

1 Identify kinetic term (continuum,first-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:

{..} 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 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}.

Express the Kinetic Hamiltonian {kinetic_symbol} using {variable} which are only on the diagonal terms, and arrange the basis in the order of {order}. [Note that the sublattice degrees of freedom is suppressed for now and will be stated later]

Use the following conventions for the symbols:

{definition_of_variables}

Excerpt:

lattice model Hamiltonian with one atomic $2p_z$ orbital per carbon site. We label the six sublattice sites illustrated in Fig. 1(a) {\em A}, {\em B}, A' , B' , A'' , B'' ; the A and B'' sites avoid near-neighbor inter-layer coupling and for this reason are {\em low-energy sites} which are dominantly occupied by electrons close to the band crossing points.

With this convention, the six band tight-binding model Hamiltonian of ABC trilayer graphene is: $\$ \{H\} = - \begin{pmatrix} 0 & \gamma_0 f & 0 \\ \gamma_3 f^* & 0 & \gamma_2 \\ \gamma_1 & 0 & 0 \end{pmatrix}$

$$\gamma_3 f^* + \gamma_N \quad 0 \quad \gamma_2$$

$$\gamma_0 f^* + \gamma_1 \gamma_4 f$$

$$0 + \gamma_4 f^* + \gamma_1 \gamma_0 f + \gamma_4 f$$

$$\gamma_3 f^* + \gamma_3 f + \gamma_N^* + \gamma_4 f^*$$

$$\gamma_0 f^* + \gamma_1 \gamma_0 + \gamma_4 f^*$$

$$\gamma_1 \gamma_0 f + \gamma_2 \gamma_0 + \gamma_3 f + \gamma_0 f^* + \end{pmatrix}$$

where

$$f(\mathbf{k}) = e^{i \mathbf{k} \cdot \mathbf{a} / \sqrt{3}} \left(1 + 2 e^{-i \mathbf{k} \cdot \mathbf{a} / \sqrt{3}} \right)$$

$$\cos \left(\frac{k_x a}{2} \right)$$

with $a = 2.46$ using the same triangular lattice vector convention as in Ref. [onlinecite{dirachf,jeilbilayer}]. The global minus sign in front of the Hamiltonian means that π -bonding bands have lower energy than anti-bonding bands when the γ parameters are positive.

In most of our calculations we have used graphite hopping parameter values which are similar to those in Ref. [onlinecite{partoens}] : $\gamma_0 = 3.12$ eV, $\gamma_1 = 0.377$ eV, $\gamma_2 = 0.01$ eV, $\gamma_3 = 0.3$ eV. We specifically address the importance of the signs of the remote γ_2 and γ_3 hopping parameters.

The near-neighbor intralayer and interlayer hopping processes γ_0 and γ_1 are responsible for broad features of the band structure, while the γ_2 and γ_3 parameters have their main impact close to the band-crossing points.

This model qualitatively reproduces the {\em ab initio} band structure in Ref. [onlinecite{latil}], in particular capturing the orientation of the triangle formed by the three band-crossing points close to the Brillouin-zone corner. We have ignored the ABC trilayer γ_4 and γ_5 processes that break particle-hole symmetry, and other small onsite terms that are often introduced in models of graphite, because they do not visibly alter the low energy features of the bands in ABC trilayer graphene.

Using a model similar to that used previously for bilayer graphene, [cite{youngwoo,kruczynski}], we have also examined the influence of a term in the Hamiltonian that is intended to capture the influence on low-energy states of an interlayer relative-translation strain.

We write $\gamma_N = \gamma_N^0 \exp(-|\mathbf{k} - \mathbf{K}^{(l)}|/k_r)$, introducing a damping factor which makes the term small away from the Brillouin-zone corners, where this form for the strain Hamiltonian becomes inaccurate, by setting

$$k_r = \gamma_1 / \hbar v_F = 0.0573^{-1}.$$

Completion

You will be instructed to describe the kinetic term of Hamiltonian in ABC trilayer graphene in the real space in the second-quantized form.

The degrees of freedom of the system are: six sublattice sites labeled as A, B, A', B', A'', B''.

Express the Kinetic Hamiltonian H_0 using variables $\gamma_0, \gamma_1, \gamma_2, \gamma_3, \gamma_N, f$ which are only on the diagonal terms, and arrange the basis in the order of A, B, A', B', A'', B''. [Note that the sublattice degrees of freedom is suppressed for now and will be stated later]

Use the following conventions for the symbols:

$f(\mathbf{k}) = e^{i \mathbf{k}_y a / \sqrt{3}} * (1 + 2 e^{-i 3 k_y a / 2\sqrt{3}} * \cos(k_x a / 2))$, where $a = 2.46 \text{ \AA}$.

$\gamma_0 = 3.12 \text{ eV}$, $\gamma_1 = 0.377 \text{ eV}$, $\gamma_2 = 0.01 \text{ eV}$, $\gamma_3 = 0.3 \text{ eV}$.

$\gamma_N = \gamma_N^0 * \exp(-|k - K'| / kr)$, where $kr = \gamma_1 / \hbar v_F = 0.0573 \text{ \AA}^{-1}$.

2 Define energy dispersion (continuum)

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 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:

lattice model Hamiltonian with one atomic $2p_z$ orbital per carbon site. We label the six sublattice sites illustrated in Fig. 1(a) {A}, {B}, A', B', A'', B''; the A and B'' sites avoid near-neighbor inter-layer coupling and for this reason are {low-energy sites} which are dominantly occupied by electrons close to the band crossing points.

With this convention, the six band tight-binding model Hamiltonian of ABC trilayer graphene is: \$\$

\label{hamil} {H} = - \begin{pmatrix} 0 & \gamma_0 f & 0 & \gamma_4 f \\

& \gamma_3 f^* + \gamma_N & 0 & \gamma_2 \\

\gamma_0 f^* & 0 & \gamma_1 & \gamma_4 f \\

& 0 & 0 & \gamma_4 f^* & 0 & \gamma_1 & 0 & \gamma_0 f & 0 & \gamma_4 f \\

& \gamma_3 f^* & \gamma_3 f + \gamma_N^* & 0 & \gamma_4 f^* \\

& \gamma_0 f^* & 0 & \gamma_1 & 0 & 0 & 0 & 0 & \gamma_4 f^* \\

& \gamma_1 & 0 & \gamma_0 f & \gamma_2 & 0 & \gamma_3 f & 0 & \gamma_0 f^* & 0 \end{pmatrix}

where

\begin{aligned} f(\mathbf{k}) &= e^{i \mathbf{k}_y a / \sqrt{3}} \left(1 + 2 e^{-i 3 k_y a / 2\sqrt{3}} \right. \\

& \left. \cos \left(\frac{k_x a}{2} \right) \right)

$\end{aligned}$$ with $a = 2.46$ using the same triangular lattice vector convention as in Ref. [dirachf,jeilbilayer]. The global minus sign in front of the Hamiltonian means that π -bonding bands have lower energy than anti-bonding bands when the γ parameters are positive.$

In most of our calculations we have used graphite hopping parameter values which are similar to those in Ref. [partoens] : $\gamma_0 = 3.12$ eV, $\gamma_1 = 0.377$ eV, $\gamma_2 = 0.01$ eV, $\gamma_3 = 0.3$ eV. We specifically address the importance of the signs of the remote γ_2 and γ_3 hopping parameters.

The near-neighbor intralayer and interlayer hopping processes γ_0 and γ_1 are responsible for broad features of the band structure, while the γ_2 and γ_3 parameters have their main impact close to the band-crossing points.

This model qualitatively reproduces the *ab initio* band structure in Ref. [latil], in particular capturing the orientation of the triangle formed by the three band-crossing points close to the Brillouin-zone corner. We have ignored the ABC trilayer γ_4 and γ_5 processes that break particle-hole symmetry, and other small onsite terms that are often introduced in models of graphite, because they do not visibly alter the low energy features of the bands in ABC trilayer graphene.

Using a model similar to that used previously for bilayer graphene, [youngwoo,kruczynski]. we have also examined the influence of a term in the Hamiltonian that is intended to capture the influence on low-energy states of an interlayer relative-translation strain.

We write $\gamma_N = \gamma_N^0 \exp(-|\mathbf{k} - \mathbf{K}^{(i)}|/k_r)$, introducing a damping factor which makes the term small away from the Brillouin-zone corners, where this form for the strain Hamiltonian becomes inaccurate, by setting

$$k_r = \gamma_1/\hbar v_F = 0.0573^{-1}.$$

Completion

Template:

You will be instructed to construct each term, namely $\{H\}_0$.

For all energy dispersions, $\{H\}_0$, it characterizes the $\{\text{Dirac}\}$ dispersion for $\{\text{electrons}\}$.

[In addition, a shift of $\{k_r\}$ in the momentum $\{k\}$ for $\{f(k)\}$, 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 $\{H\}_0$ 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):

$$\{f(\mathbf{k})\} \equiv e^{i \mathbf{k} \cdot \mathbf{a} / \sqrt{3}} \left(1 + 2 e^{-i 3 \mathbf{k} \cdot \mathbf{a} / 2\sqrt{3}} \right)$$

$$\cos \left(\frac{k_x a}{2} \right)$$

$\end{aligned}$$ with $a = 2.46$ using the same triangular lattice vector convention as in Ref. [dirachf,jeilbilayer]. The global minus sign in front of the Hamiltonian means that π -bonding bands have lower energy than anti-bonding bands when the γ parameters are positive.$

In most of our calculations we have used graphite hopping parameter values which are similar to those in Ref. [partoens] : $\gamma_0 = 3.12$ eV, $\gamma_1 = 0.377$ eV, $\gamma_2 = 0.01$ eV, $\gamma_3 = 0.3$ eV. We specifically address the importance of the signs of the remote γ_2 and γ_3 hopping parameters.

The near-neighbor intralayer and interlayer hopping processes γ_0 and γ_1 are responsible for broad features of the band structure, while the γ_2 and γ_3 parameters have their main impact close to the band-crossing points.

This model qualitatively reproduces the *ab initio* band structure in Ref. [latil], in particular capturing the orientation of the triangle formed by the three band-crossing points close to the Brillouin-zone corner. We have ignored the ABC trilayer γ_4 and γ_5 processes that break particle-hole symmetry, and other small onsite terms that are often introduced in models of graphite, because they do not visibly alter the low energy features of the bands in ABC trilayer graphene.

Using a model similar to that used previously for bilayer graphene, [youngwoo,kruczynski]. we have also examined the influence of a term in the Hamiltonian that is intended to capture the influence on low-energy states of an interlayer relative-translation strain.

We write $\gamma_N = \gamma_N^0 \exp(-|\mathbf{k} - \mathbf{K}^{(i)}|/k_r)$, introducing a damping factor which makes the term small away from the Brillouin-zone corners, where this form for the strain Hamiltonian becomes inaccurate, by setting

$$k_r = \gamma_1/\hbar v_F = 0.0573^{-1}.$$

3 Second-quantization (matrix)

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 second quantized form of the total noninteracting Hamiltonian in the {real|momentum} space.

The noninteracting Hamiltonian in the {real|momentum} space {nonint_symbol} is the sum of Kinetic Hamiltonian {kinetic_symbol} and Potential Hamiltonian {potential_symbol}.

To construct the second quantized form of a Hamiltonian. You should construct the creation and annihilation operators from the basis explicitly. You should follow the EXAMPLE below to convert a Hamiltonian from the single-particle form to second-quantized form.

Finally by "total", it means you need to take a summation over the {real|momentum} space position {r|k}.

Return the second quantized form of the total noninteracting Hamiltonian {second_nonint_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:

lattice model Hamiltonian with one atomic $2p_z$ orbital per carbon site. We label the six sublattice sites illustrated in Fig. 1(a) {em A}, {em B}, A' , B' , A'' , B'' ; the A and B'' sites avoid near-neighbor inter-layer coupling and for this reason are {em low-energy sites} which are dominantly occupied by electrons close to the band crossing points.

With this convention, the six band tight-binding model Hamiltonian of ABC trilayer graphene is: \$\$

\label{hamil} \{H\}0= - \begin{pmatrix} 0 & \gamma_0 f & 0 \\ \gamma_4 f & 0 & \gamma_4 f \\ \gamma_3 f^* & \gamma_3 f & 0 \end{pmatrix}

& \gamma_3 f^* + \gamma_N & 0 & \gamma_2 & \\

\gamma_0 f^* & 0 & \gamma_1 & \gamma_4 f \\

& 0 & 0 & \gamma_4 f^* & 0 & \gamma_1 & 0 & \gamma_0 f & 0 \\

& \gamma_3 f^* & \gamma_3 f & + \gamma_N^* & 0 \\

& \gamma_0 f^* & 0 & \gamma_1 & 0 & 0 & 0 & \gamma_4 f^* \\

& \gamma_1 & 0 & \gamma_0 f & \gamma_2 & 0 & \gamma_3 f & 0 & \gamma_0 f^* & 0 \end{pmatrix}

where

\begin{aligned} f \left(\bm{k} \right) &= e^{i k_y a / \sqrt{3}} \left(1 + 2 e^{-i 3 k_y a / 2\sqrt{3}} \right) \end{aligned}

\cos \left(\frac{k_x a}{2} \right)

with $a = 2.46$ using the same triangular lattice vector convention as in Ref. [onlinecite{dirachf,jeilbilayer}]. The global minus sign in front of the Hamiltonian means that π -bonding bands have lower energy than anti-bonding bands when the γ parameters are positive.

In most of our calculations we have used graphite hopping parameter values which are similar to those in Ref. [onlinecite{partoens}] : $\gamma_0 = 3.12$ eV, $\gamma_1 = 0.377$ eV, $\gamma_2 = 0.01$ eV, $\gamma_3 = 0.3$ eV. We specifically address the importance of the signs of the remote γ_2 and γ_3 hopping parameters.

The near-neighbor intralayer and interlayer hopping processes γ_0 and γ_1 are responsible for broad features of the band structure, while the γ_2 and γ_3 parameters have their main impact close to the band-crossing points.

This model qualitatively reproduces the {em ab initio} band structure in Ref. [onlinecite{latil}], in particular capturing the orientation of the triangle formed by the three band-crossing points close to the Brillouin-zone corner. We have ignored the ABC trilayer γ_4 and γ_5 processes that break particle-hole symmetry, and other small onsite terms that are often introduced in models of graphite, because they do not visibly alter the low energy features of the bands in ABC trilayer graphene.

Using a model similar to that used previously for bilayer graphene,\cite{youngwoo,kruczynski}. we have also examined the influence of a term in the Hamiltonian that is intended to capture the influence on low-energy states of an interlayer relative-translation strain.

We write $\gamma_N = \gamma_N^0 \exp(-|\mathbf{k} - \mathbf{K}^{(i)}|/k_r)$, introducing a damping factor which makes the term small away from the Brillouin-zone corners, where this form for the strain Hamiltonian becomes inaccurate, by setting

$$k_r = \gamma_1/\hbar v_F = 0.0573^{-1}.$$

Completion

You will be instructed to construct the second quantized form of the total noninteracting Hamiltonian in the momentum space.

The noninteracting Hamiltonian in the momentum space H_0 is the sum of Kinetic Hamiltonian and Potential Hamiltonian.

To construct the second quantized form of a Hamiltonian. You should construct the creation and annihilation operators from the basis explicitly. You should follow the EXAMPLE below to convert a Hamiltonian from the single-particle form to second-quantized form.

Finally by "total", it means you need to take a summation over the momentum space position k .

Return the second quantized form of the total noninteracting Hamiltonian.

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):

$$\psi(\mathbf{k}) = e^{i\mathbf{k} \cdot \mathbf{a} / \sqrt{3}} \sqrt{1 + 2e^{-i3\mathbf{k} \cdot \mathbf{a} / 2\sqrt{3}}}$$

$$\cos\left(\frac{k_x a}{2}\right) \quad \text{right)}, \text{ where } a = 2.46 \text{ \AA}.$$

$$\gamma_0 = 3.12 \text{ eV}, \gamma_1 = 0.377 \text{ eV}, \gamma_2 = 0.01 \text{ eV}, \gamma_3 = 0.3 \text{ eV}. \gamma_N = \gamma_N^0 \exp(-|\mathbf{k} - \mathbf{K}^{(i)}|/k_r), \text{ where } k_r = \gamma_1/\hbar v_F = 0.0573^{-1}.$$

4 Second-quantization (summation)

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 expand the second-quantized form Hamiltonian {second_nonint_symbol} using {matrix_element_symbol} and {basis_symbol}. You should follow the EXAMPLE below to expand the Hamiltonian.

You should use any previous knowledge to simplify it. For example, if any term of {matrix_element_symbol} is zero, you should remove it from the summation. Return the expanded form of {second_nonint_symbol} after simplification.

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

{definition_of_variables}

Excerpt:

lattice model Hamiltonian with one atomic $2p_z$ orbital per carbon site. We label the six sublattice sites illustrated in Fig. 1(a) {em A}, {em B}, A' , B' , A'' , B'' ; the A and B'' sites avoid near-neighbor inter-layer coupling and for this reason are {em low-energy sites} which are dominantly occupied by electrons close to the band crossing points.

With this convention, the six band tight-binding model Hamiltonian of ABC trilayer graphene is:
$$\text{\label{hamil}} \begin{pmatrix} H & 0 & \gamma_0 f & 0 & \gamma_2 & 0 \\ \gamma_0 f^* & 0 & \gamma_1 & \gamma_4 f & 0 & 0 \\ \gamma_3 f^* & \gamma_3 f & \gamma_4 N^* & 0 & \gamma_4 f^* & 0 \\ \gamma_0 f^* & 0 & \gamma_1 & 0 & 0 & 0 \\ \gamma_1 & 0 & \gamma_0 f & \gamma_2 & 0 & \gamma_3 f \\ 0 & \gamma_0 f^* & 0 & 0 & \gamma_3 f^* & 0 \end{pmatrix}$$

$$\gamma_3 f^* + \gamma_N \quad 0 \quad \gamma_2 \quad \backslash$$

$$\gamma_0 f^* \quad 0 \quad \gamma_1 \quad \gamma_4 f$$

$$0 \quad 0 \quad \gamma_4 f^* \quad 0 \quad \gamma_1 \quad 0 \quad \gamma_0 f \quad 0 \quad \gamma_4 f$$

$$\gamma_3 f^* \quad \gamma_3 f + \gamma_4 N^* \quad 0 \quad \gamma_4 f^*$$

$$\gamma_0 f^* \quad 0 \quad \gamma_1 \quad 0 \quad 0 \quad 0 \quad \gamma_4 f^*$$

$$\gamma_1 \quad 0 \quad \gamma_0 f \quad \gamma_2 \quad 0 \quad \gamma_3 f \quad 0 \quad \gamma_0 f^* \quad 0 \quad \text{\end{pmatrix}}$$

where

$f(\mathbf{k}) = e^{i \mathbf{k} \cdot \mathbf{a} / \sqrt{3}} \left(1 + 2 e^{-i 3 \mathbf{k} \cdot \mathbf{a} / 2\sqrt{3}} \right)$

$$\cos \left(\frac{k_x a}{2} \right) \right)$$

with $a = 2.46$ using the same triangular lattice vector convention as in Ref. [dirachf,jeilbilayer]. The global minus sign in front of the Hamiltonian means that π -bonding bands have lower energy than anti-bonding bands when the γ parameters are positive.

In most of our calculations we have used graphite hopping parameter values which are similar to those in Ref. [partoens] : $\gamma_0 = 3.12$ eV, $\gamma_1 = 0.377$ eV, $\gamma_2 = 0.01$ eV, $\gamma_3 = 0.3$ eV. We specifically address the importance of the signs of the remote γ_2 and γ_3 hopping parameters.

The near-neighbor intralayer and interlayer hopping processes γ_0 and γ_1 are responsible for broad features of the band structure, while the γ_2 and γ_3 parameters have their main impact close to the band-crossing points.

This model qualitatively reproduces the *ab initio* band structure in Ref. [latil], in particular capturing the orientation of the triangle formed by the three band-crossing points close to the Brillouin-zone corner. We have ignored the ABC trilayer γ_4 and γ_5 processes that break particle-hole symmetry, and other small onsite terms that are often introduced in models of graphite, because they do not visibly alter the low energy features of the bands in ABC trilayer graphene.

Using a model similar to that used previously for bilayer graphene, [cite{youngwoo,kruczynski}], we have also examined the influence of a term in the Hamiltonian that is intended to capture the influence on low-energy states of an interlayer relative-translation strain.

We write $\gamma_N = \gamma_N^0 \exp(-|\mathbf{k} - \mathbf{K}^{(l)}|/k_r)$, introducing a damping factor which makes the term small away from the Brillouin-zone corners, where this form for the strain Hamiltonian becomes inaccurate, by setting

$$k_r = \gamma_1 / \hbar v_F = 0.0573^{-1}.$$

Completion

You will be instructed to expand the second-quantized form Hamiltonian H_0 using γ and f as matrix elements and basis respectively. You should follow the EXAMPLE below to expand the Hamiltonian. You should use any previous knowledge to simplify it. For example, if any term of γ is zero, you should remove it from the summation. Return the expanded form of H_0 after simplification.

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

$$f(\mathbf{k}) = e^{i \mathbf{k} \cdot \mathbf{a} / \sqrt{3}} \left(1 + 2 e^{-i 3 \mathbf{k} \cdot \mathbf{a} / 2\sqrt{3}} \right)$$

$$\cos \left(\frac{k_x a}{2} \right) \right), \text{ where } a = 2.46 \text{ \AA}.$$

$$\gamma_0 = 3.12 \text{ eV}, \gamma_1 = 0.377 \text{ eV}, \gamma_2 = 0.01 \text{ eV}, \gamma_3 = 0.3 \text{ eV}. \gamma_N = \gamma_N^0 \exp(-|\mathbf{k} - \mathbf{K}^{(l)}|/k_r), \text{ where } k_r = \gamma_1 / \hbar v_F = 0.0573^{-1}.$$

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 $V(q) = \text{int_form}$, 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:

which allows symmetries to be broken:

$$V_{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} \left[\sum_{\mathbf{k}'} \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \right\rangle \right] c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda}$$

$$\% - \sum_{\mathbf{k}'\lambda\lambda'} U_X^{\lambda\lambda'} (\mathbf{k}' - \mathbf{k}) \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \right\rangle c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where $c_{\mathbf{k}\lambda}^\dagger$, $c_{\mathbf{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgen}), $\begin{aligned} U_H^{\lambda\lambda'} &= \frac{1}{A} \sum_{\mathbf{G}} e^{i \mathbf{G} \cdot \left(\mathbf{s}_l - \mathbf{s}_{l'} \right)} \left| \widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{G} \right| \right) \right|^2 \\ , \quad U_X^{\lambda\lambda'} &= \frac{1}{A} \sum_{\mathbf{G}} ; e^{i \mathbf{G} \cdot \left(\mathbf{s}_l - \mathbf{s}_{l'} \right)} \left| \widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{G} \right| - \left| \mathbf{q} \right| \right) \right|^2 \end{aligned}$ involve sums over reciprocal lattice vectors \mathbf{G} . In these equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

Completion

You will be instructed to construct the interaction part of the Hamiltonian V_{HF} 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 λ and λ' , and 1, 2, 3, 4 for the \mathbf{k} . The second part is the constraint of total momentum conservation, namely the total momentum of all creation operators should be the same as that of all annihilation operators. The third part is the interaction form. You should use $U_H^{\lambda\lambda'}$ and $U_X^{\lambda\lambda'}$ with $V(q) = U_H^{ll'}$ and $U_X^{ll'}(q)$, where q is the transferred total momentum between a creation operator and an annihilation operator with the same λ , namely $q = \mathbf{k}' - \mathbf{k}$.

The fourth part is the normalization factor, you should use $\frac{1}{A}$ here. Finally, the summation should be running over all λ and \mathbf{k} Return the interaction term V_{HF} in terms of $c_{\mathbf{k}\lambda}^\dagger$, $c_{\mathbf{k}\lambda}$ and $V(q)$ (with q expressed in terms of \mathbf{k}).

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):

$c_{\mathbf{k}\lambda}^\dagger$, $c_{\mathbf{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgen}), $U_H^{ll'}$ and $U_X^{ll'}(q)$ involve sums over reciprocal lattice vectors \mathbf{G} . In these equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

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:

{..} 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 {{..}}.

which allows symmetries to be broken:

$$V_{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} \left[\sum_{\mathbf{k}'} \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda'} \right\rangle \right] c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda} \\ \% - \sum_{\mathbf{k}'\lambda\lambda'} U_X^{\lambda\lambda'} (\mathbf{k}' - \mathbf{k}) \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \right\rangle c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where $c_{k\lambda}^\dagger$, $c_{k\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgn}),
$$\begin{aligned} U_{\mathbf{l} \mathbf{l}'}^{\prime} &= \frac{1}{A} \sum_{\mathbf{G}} e^{i \sum_{\mathbf{G}} \mathbf{G} \cdot \left(\sum_{\mathbf{s}} \mathbf{s} - \sum_{\mathbf{s}'} \mathbf{s}' \right)} \left| \widetilde{V}^{\mathbf{l} \mathbf{l}'} \right| \left(\left| \mathbf{G} \right| \right) \left| \widetilde{V}^{\mathbf{l} \mathbf{l}'} \right| \left(\left| \mathbf{G} \right| \right) \quad \text{label{mom1}} \\ &= \frac{1}{A} \sum_{\mathbf{G}} e^{i \sum_{\mathbf{G}} \mathbf{G} \cdot \left(\sum_{\mathbf{s}} \mathbf{s} - \sum_{\mathbf{s}'} \mathbf{s}' \right)} \left| \widetilde{V}^{\mathbf{l} \mathbf{l}'} \right| \left(\left| \mathbf{q} - \mathbf{G} \right| \right) \left| \widetilde{V}^{\mathbf{l} \mathbf{l}'} \right| \left(\left| \mathbf{q} - \mathbf{G} \right| \right), \quad \text{label{mom2}} \end{aligned}$$
 involve sums over reciprocal lattice vectors \mathbf{G} . In these equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

$c_{\mathbf{k}\lambda}^\dagger$, $c_{\mathbf{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hngen}), $U_H^{ll'}$ and $U_X^{ll'}(\mathbf{q})$ involve sums over reciprocal lattice vectors \mathbf{G} . In these equations s_l is the (2D) projection of the position of the sublattice in the unit cell.

[..] 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:

which allows symmetries to be broken:

$$V_{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} \left[\sum_{\mathbf{k}'} \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda'} \right\rangle \right] c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda}$$

$$\% - \sum_{\mathbf{k}'\lambda\lambda'} U_X^{\lambda\lambda'} (\mathbf{k}' - \mathbf{k}) \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \right\rangle c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where $c_{\mathbf{k}\lambda}^\dagger$, $c_{\mathbf{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgen}),
$$U_H^{\lambda\lambda'} = \frac{1}{A} \sum_{\mathbf{G}} e^{i \mathbf{G} \cdot \left(\mathbf{r}_s - \mathbf{r}_{s'} \right)} \left| \widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{G} \right| \right) \right|^2$$
 „ $\widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right) = U_X^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right) \left(\left| \mathbf{q} \right| - \left| \mathbf{G} \right| \right)$ \quad \quad \quad \label{mom2}

involve sums over reciprocal lattice vectors \mathbf{G} . In these equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

Completion

You will be instructed to extract the quadratic terms in the Hartree-Fock term, denoted as V_{HF} .

The quadratic terms mean terms that are proportional to $c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda}$ and $c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$, which excludes terms that are solely expectations or products of expectations.

You should only preserve the quadratic terms in V_{HF} , denoted as $V_{HF}^{(2)}$.

Return $V_{HF}^{(2)}$.

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):

$c_{\mathbf{k}\lambda}^\dagger$ and $c_{\mathbf{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgen}), denoted as $U_H^{ll'}$ and $U_X^{ll'}(\mathbf{q})$, involve sums over reciprocal lattice vectors \mathbf{G} . In these equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

8 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:

`{{..}}` 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:

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:

which allows symmetries to be broken:

$$V_{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} \left[\sum_{\mathbf{k}'} \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda'} \right\rangle \right] c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda}$$

$$\% - \sum_{\mathbf{k}'\lambda\lambda'} U_X^{\lambda\lambda'} (\mathbf{k}' - \mathbf{k}) \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \right\rangle c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where $c_{\mathbf{k}\lambda}^\dagger, c_{\mathbf{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgn}),
$$U_H^{\lambda\lambda'} = \frac{1}{A} \sum_{\mathbf{G}} e^{i \mathbf{G} \cdot \left(\mathbf{s}_l - \mathbf{s}_{l'} \right)} \left| \widetilde{f} \left(\left| \mathbf{G} \right| \right) \right|^2$$
 „ $\widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right) \left| \widetilde{f} \left(\left| \mathbf{q} - \mathbf{G} \right| \right) \right|^2$ „ $\widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right)$,
$$U_X^{\lambda\lambda'} = \frac{1}{A} \sum_{\mathbf{G}} e^{i \mathbf{G} \cdot \left(\mathbf{s}_l - \mathbf{s}_{l'} \right)} \left| \widetilde{f} \left(\left| \mathbf{q} - \mathbf{G} \right| \right) \right|^2$$
 „ $\widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right)$,
$$\widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right) \left| \widetilde{f} \left(\left| \mathbf{q} - \mathbf{G} \right| \right) \right|^2$$
 „ $\widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right)$,
$$\widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right) \left| \widetilde{f} \left(\left| \mathbf{q} - \mathbf{G} \right| \right) \right|^2$$
 „ $\widetilde{V}^{\lambda\lambda'} \left(\left| \mathbf{q} \right| \right)$ involve sums over reciprocal lattice vectors \mathbf{G} . In these equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

Completion

You will be instructed to simplify the Hartree term in V_{HF} by reducing the momentum inside the expected value $\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda'} \rangle$.

The expected value $\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda'} \rangle$ is only nonzero when the two momenta \mathbf{k}' are the same, namely, $\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda'} \rangle \neq 0$.

You should use the property of Kronecker delta function $\delta_{\mathbf{k}', \mathbf{k}'}$ to reduce one momentum \mathbf{k}' but not $c_{\mathbf{k}'\lambda'}$. Once you reduce one momentum inside the expected value $\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda'} \rangle$. 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 V_{HF} .

10 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 .

$$V_{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} \left[\sum_{\mathbf{k}'} \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda'} \right\rangle \right] c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda}$$

$$\% - \sum_{\mathbf{k}'\lambda\lambda'} U_X^{\lambda\lambda'} (\mathbf{k}' - \mathbf{k}) \left\langle c_{\mathbf{k}'\lambda'}^\dagger c_{\mathbf{k}'\lambda} \right\rangle c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda'}$$

where $c_{\mathbf{k}\lambda}^\dagger$, $c_{\mathbf{k}\lambda}$ are Bloch state creation and annihilation operators, and $\lambda = (l, \sigma)$ lumps lattice and spin indices. The Hartree and Exchange Coulomb integrals in Eq.(~\ref{hfgen}),
$$\begin{aligned} U_H^{ll'} &= \frac{1}{A} \sum_{\mathbf{G}} e^{i \mathbf{G} \cdot (\mathbf{s}_l - \mathbf{s}_{l'})} \left| \widetilde{f}(\mathbf{G}) \right|^2 \\ U_X^{ll'} &= \frac{1}{A} \sum_{\mathbf{G}} e^{i \mathbf{G} \cdot (\mathbf{s}_l - \mathbf{s}_{l'})} \left| \widetilde{f}(\mathbf{q} - \mathbf{G}) \right|^2 \end{aligned}$$
 involve sums over reciprocal lattice vectors \mathbf{G} . In these equations s_l is the (2D projection of the) position of the sublattice in the unit cell.

Completion

You will now be instructed to combine the Hartree term $U_H^{\lambda\lambda'}$ and the Fock term $U_X^{\lambda\lambda'}$. You should perform the same trick of relabeling the index in the Fock term to make the quadratic operators in the Fock term the same as those in the Hartree term. The relabeling should be done with a swap : $\mathbf{k}'\lambda'$ with $\mathbf{k}\lambda$. You should add them, relabel the index in Fock term, and simply their sum. Return the final sum of Hartree and Fock term.