.

Use the following conventions for the symbols (You should also obey the conventions in all my previous prompts if you encounter undefined symbols. If you find it is never defined or has conflicts in the conventions, you should stop and let me know): t_s is the hopping parameter, $c_{i,s}^\dagger$ and $c_{j,s}$ are the creation and annihilation operators, respectively, $U(\mathbf{R}_i - \mathbf{R}_j)$ is the repulsion between sites i and j , and ϵ is the effective background dielectric constant.

3 Fourier transform noninteracting term to momentum space (lattice)

Prompt

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Template:

You will be instructed to convert the noninteracting Hamiltonian {nonint_symbol} in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to {real_creation_op} in the real space to the {momentum_creation_op} in the momentum space, which is defined as {definition_of_Fourier_Transformation}, where {real_variable} is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that hopping have no position dependence now.] Express the total noninteracting Hamiltonian {nonint_symbol} in terms of {momentum_creation_op}. Simplify any summation index if possible.

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

Excerpt:

$$H_{\text{TB}} = \sum_s \sum_{i,j} t_s(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s},$$

where $s = \uparrow, \downarrow$ represents spin \uparrow and \downarrow states associated respectively with $+K$ and $-K$ valleys, \mathbf{R}_i represents a site in the triangular lattice, and $c_{j,s}$ ($c_{j,s}^\dagger$) is electron annihilation (creation) operator. $t_s(\mathbf{R}_i - \mathbf{R}_j)$ is the hopping parameter, which is constrained by the following relations. (1) Hermiticity of Hamiltonian~\eqref{eq:tb} requires that $t_s(\mathbf{R}) = t_s^*(-\mathbf{R})$; (2) threefold rotational symmetry (C_3) requires that $t_s(\mathbf{R}) = t_s(\hat{R}(2\pi/3)\mathbf{R})$, where $\hat{R}(2\pi/3)$ is a $2\pi/3$ rotation matrix; (3) time-reversal symmetry (\mathcal{T}) requires that $t_s(\mathbf{R}) = t_{-s}^*(\mathbf{R})$. In Fig.~\ref{fig:lattice}, we use $|t_n|$ and ϕ_n^\uparrow to denote the magnitude and phase for \{it representative\} hopping parameters between n -th nearest neighbors in the spin \uparrow channel. Since all the hopping terms within the n -th hopping shell are related by the aforementioned three relations, they can be determined once $|t_n|$ and ϕ_n^\uparrow are determined.

Completion

You will be instructed to convert the noninteracting Hamiltonian {nonint_symbol} in the second quantized form from the basis in real space to the basis in momentum space. To do that, you should apply the Fourier transformation to {real_creation_op} in the real space to the {momentum_creation_op} in the momentum space, which is defined as {definition_of_Fourier_Transformation}, where {real_variable} is integrated over all sites in the entire real space. You should follow the EXAMPLE below to apply the Fourier transformation. [Note that hopping have no position dependence now.] Express the total noninteracting Hamiltonian {nonint_symbol} in terms of {momentum_creation_op}. Simplify any summation index if possible.

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

4 Fourier transform interacting term to momentum space (lattice)

Prompt

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Template:

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

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

Excerpt:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where the repulsion $U(\mathbf{R}_i - \mathbf{R}_j)$ between sites i and j is calculated by projecting the Coulomb repulsion $\tilde{U}(\mathbf{r}) = e^2/(\epsilon r)$ onto the Wannier states. Here ϵ is the effective background dielectric constant that can be controlled by the three-dimensional dielectric environment. We take ϵ as a free parameter in our theory since its precise value is tunable (and not always precisely known). Numerical values of U_0 (on site repulsion) and U_n ($n = 1, 2, 3$ for repulsion between n -th nearest neighbors) are presented in Fig.~\ref{fig:hopping}(b). For a typical value of ϵ about 10, the on-site interaction U_0 can be at least one order-of-magnitude greater than the hopping parameters for twist angle θ below 5° . Therefore, tWSe₂ provides a platform to simulate the generalized Hubbard model on a triangular lattice. Moreover, the hopping parameters can be {\it in situ} controlled by an external displacement field. The effective interacting model is a generalized Hubbard model since both interaction and hopping in Eq.~\ref{eq:hubbard} are not necessarily restricted to being on-site or nearest-neighbor, respectively as the whole many-body Hamiltonian matrix of Eq.~\ref{eq:hubbard} can be calculated from our moir'e band calculations for a given ϵ .

Completion

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

5 Wick's theorem expansion

Prompt

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Template:

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

You should use Wick's theorem to expand the four-fermion term in {second_int_symbol} into quadratic terms. You should strictly follow the EXAMPLE below to expand using Wick's theorem, select the correct EXAMPLE by noticing the order of four term product with and without \dagger , 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:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where the repulsion $U(\mathbf{R}_i - \mathbf{R}_j)$ between sites i and j is calculated by projecting the Coulomb repulsion $\tilde{U}(\mathbf{r}) = e^2/(\epsilon r)$ onto the Wannier states. Here ϵ is the effective background dielectric constant that can be controlled by the three-dimensional dielectric environment. We take ϵ as a free parameter in our theory since its precise value is tunable (and not always precisely known). Numerical values of U_0 (on site repulsion) and U_n ($n = 1, 2, 3$ for repulsion between n -th nearest neighbors) are presented in Fig.~\ref{fig:hopping}(b). For a typical value of ϵ about 10, the on-site interaction U_0 can be at least one order-of-magnitude greater than the hopping parameters for twist angle θ below 5° . Therefore, tWSe₂ provides a platform to simulate the generalized Hubbard model on a triangular lattice. Moreover, the hopping parameters can be {it in situ} controlled by an external displacement field. The effective interacting model is a generalized Hubbard model since both interaction and hopping in Eq.~\eqref{eq:hubbard} are not necessarily restricted to being on-site or nearest-neighbor, respectively as the whole many-body Hamiltonian matrix of Eq.~\eqref{eq:hubbard} can be calculated from our moir'e band calculations for a given ϵ .

Completion

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 \dagger , 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}

6 Drop constant terms

Prompt

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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:

$$H = \sum_s \sum_{i,j} t_s (\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\mathbf{R}_i - \mathbf{R}_j) c_{i,s}^\dagger c_{j,s'}^\dagger c_{j,s'} c_{i,s},$$

where the repulsion $U(\mathbf{R}_i - \mathbf{R}_j)$ between sites i and j is calculated by projecting the Coulomb repulsion $\tilde{U}(\mathbf{r}) = e^2/(\epsilon r)$ onto the Wannier states. Here ϵ is the effective background dielectric constant that can be controlled by the three-dimensional dielectric environment. We take ϵ as a free parameter in our theory since its precise value is tunable (and not always precisely known). Numerical values of U_0 (on site repulsion) and U_n ($n = 1, 2, 3$ for repulsion between n -th nearest neighbors) are presented in Fig.~\ref{fig:hopping}(b). For a typical value of ϵ about 10, the on-site interaction U_0 can be at least one order-of-magnitude greater than the hopping parameters for twist angle θ below 5° . Therefore, tWSe₂ provides a platform to simulate the generalized Hubbard model on a triangular lattice. Moreover, the hopping parameters can be {it in situ} controlled by an external displacement field. The effective interacting model is a generalized Hubbard model since both interaction and hopping in Eq.~\eqref{eq:hubbard} are not necessarily restricted to being on-site or nearest-neighbor, respectively as the whole many-body Hamiltonian matrix of Eq.~\eqref{eq:hubbard} can be calculated from our moir'e band calculations for a given ϵ .

Completion

In this paper, we will be focusing on the Hartree-Fock term, denoted as H. The quadratic terms refer to terms that are proportional to the bilinear operator, denoted as B. These terms exclude those that are solely expectations or products of expectations. We will only preserve the quadratic terms in H, which we will denote as H'.

The following conventions for the symbols are used: H represents the Hartree-Fock term, B represents the bilinear operator, and H' represents the Hartree-Fock term with only the quadratic terms preserved.

Template:

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

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

You should only preserve the quadratic terms in {H}, denoted as {H'}.

Return {H'}.

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 represents the Hartree-Fock term, B represents the bilinear operator, and H' represents the Hartree-Fock term with only the quadratic terms preserved.