

1. Question:

For the following mean-field Hamiltonian, if we want to code and numerically solve the self-consistent equation, what is the dimension of the mean-field Hamiltonian matrix at a given momentum k ?

Consider the mean-field Hamiltonian: $H = H_{\text{Kinetic}} + H_{\text{Hartree}} + H_{\text{Fock}}$, with each term defined below:

$$H_{\text{Kinetic}} = \sum_{s,k} E_s(k) c_s^\dagger(k) c_s(k), \text{ where } E_s(k) = \sum_n t_s(n) e^{-ik \cdot n}$$

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(0) \langle c_s^\dagger(k_1) c_s(k_1) \rangle c_{s'}^\dagger(k_2) c_{s'}(k_2)$$

$$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(k_1 - k_2) \langle c_s^\dagger(k_1) c_{s'}(k_1) \rangle c_{s'}^\dagger(k_2) c_s(k_2)$$

$U(k) = \sum_n U_n e^{-ik \cdot n}$, where U_0 is the on-site interaction, U_1 is the nearest neighbor interaction, and U_n is the n -th shell neighbor interaction. Here, we consider only the on-site interaction and the nearest neighbor interaction.

Hopping parameters are $t_1 = 6$ meV for nearest-neighbor hopping and $t_2 = 1$ meV for next-nearest-neighbor hopping, which correspond to $t_s(n)$ in the kinetic energy term. $s = \{\uparrow, \downarrow\}$ is the spin index.

The lattice is a two-dimensional triangular lattice.

Answer:

2×2 matrix.

2. Question:

For the following mean-field Hamiltonian, what do you think is the possible order parameter we can write down for the system without breaking the translational symmetry?

Consider the mean-field Hamiltonian: $H = H_{\text{Kinetic}} + H_{\text{Hartree}} + H_{\text{Fock}}$, with each term defined below:

$$H_{\text{Kinetic}} = \sum_{s,k} E_s(k) c_s^\dagger(k) c_s(k), \text{ where } E_s(k) = \sum_n t_s(n) e^{-ik \cdot n}$$

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(0) \langle c_s^\dagger(k_1) c_s(k_1) \rangle c_{s'}^\dagger(k_2) c_{s'}(k_2)$$

$$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(k_1 - k_2) \langle c_s^\dagger(k_1) c_{s'}(k_1) \rangle c_{s'}^\dagger(k_2) c_s(k_2)$$

$U(k) = \sum_n U_n e^{-ik \cdot n}$, where U_0 is the on-site interaction, U_1 is the nearest neighbor interaction, and U_n is the n-th shell neighbor interaction. Here, we consider only the on-site interaction and the nearest neighbor interaction.

Hopping parameters are $t_1 = 6$ meV for nearest-neighbor hopping and $t_2 = 1$ meV for next-nearest-neighbor hopping, which correspond to $t_s(n)$ in the kinetic energy term. $s = \{\uparrow, \downarrow\}$ is the spin index.

The lattice is a two-dimensional triangular lattice.

Answer:

$$\langle c_s^\dagger c_{s'} \rangle \text{ with } s, s' = \uparrow, \downarrow.$$

3. Question:

For the following mean-field Hamiltonian, if we want to code and solve the problem in the momentum space, what are the coordinates of the 6 Brillouin zone corners, K point? Round to 2 decimal places.

Consider the mean-field Hamiltonian: $H = H_{\text{Kinetic}} + H_{\text{Hartree}} + H_{\text{Fock}}$, with each term defined below:

$$H_{\text{Kinetic}} = \sum_{s,k} E_s(k) c_s^\dagger(k) c_s(k), \text{ where } E_s(k) = \sum_n t_s(n) e^{-ik \cdot n}$$

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(0) \langle c_s^\dagger(k_1) c_s(k_1) \rangle c_{s'}^\dagger(k_2) c_{s'}(k_2)$$

$$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(k_1 - k_2) \langle c_s^\dagger(k_1) c_{s'}(k_1) \rangle c_{s'}^\dagger(k_2) c_s(k_2)$$

$U(k) = \sum_n U_n e^{-ik \cdot n}$, where U_0 is the on-site interaction, U_1 is the nearest neighbor interaction, and U_n is the n -th shell neighbor interaction. Here, we consider only the on-site interaction and the nearest neighbor interaction.

Hopping parameters are $t_1 = 6$ meV for nearest-neighbor hopping and $t_2 = 1$ meV for next-nearest-neighbor hopping, which correspond to $t_s(n)$ in the kinetic energy term. $s = \{\uparrow, \downarrow\}$ is the spin index.

The lattice is a two-dimensional triangular lattice.

Answer:

- (0, 4.19)
- (0, -4.19)
- (3.62, 2.09)
- (-3.62, 2.09)
- (3.62, -2.09)
- (-3.62, -2.09)

4. Question:

For the following mean-field Hamiltonian, if we want to code and solve the problem in the momentum space, what are the coordinates of the center of Brillouin zone, Γ point? Round to 2 decimal places.

Consider the mean-field Hamiltonian: $H = H_{\text{Kinetic}} + H_{\text{Hartree}} + H_{\text{Fock}}$, with each term defined below:

$$H_{\text{Kinetic}} = \sum_{s,k} E_s(k) c_s^\dagger(k) c_s(k), \text{ where } E_s(k) = \sum_n t_s(n) e^{-ik \cdot n}$$

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(0) \langle c_s^\dagger(k_1) c_s(k_1) \rangle c_{s'}^\dagger(k_2) c_{s'}(k_2)$$

$$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(k_1 - k_2) \langle c_s^\dagger(k_1) c_{s'}(k_1) \rangle c_{s'}^\dagger(k_2) c_s(k_2)$$

$U(k) = \sum_n U_n e^{-ik \cdot n}$, where U_0 is the on-site interaction, U_1 is the nearest neighbor interaction, and U_n is the n -th shell neighbor interaction. Here, we consider only the on-site interaction and the nearest neighbor interaction.

Hopping parameters are $t_1 = 6$ meV for nearest-neighbor hopping and $t_2 = 1$ meV for next-nearest-neighbor hopping, which correspond to $t_s(n)$ in the kinetic energy term. $s = \{\uparrow, \downarrow\}$ is the spin index.

The lattice is a two-dimensional triangular lattice.

Answer:

(0,0)

5. Question:

For the following mean-field Hamiltonian, if we want to code and solve the noninteracting band structure, what are the energies at the center of Brillouin zone, Γ point, for all bands?

Consider the mean-field Hamiltonian: $H = H_{\text{Kinetic}} + H_{\text{Hartree}} + H_{\text{Fock}}$, with each term defined below:

$$H_{\text{Kinetic}} = \sum_{s,k} E_s(k) c_s^\dagger(k) c_s(k), \text{ where } E_s(k) = \sum_n t_s(n) e^{-ik \cdot n}$$

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(0) \langle c_s^\dagger(k_1) c_s(k_1) \rangle c_{s'}^\dagger(k_2) c_{s'}(k_2)$$

$$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(k_1 - k_2) \langle c_s^\dagger(k_1) c_{s'}(k_1) \rangle c_{s'}^\dagger(k_2) c_s(k_2)$$

$U(k) = \sum_n U_n e^{-ik \cdot n}$, where U_0 is the on-site interaction, U_1 is the nearest neighbor interaction, and U_n is the n -th shell neighbor interaction. Here, we consider only the on-site interaction and the nearest neighbor interaction.

Hopping parameters are $t_1 = 6$ meV for nearest-neighbor hopping and $t_2 = 1$ meV for next-nearest-neighbor hopping, which correspond to $t_s(n)$ in the kinetic energy term. $s = \{\uparrow, \downarrow\}$ is the spin index.

The lattice is a two-dimensional triangular lattice.

Answer:

(48 meV, 48 meV)

6. Question:

For the following mean-field Hamiltonian, if we want to code and solve the noninteracting band structure, what are the energies at the first Brillouin zone corners, K point, for all bands?

Consider the mean-field Hamiltonian: $H = H_{\text{Kinetic}} + H_{\text{Hartree}} + H_{\text{Fock}}$, with each term defined below:

$$H_{\text{Kinetic}} = \sum_{s,k} E_s(k) c_s^\dagger(k) c_s(k), \text{ where } E_s(k) = \sum_n t_s(n) e^{-ik \cdot n}$$

$$H_{\text{Hartree}} = \frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(0) \langle c_s^\dagger(k_1) c_s(k_1) \rangle c_{s'}^\dagger(k_2) c_{s'}(k_2)$$

$$H_{\text{Fock}} = -\frac{1}{N} \sum_{s,s'} \sum_{k_1,k_2} U(k_1 - k_2) \langle c_s^\dagger(k_1) c_{s'}(k_1) \rangle c_{s'}^\dagger(k_2) c_s(k_2)$$

$U(k) = \sum_n U_n e^{-ik \cdot n}$, where U_0 is the on-site interaction, U_1 is the nearest neighbor interaction, and U_n is the n -th shell neighbor interaction. Here, we consider only the on-site interaction and the nearest neighbor interaction.

Hopping parameters are $t_1 = 6$ meV for nearest-neighbor hopping and $t_2 = 1$ meV for next-nearest-neighbor hopping, which correspond to $t_s(n)$ in the kinetic energy term. $s = \{\uparrow, \downarrow\}$ is the spin index.

The lattice is a two-dimensional triangular lattice.

Answer:

(-15 meV, -15 meV)

7. Question:

For the following problem, derive the kinetic term of the Hamiltonian in second-quantized form (H_{TB}) for this triangular lattice system. Express your final answer as the complete tight-binding Hamiltonian, clearly showing the summations and indices.

Consider a triangular lattice system where the degrees of freedom are spin states associated with $+K$ and $-K$ valleys. The kinetic term of the Hamiltonian can be described by a tight-binding model with the following properties:

Electrons hop between sites with amplitude $t_s(R_i - R_j)$.

$s = \uparrow, \downarrow$ represents spin states associated with $+K$ and $-K$ valleys respectively.

R_i represents a site position in the triangular lattice.

$c_{R_i,s}$ is the electron annihilation operator at site with position R_i with spin s .

$c_{R_i,s}^\dagger$ is the electron creation operator at site with position R_i with spin s .

The hopping process occurs between sites at positions R_i and R_j .

The summation should be taken over all spin states and all real space positions.

Answer:

$$H_{TB} = - \sum_{R_i, R_j, s} t_s(R_i - R_j) c_{R_i, s}^\dagger c_{R_j, s}$$

8. Question:

For the following problem, derive the interaction part of the Hamiltonian H^{int} in the second-quantized form for this triangular lattice system. Express your final answer in terms of the number operators $n_s(R_i)$.

Consider a triangular lattice system with spin degrees of freedom associated with $+K$ and $-K$ valleys. We want to examine the interaction term of the Hamiltonian in the second-quantized form, which complements the kinetic term.

The system has a density-density interaction between sites with the following properties:

The interaction occurs between sites at positions R_i and R_j with interaction strength $U(R_i - R_j)$.

R_i and R_j represent site positions in the triangular lattice.

$c_{R_i,s}$ and $c_{R_i,s}^\dagger$ are the electron annihilation and creation operators.

The summation should be taken over all spin states s, s' and all real space positions.

The number operator for electrons with spin s at site position R_i is defined as $n_s(R_i) = c_{R_i,s}^\dagger c_{R_i,s}$.

Answer:

$$H^{\text{int}} = \frac{1}{2} \sum_{s,s'=\uparrow,\downarrow} \sum_{R_i,R_j} U(R_i - R_j) n_s(R_i) n_{s'}(R_j)$$

9. Question:

For the following problem, express the noninteracting Hamiltonian \hat{H}_{Kinetic} in terms of the second quantized operators $c_s^\dagger(k)$ and $c_s(k)$ in the momentum space. Simplify any summation indices if possible.

Consider a triangular lattice system with spin degrees of freedom associated with $+K$ and $-K$ valleys. We have a noninteracting Hamiltonian in the second-quantized form expressed in the real space basis as:

$$\hat{H}_{\text{Kinetic}} = \sum_{R_i, R_j} \sum_{s=\uparrow, \downarrow} t_s(R_i - R_j) c_s^\dagger(R_i) c_s(R_j)$$

where:

$c_s^\dagger(R_i)$ and $c_s(R_j)$ are creation and annihilation operators in real space

$t_s(R_i - R_j)$ is the hopping parameter

The summation is over all sites and spin states

The Fourier transformation from real space to momentum space is defined as:

$$c_s^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_s^\dagger(R_i) e^{ik \cdot R_i}$$

where N is the number of unit cells in the real space.

Answer:

$$\hat{H}_{\text{Kinetic}} = \sum_{s=\uparrow, \downarrow} \sum_k E_s(k) c_s^\dagger(k) c_s(k)$$

where $E_s(k) = \sum_n t_s(n) e^{-ik \cdot n}$

10. **Question:**

For the following problem, express the interaction Hamiltonian \hat{H}^{int} in terms of second quantized operators $c_s^\dagger(k)$ and $c_s(k)$ in the momentum space. Simplify any summation indices if possible.

Consider a triangular lattice system with spin degrees of freedom associated with $+K$ and $-K$ valleys. We have an interaction Hamiltonian in the second-quantized form expressed in the real space basis as:

$$\hat{H}^{\text{int}} = \frac{1}{2} \sum_{R_i, R_j} \sum_{s, s'=\uparrow, \downarrow} U(R_i - R_j) n_s(R_i) n_{s'}(R_j)$$

where:

$n_s(R_i) = c_s^\dagger(R_i) c_s(R_i)$ is the number operator at site R_i with spin s

$U(R_i - R_j)$ is the interaction strength between sites i and j

The summation is over all sites and spin states

The Fourier transformation from real space to momentum space is defined as:

$$c_s^\dagger(k) = \frac{1}{\sqrt{N}} \sum_i c_s^\dagger(R_i) e^{ik \cdot R_i}$$

where k is defined within the first Brillouin zone and N is the number of unit cells in the real space.

Answer:

$$\hat{H}^{\text{int}} = \frac{1}{2N} \sum_{s, s'=\uparrow, \downarrow} \sum_{k, k', k'', k'''} U(k - k') c_s^\dagger(k) c_s(k') c_{s'}^\dagger(k'') c_{s'}(k''') \sum_G \delta(k - k' + k'' - k''', G)$$

where $U(k) = \sum_n U(n) e^{-ik \cdot n}$ and G is a reciprocal lattice vector.