Interaction-driven phases in a Dirac semimetal: exact diagonalization results

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Abstract
The interaction-driven phases in the Dirac semimetal (SM) of the \( \pi \)-flux model on the square lattice are studied with nearest-(NN), next-nearest-(NNN) and next-next-nearest-neighbor (NNNN) interactions using the exact diagonalization method. We find that the NN interaction drives a phase transition from the SM phase to a charge density wave insulator. In the presence of the NNN interaction, the system becomes an anisotropic SM for small interactions and an insulator with the stripe order for large ones. The NNNN interaction drives the Dirac SM to a dimmerized insulator. The interplay of the NNN and NNNN interactions is also studied. We find that the NNNN interaction firstly eliminates the effect of the NNN interaction and then develops its favorable order. In the calculations, the signature of the interaction-driven quantum anomalous Hall phase is not found.

Keywords: Dirac semimetal, interaction, topological insulator
(Some figures may appear in colour only in the online journal)

1. Introduction
The discovery of topological insulators (TIs) has generated great interest in the field of condensed matter physics due to its many exotic electronic properties and application potentials [1–4]. Many efforts have been devoted to the studies of TIs, particularly to the interplay between the interactions and the topological property [5]. The effects of the interactions on TIs have been extensively studied with different models. Consistent results have been obtained using various analytical and numerical methods [5–9].

Another important related problem is the possibility of the interaction-driven topological phase, which is firstly suggested on the honeycomb lattice within the mean-field approximation [10]. This provides a new approach to generating the topological phase without strong intrinsic spin–orbit coupling and greatly extends the class of the topologically nontrivial materials. Though the phase has also been predicted in other models [11–14], the mechanism is still within the mean-field framework. Since in 2D the quantum fluctuation may render the mean-field theory a poor approximation, its use is warranted to verify the relevant physics with the exact methods. Recently, works have addressed the problem using numerical exact diagonalization (ED), but inconsistent conclusions have been drawn [15–18]. Before large-scale numerical studies come out to clarify the problem, it is important to have consistent results from the ED calculations.

Though the ED method is limited by its small size, it is an important method in dealing with interacting systems. In the paper, based on the \( \pi \)-flux model on the square lattice, the interaction-driven phases in the Dirac semimetal (SM) are studied. The ED method using the Lanczos algorithm with the momentum state as the basis is used, from which the eigenstates are distinguished by their momenta. We show that this is very helpful in identifying the different quantum phases. In the calculations, the signature of the interaction-driven quantum anomalous Hall phase is not found.
calculations, the signature of the interaction-driven quantum anomalous Hall (QAH) phase is not found.

2. The model and method

We consider a $\pi$-flux model on the square lattice with a tight-binding Hamiltonian \[ H_0 = \sum_{ij} t_{ij} e^{i\hat{\delta}_{ij}/2} c_i^+ c_j, \] where $c_i^+$ and $c_i$ are the annihilation and creation operators at site $r_i = (i_x, i_y)$. For the case of sites $i$ and $j$ NN neighbors, $t_{ij} = t_1$ and $\hat{\delta}_{ij} = 0$, $\hat{\delta}_{i,i+x} = \pi t_2$ with $\hat{\delta}(\hat{\delta})$ is the lattice constant in the $xy$-direction. A unit cell contains two sites along the $x$-direction (see figure 1). In the reciprocal space, the Hamiltonian is written as $H_0 = \sum_k \psi_k^* H_0(k) \psi_k$ with $\psi_k = (c_i, c_j)^T$ and $H_0(k) = 2t_1 \cos k_x \sigma_x - 2t_1 \cos k_y \sigma_y$, where $\sigma_x, \sigma_y$ are the Pauli matrices. The energy spectrum is given by $E_k = \pm \sqrt{4t_1^2 (\cos^2 k_x + \cos^2 k_y)}$. The system is an SM with two inequivalent Dirac points at $k_{1,2} = (\pi/2, \pm \pi/2)$. Before the effect of the interactions is studied, we first study the perturbations of the static orders favored by the interaction toward the Dirac SM.

The gapless Dirac points can be gapped by the NNN hopping with the pattern: $t_{ij} = t_2$ and $\chi_{i,i+x} = \chi_{i,i+x} = \pi t_2$. In the momentum space it is: $\mathcal{H}_\text{NNN}(k) = -4t_2 \sin k_x \sin k_y \sigma_y$, and the energy spectrum becomes

\[ E_k^{(1)} = \pm \sqrt{4t_1^2 (\cos^2 k_x + \cos^2 k_y)} + 16t_2^2 \sin^2 k_x \sin^2 k_y, \]

where $k$ is in the reduced Brillouin zone $|k| \leq \pi/2$ and $|k_y| \leq \pi$. A nontrivial gap $4|t_2|$ opens at $K_{1,2}$. The system is topological with gapless states associated with the edges traversing the gap and can be characterized by a nonzero Chern number.

The gapless Dirac points can also be gapped by the staggered CDW order $H_{\text{cdw}} = V_c \sum_i (-1)^{i_y} c_i^+ c_i$. Then, a unit cell contains four sites. The Hamiltonian can be written as

$\mathcal{H}_0(k) = 2t_1 \cos k_x \sigma_x \otimes I + 2t_1 \cos k_y \sigma_y \otimes \sigma_y + V_c \sigma_z \otimes I$, and the energy spectrum is

\[ E_k^{(2)} = \pm \sqrt{4t_1^2 (\cos^2 k_x + \cos^2 k_y) + V_c^2}, \]

where $k$ is in the reduced Brillouin zone $|k| \leq |k_x| \leq \pi/2$. A gap $|V_c|$ opens at $K_{1,2}$ and the resulting system is a trivial insulator.

We are also interested in the stripe order $H_{\text{stripe}} = V_s \sum_i (-1)^{i_y} c_i^+ c_i$. In the four-site unit cell as that in the case of the CDW order, it can be written as $H_{\text{stripe}}(k) = V_s \sigma_z \otimes \sigma_z$. The energy spectrum becomes

\[ E_k^{(3)} = \pm \sqrt{4t_1^2 \cos^2 k_x + (2t_1 \cos k_y \pm V_s)^2}. \]

For $|V_s| \leq |2t_1|$, the SM phase remains, but the touching points are anisotropic and are moved to other momenta. The anisotropic Dirac points can be gapped by the above NNN hopping, but no longer by the CDW order.

In the following section, we use ED to study the effects of the NN, NNN and NNNN interactions on equation (1),

\[ H_{\text{int1}} = V_1 \sum_{\langle ij \rangle} n_i n_j, \]

\[ H_{\text{int2}} = V_2 \sum_{\langle\langle ij \rangle\rangle} n_i n_j, \]

\[ H_{\text{int3}} = V_3 \sum_{\langle\langle\langle ij \rangle\rangle\rangle} n_i n_j, \]

with $V_1, V_2, V_3$ the strengths of the interactions and $n_i = c_i^+ c_i$ the number operator. Since the total Hamiltonian is translationally invariant, the momentum states can be constructed as the basis of the ED calculations and the eigenenergies in each momentum sector are calculated. The momentum-dependent eigenenergies provide more information when distinguishing the interaction-driven quantum phases. In the following, we set $t_1 = 1$ as the energy scale and all ED calculations are performed on a $4 \times 4$ system. The momentum is discrete as $k = (q_x \pi^2, q_y \pi^2, q_x, q_y)$, $q_x, q_y = 0, \ldots, N_{\text{ext}}$, with $N_{\text{ext}}$ the number of unit cell in $x(y)$-direction. For convenience, we label the momentum $k$ using $(q_x, q_y)$ or one integer $Q = q_x + N_{\text{ext}} q_y$.

3. The non-interacting SM phase

The main shortcoming of the ED calculation is the limited sizes. To understand the results on the small lattice, we first study the non-interacting SM phase using the ED method. The energy spectrum of the SM phase is shown in figure 2. At half filling, the ground state is six-fold degenerate, four of which are in the momentum sector $0(0)$ and two in $0(2)$. This is consistent with the analysis from the band structure. For the
4 × 4 lattice, the momenta are discrete as $k = (q_x, q_y)$, $q_x = 0, 1, q_y \in [0, 3]$. Since the eigenenergy is two-fold degenerate at the Dirac points $K_1 = (1, 1)$ and $K_2 = (1, 3)$, two particles are chosen from the four states and the degeneracy is 6. Out of the six cases, four cases have one particle at $K_1$ and the other one at $K_2$, thus the four states have a total momentum $(0,0)$ or $Q = 0$. Having both particles at $K_1$ or $K_2$ results in a total momentum $(0, 2)$ or $Q = 4$. Since the system is an SM, the energy spectrum is continuous. The gap between the six degenerate states and higher states ($\Delta E$ in figure 2) is due to the finite-size effect and will decrease as the sizes become larger.

If we use the above NNN hopping or CDW or stripe order to perturb the SM phase, the six-fold degenerate ground state is split and the ground state becomes non-degenerate. However, for the case of the stripe order, it is known that the resulting phase is still SM, so the splitting is due to the finite-size effect. For the cases of the NNN hopping and the CDW order, the split non-degenerate ground state corresponds to a kind of insulating phase. Therefore, to identify the quantum phase in the system, it is important to distinguish the true gap and the finite-size effect. As the interaction is increased, $\Delta E_1$ is increased, while $\Delta E_2$ is decreased. Thus, after a critical interaction, $\Delta E_1$ should become a true gap. Then, the ground state is two-fold degenerate. The realistic ground state is a spontaneous symmetry breaking CDW insulator. Therefore, the NN interaction drives a phase transition from the SM phase to a CDW insulator.

There are two possible configurations for the CDW order supposing they are: $\varphi_1, \varphi_2$. The momentum states are constructed from the representative states using the translating operator $T^r$, which translates a state by the vector $r$. Since some translating operators translate $\varphi_1 (\varphi_2)$ to $\varphi_2 (\varphi_1)$, one of $\varphi_1, \varphi_2$ is representative and we chose $\varphi_1$. The momentum state is [21],

$$\varphi'(k) \propto \sum_r e^{-i r \cdot k} T^r \varphi_1.$$ 

It is straightforward that $\varphi'(k)$ is nonzero at $(0,0)$ or $Q = 0$ and $(0, 2)$ or $Q = 4$. The resulting momentum states are: $\varphi'_1 = (\varphi_1 + \varphi_2)/2$ and $\varphi'_2 = (\varphi_1 - \varphi_2)/2$, respectively. $\varphi'_1(2)$ is translationally invariant and is the state obtained in the ED calculations. Thus, the momenta helped us pick out the eigenstates with specific orders.

**Figure 2.** The energy spectrum in the momentum sector: (a) $V_1 = 0$; (b) $V_1 = 1$; (c) $V_1 = 2$. (d) $\Delta E_1$ and $\Delta E_2$ versus $V_1$. The eigenvalues are marked by different symbols (cross, horizontal mark, etc). $\Delta E_1, \Delta E_2$ are the dominated energy scales between the ground state and the excited states. If not mentioned, they are the same in the following figures.

4. The effect of the NN interaction

We firstly study the effect of the NN interaction described by equation (2) on the Dirac SM. The energy spectrums in the momentum sectors are shown in figure 2. When the NN interaction is added, the six-fold degenerate state is split into two groups, one of which contains two states and the other four states (see figure 2(b)). There are two energy scales $\Delta E_1$ and $\Delta E_2$. For small interactions, it is expected that the ground state is still the Dirac SM [20]. Thus, $\Delta E_1$ and $\Delta E_2$ are due to the finite-size effect. As the interaction is increased, $\Delta E_1$ is increased, while $\Delta E_2$ is decreased. Thus, after a critical interaction, $\Delta E_1$ should become a true gap. Then, the ground state is two-fold degenerate. The realistic ground state is a spontaneous symmetry breaking CDW insulator. Therefore, the NN interaction drives a phase transition from the SM phase to a CDW insulator.
represent the moving direction of the nearby states as \( V \) increases, it is expected that at large \( \Delta E \) by equation (3) in the Dirac SM. The energy spectrums in the momentum sector: (Figure 3. The effect of the NNN interaction

Next, we study the effect of the NNN interaction described by equation (4) and its interplay with the NNNN interaction described by equation (5) in the Dirac SM. The energy spectrums in the momentum sectors are shown in figure 3. As the interaction is increased, the following processes occur in sequence (see figure 3(a)):

1. \( \Delta E_1 \) increases and \( \Delta E_2 \) tends to vanish.
2. \( \Delta E_1 \) tends to vanish and \( \Delta E_2 \) increases.
3. \( \Delta E_1 \) increases and \( \Delta E_2 \) tends to vanish.

In the third process, since \( \Delta E_1 \) increases as \( V_2 \) increases, \( \Delta E_1 \) is a true gap. The ground state is four-fold degenerate and is of the stripe order, which can be probed by adding a very small specific stripe order to induce spontaneous symmetry breaking. Also similar to the analysis in the previous section, three configurations of the stripe order are at \( Q = 0 \) and one at \( Q = 4 \).

So the phases driven by the small and large NNN interactions are identified. The more interesting region is the moderate NNN interactions, where an important question is whether the QAH topological phase needs to be stabilized by an additional NNNN interaction [13]. Therefore, in this section, we study the effect of the NNNN interaction described by equation (5) and its interplay with the NNN interaction in the Dirac SM.

First, we study the effect of the sole NNNN interaction.

In the mean-field approximation, the interaction-driven QAH phase needs to be stabilized by an additional NNNN interaction. Therefore, in this section, we study the effect of the NNNN interaction described by equation (5) and its interplay with the NNN interaction in the Dirac SM. In the mean-field approximation, the interaction-driven QAH phase needs to be stabilized by an additional NNNN interaction. Therefore, in this section, we study the effect of the NNNN interaction described by equation (5) and its interplay with the NNN interaction in the Dirac SM. In the mean-field approximation, the interaction-driven QAH phase needs to be stabilized by an additional NNNN interaction. Therefore, in this section, we study the effect of the NNNN interaction described by equation (5) and its interplay with the NNN interaction in the Dirac SM.
defined, with $\Delta E_1$ splitting the sixteen low-energy states and $\Delta E_2$ the gap from the higher states. At large interaction and as it increases, $\Delta E_1$ decreases while $\Delta E_2$ increases, suggesting that the ground state is an insulator with the order shown in figure 4. Particularly in a system with this kind of order, the NN hopping amplitudes form 8 different patterns in which the NN hopping amplitudes are dimmerized along the $x$- and $y$-directions. Thus, the ED results suggest a phase transition from the Dirac SM to the insulator with the dimmerization driven by the NNNN interaction. However, the detail of the phase transition is beyond the scope of the present ED method.

Next, we study the interplay of the NNNN interaction with the NNN interaction and the possible QAH phase driven by them. We add the NNNN interaction to a system with the NNN interaction. It is found that as the NNNN interaction is increased, it first eliminates the effect of the NNN interaction and then develops its favorable order. An example at $V_2 = 1.4$ is shown in figure 6. As shown in figure 3(b), when only the NNN interaction exists, the upper group containing four states begins to decrease as the interaction is increased. After the NNNN interaction is added, it can be observed that the group begins to increase. Then, the number of the states in the group becomes two and begins to decrease. Finally, at relatively large interactions, 16 low-energy states are developed, which is favored by the NNNN interaction. We also performed the calculations at other values of $V_2$ and are with the same results.

It was suggested in previous works that the QAH phase preserving the symmetry of the system should be two-fold degenerate. However, from the above calculations, we find no such signature, which is consistent with our previous work [15].

7. Conclusion and discussion

We study the interaction-driven phases in the Dirac SM of the $\pi$-flux model on the square lattice. To properly identify the quantum phases from the ED results, the effects of the static orders are first studied. We consider the staggered CDW, the stripe order and the nontrivial NNN hopping, which are favored by the considered interactions. Then, we show that the non-interacting SM phase is characterized by a six-fold degenerate ground state, whose momenta are consistent with those from the analysis of the band structure. The gapping of the SM by the orders becomes the splitting of the degeneracy.

The effect of the NN interaction is firstly considered. We calculate the energy spectrum in the momentum sector. Though the results are affected by the finite-size effect, a phase transition from the SM phase to a CDW insulator is still identified. Next, we study the effect of the NNN interaction. The results show that for small interactions, the SM phase is robust but becomes anisotropic, while for large interactions, it is an insulator with the stripe order.

To explore the interaction-driven QAH phase, we study the effect of the NNNN interaction. It is found that the sole NNNN interaction drives a phase transition from the SM to a dimmerized insulator. In the presence of the NNNN interaction, it is found to first eliminate the effect of the NNN interaction and then develop its favorable order. However, the signature of the interaction-driven QAH is not found. 

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Figure 4. The sixteen degenerate configurations favored by the NNNN interaction. The spheres represent the electrons. The thick (thin) solid bonds represent strengthened (weakened) hopping amplitudes in the presence of small $t_1$. 
Finally, we want to emphasize that the present results are in the scope of the ED method and are limited by small sizes. Large-scale numerical calculations are warranted to verify them.

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