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Hubbard interaction in the arbitrary Chern number insulator: A mean-field study

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ABSTRACT

The low-dimensional electron gas owing topological property has attracted many interests recently. In this work, we study the influence of the electron-electron interaction on the arbitrary Chern number insulator. Using the mean-field method, we approximately solve the Hubbard model in the half-filling case and obtain the phase diagrams in different parametric spaces. We further verify the results by calculating the entanglement spectrum, which contains C chiral modes and corresponds to a real space partitioning.

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1. Introduction

The realization of different topological states of matter is one of the major challenges in condensed matter field for both fundamental and technological reasons [1,2]. The quantum anomalous Hall (QAH) effect, or called the Chern insulator in which the quantum Hall effect can arise without the net magnetic flux was first proposed by Haldane on the honeycomb lattice [3]. The Chern insulator has been theoretically predicted in a broad range of systems, such as the magnetically doped topological insulators and honeycomb lattices formed by transition-metal or heavy-metal ions [4–6], but was only recently realized in experiment in the magnetic Cr-doped $(\text{Bi}_{1-x}\text{Sb})_x\text{Te}_3$ thin film [7].

Among the studies of the Chern insulator, the interplay between the electron-electron correlation effect and band topology has also aroused people's interests. It was found that in the prototype Haldane–Hubbard (HH) model, the local onsite interaction favors an antiferromagnetic (AFM) insulator phase in the strong coupling regime [8,9]. The static mean-field study [10–12] reported a spin-density wave state at the intermediate strength. More interestingly, with the dynamical mean-field study, a spontaneous symmetry breaking quantum Hall phase was found as the intermediate phase between the band insulator and the Mott insulator [13]. Beyond the mean-field, the fluctuation-induced interaction can further open the gap in the system, rendering a first-order transition [14].

It was worthy pointing out that besides the honeycomb lattice, the Chern insulator can also be realized on other lattice structures, such as the square lattice with the proper hopping integrals and spin-orbit couplings [15–18]. In this work, we investigate the influence of on-site Hubbard interaction on the arbitrary Chern number insulator and take the single-site square lattice model as an example [19]. In the model, the valley-degeneracy breaking plays a decisive role in forming the different topological states. As the unit cell only owns one site in the square lattice, the magnetic property is much simpler than the honeycomb lattice where the AFM phase is common [8,9,20]. Such a model is excited by two aspects: first, the model can be considered as a simplified version to describe the electron motion in the double-perovskite monolayers [21]; second, the ultracold atomic gases which can be controlled to a high degree offers a unique opportunity to investigate the correlation effect [22]. In Ref. [23], Cook et al. studied a similar single-site Chern insulator model and found an emergent dome of nematic order around the Chern insulator-normal insulator topological critical point that is driven by a quadratic band touching point.

Using the mean-field method, we self-consistently solve the half-filled Hubbard model. The main results are as follows: 1. We make a detailed discussion of how the mean-field parameter and local magnetization are intimately related with the Zeeman field and hopping integrals; 2. the mean-field phase diagrams are obtained in different parametric spaces and we point out that the Hubbard interaction gives a rather effective route in modulating the Chern insulator phase transitions; 3. the Chern number phases are demonstrated by calculating the entanglement spec-

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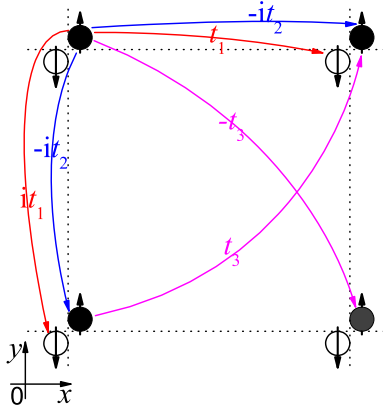


Fig. 1. (Color online.) Schematic plot of the square lattice, where the two spin orbits are separated for clarity. The hopping terms are shown explicitly by the arrows. Note the downspin–downspin hoppings are opposite to the upspin–upspin ones and are not shown.

trum, which contains C chiral modes corresponding to a real space partitioning.

2. Model and mean-field theory

We start from a tight-binding model of spinful fermions on the single-site square lattice. When the onsite Hubbard interaction is included, the system can be described by the Hamiltonian:

$$H = \sum_{(ij)} t_{ij}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} + \sum_{\langle\langle ij \rangle\rangle} t'_{ij}{}^{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \Delta_0 \sum_i (c_{i\uparrow}^{\dagger} c_{i\uparrow} - c_{i\downarrow}^{\dagger} c_{i\downarrow}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) denotes the creation (annihilation) operator at site i with spin σ , t_{ij} and t'_{ij} are the nearest-neighbor (NN) and next-nearest-neighbor (NNN) hopping integrals, Δ_0 gives the local Zeeman splitting field, and U is the Hubbard repulsive strength. Explicitly, the NN hopping terms that are spin-conserving are given as $t_{i+x,i}^{\uparrow\uparrow} = t_{i+y,i}^{\uparrow\uparrow} = -t_{i+x,i}^{\downarrow\downarrow} = -t_{i+y,i}^{\downarrow\downarrow} = -it_2$, while the spin-flip NN hopping terms are chosen as $t_{i\pm x,i}^{\uparrow\downarrow} = -it_2^{\downarrow\uparrow} = t_1$, which can be considered as the Rashba SOC and represent the kinetic terms. On the other hand, the spin-conserving NNN hopping terms that can be related to the intrinsic SOC are given as $t_{i+x+y,i}^{\uparrow\uparrow} = -t_{i-x+y,i}^{\uparrow\uparrow} = -t'_{i+x+y,i}{}^{\downarrow} = t'_{i-x+y,i}{}^{\downarrow} = t_3$. Here the spin-flip NNN hoppings have been neglected and the schematic plot of the spinful square lattice model is given in Fig. 1. The complex hopping which is related to a nonzero phase factor breaks the time-reversal symmetry and the Zeeman term breaks the inversion symmetry, where both terms can open the gap at Dirac points.

The tight-binding model can well describe the electron motion in {001} double-perovskite monolayers, such as the crystal of $\text{La}_2\text{MnIrO}_6$ [21]. In their work, the effective intersite SOC between different orbits are also taken into account. Although our model is a simplified version, it still captures the main mechanism of the valley-degeneracy breaking that induces the high-Chern number phase.

Without interactions, $U = 0$, the model can support the non-trivial Chern bands. In the basis of $(c_{\mathbf{k}\uparrow}^{\dagger}, c_{\mathbf{k}\downarrow}^{\dagger})^T$, the Hamiltonian in the momentum space becomes

$$H(\mathbf{k}) = \begin{pmatrix} A_{\mathbf{k}} + \Delta_0 & B_{\mathbf{k}} \\ B_{\mathbf{k}}^* & -A_{\mathbf{k}} - \Delta_0 \end{pmatrix}, \tag{2}$$

in which the matrix elements are

$$A_{\mathbf{k}} = 2t_2(\text{sink}_x + \text{sink}_y) + 2t_3[\cos(k_x + k_y) - \cos(k_x - k_y)],$$

$$B_{\mathbf{k}} = 2t_1(\text{cos}k_x - i\text{cos}k_y),$$

where the lattice constant has been taken as $a = 1$. The 2×2 Hamiltonian gives the minimum structure to realize the arbitrary Chern number phase [24,25]. The different topological phases can be well characterized by the Chern number of the occupied bands. When the Chern number changes, the topological phase transition occurs, via a mass gap closing at the corners of the Brillouin zone (the low-energy valleys), which are $\mathbf{K}_1 = (\frac{\pi}{2}, \frac{\pi}{2})$, $\mathbf{K}_2 = (-\frac{\pi}{2}, \frac{\pi}{2})$, $\mathbf{K}_3 = (-\frac{\pi}{2}, -\frac{\pi}{2})$ and $\mathbf{K}_4 = (\frac{\pi}{2}, -\frac{\pi}{2})$. In momentum space, the Berry curvature Ω_{α} in the vicinity of \mathbf{K}_{α} is given as:

$$\Omega_{\alpha}(\mathbf{k}) = \eta \frac{\Delta_{\alpha}}{2(k^2 + \Delta_{\alpha}^2)^{\frac{3}{2}}}, \tag{3}$$

where \mathbf{k} is the deviation of the momentum vector from \mathbf{K}_{α} , $\eta = 1(-1)$ for valley $\mathbf{K}_{1,3}$ ($\mathbf{K}_{2,4}$) and the mass terms are $\Delta_1 = \Delta_0 + 4t_2 - 4t_3$, $\Delta_2 = \Delta_4 = \Delta_0 + 4t_3$ and $\Delta_3 = \Delta_0 - 4t_2 - 4t_3$. From the Berry curvature, it shows that the introduction of t_2 breaks the valley degeneracy between \mathbf{K}_1 and \mathbf{K}_3 , while the degeneracy between \mathbf{K}_2 and \mathbf{K}_4 is still preserved [25].

When the interaction is much stronger than the energy scale of the system, $U \gg t_{1,2,3}$ and we consider the half-filled lattice with one electron per site, it is evidently that the ground state of the system is a charge-localized Mott insulator [20]. While for intermediate interaction strength, $U \sim t_{1,2,3}$, the correlation effect between electrons will compete with the topological bands. In this case, the correlation effect can be adequately captured by the mean-field theory, whose underlying idea is that the many-body interaction can be approximated as the interaction between the degrees of freedom on that site with an external bath that is created by all other degrees of freedom on other sites [26].

With the Hatree-Fock mean-field approximation, the Hubbard interaction can be decoupled as:

$$U \sum_i n_{i\uparrow} n_{i\downarrow} = U \sum_i [(n_{i\uparrow} \langle n_{i\downarrow} \rangle + n_{i\downarrow} \langle n_{i\uparrow} \rangle) - (\sigma_i^+ \langle \sigma_i^- \rangle + \sigma_i^- \langle \sigma_i^+ \rangle)], \tag{4}$$

where $\langle n_{i\sigma} \rangle = \frac{N_{\sigma}}{N_s}$ denotes the average occupation number of electrons at site i with spin σ , N_{σ} and N_s are respectively the electron number with spin σ and the site number, $\sigma_i^+ = c_{i\uparrow}^{\dagger} c_{i\downarrow}$ and $\sigma_i^- = c_{i\downarrow}^{\dagger} c_{i\uparrow}$. We have dropped the constant terms that are unimportant for the calculation. The first two terms are the Hatree terms, which represent the decoupling in a direct channel and favor Ising-type ordering in the z -direction. The Hatree term can well describe spontaneous symmetry breaking along a chosen axis and capture the magnetic property of the system [27,28]. The last two terms are the Fock exchange terms, which only affect the nondiagonal terms in $H(\mathbf{k})$. However, as the Fock terms will not change the chirality of the low-energy valleys, they have no influence on the topological properties and will not be considered. In addition, the decoupling mechanism of pairing channel is related with superconducting phase, which is not the topic in this work.

We consider the half-filling case, so the particle number conservation can be written as

$$\langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle = 1. \tag{5}$$

In momentum space, the particle density gives the form of

$$\langle n_{\sigma} \rangle = \frac{1}{N_s} \sum_{\mathbf{k}} \langle \psi_{\sigma}^{\dagger}(\mathbf{k}) \psi_{\sigma}(\mathbf{k}) \rangle = \frac{1}{N_s} \sum_{\mathbf{k}, a} \psi_{a\sigma}^{\dagger}(\mathbf{k}) \psi_{a\sigma}(\mathbf{k}) f[E_a(\mathbf{k})], \tag{6}$$

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