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Interplay between the spin-orbit coupling and lattice modulation on the Lieb lattice

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Abstract. The interplay between the spin-orbit coupling and a lattice modulation in the Lieb lattice is studied. The electron structure of the tight-binding model on the Lieb lattice features both the flat and the Dirac linearly dispersing bands. Within the Lieb lattice the spin-orbit coupling can induce a topological insulating state, while the lattice modulation breaks the topology. As a result of the interplay, a topological competition between the spin-orbit coupling and the lattice modulation occurs. The topology of the system is detected by the edge modes in open boundaries.

1. Introduction

The interplay between the band flatness, spin-orbit coupling (SOC) and lattice modulation has attracted research attention. Dispersionless electrons create a special feature that any electron interaction becomes dominant over the kinetic energy. As a consequence, this leads to many intriguing phenomena of electron correlations [1–10]. A prominent example is the fractional Hall effect, where the interplay between the band flatness and the Coulomb interaction is essential [3–6]. The other examples are the special Kondo effect due to the presence of flat bands [8–10]. The spin-orbit coupling (SOC) is a relativistic effect of the Coulomb interaction of ions acting on electrons [11]. It is a one-body interaction in comparison with the two-body Coulomb interaction between electrons. The SOC often opens a gap in the single-particle spectra, and can induce a topological insulating state [12–14]. In flat-band lattices, such as the Lieb lattice [1], the SOC can also induce a topological insulating state [14]. On the other hand, a modulation of the electron hopping in the Lieb lattice can also lead to a gap opening in the single-particle spectra [14, 15]. However, in contrast to the SOC, the insulating state induced by the lattice modulation is topologically trivial [14]. When both the SOC and the lattice modulation are present, they may compete each other. As a result of the competition, the insulating state can change from topological to non-topological one.

In this paper we report the interplay between the SOC and the lattice modulation in the Lieb lattice. The lattice modulation is achieved by staggered hoppings. The topology of the ground state can be determined by different methods. One is directly calculating the Chern number [16–18]. The other is using the index of edge modes [19]. The topological classification of insulators can be based on the bulk-edge correspondence [19]. If across the interface between two insulators the topological invariants change then gapless conducting states exist at the interface [19]. Such

edge modes are deeply related to the topology of bulk. The number of edge modes determines the topology of bulk. In this paper we determine the topology of the system through monitoring the edge modes. The edge modes can be obtained by exact diagonalization of a ribbon structure [20].

The present paper is organized as follows. In Sec. 2 we describe the tight-binding model with the SOC and a hopping modulation on the Lieb lattice. The numerical results are presented in Sec. 3. Finally, Sec. 4 is the conclusion.

2. Tight-binding model with the spin-orbit coupling and lattice modulation on the Lieb lattice

We consider a tight-binding model with the spin-orbit coupling and lattice modulation on the Lieb lattice

$$H \;\; = \;\; \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + i\lambda \sum_{\langle\langle i,j \rangle\rangle, s, s'} \nu_{ij} c_{is}^{\dagger} \sigma_{ss'}^{z} c_{js'}, \tag{1}$$

where $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron with spin σ at lattice site i. $\sigma_{ss'}^{z} = s\delta_{ss'}$ with $s = \pm 1$ for up (down) spin is the z-component Pauli matrix. t_{ij} is the hopping parameter between sites i and j. $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ denote the nearest-neighbor and next-nearest-neighbor diagonal sites in the lattice, respectively. λ is the SOC which is realized through the spin and direction dependent hopping between next-nearest-neighbor diagonal sites. The sign $\nu_{ij} = \pm 1$ depends on the hopping direction as shown in Fig. 1. The Lieb lattice is an edge centered square lattice (see Fig. 1). It can be considered as the basic structure of layered cuprate superconductors [1]. The square with three sites A, B, C can be chosen for the unit cell, as shown in Fig. 1. We take the lattice parameter $a = 1$. The lattice modulation is achieved through a staggered hopping between nearest-neighbor sites along the x and y axes

$$t_{ij} = -t(1 \pm \delta), \tag{2}$$

as it is shown in Fig. 1 [14, 15]. δ is the modulation parameter. Without loss of generality we consider $0 \leq \delta \leq 1$. We use $t = 1$ as the energy unit.

The edge modes are obtained by exact diagonalization of a ribbon structure [20]. The ribbon is constructed by allowing the periodic boundary in the x-axis and open boundaries in the y-axis. For the Lieb lattice there are different open boundaries [20]. Different open boundaries may lead to different edge modes [20]. However, in this paper we present only the results with the straight open boundaries as shown in Fig. 1. The results with other open boundaries will be published somewhere else.
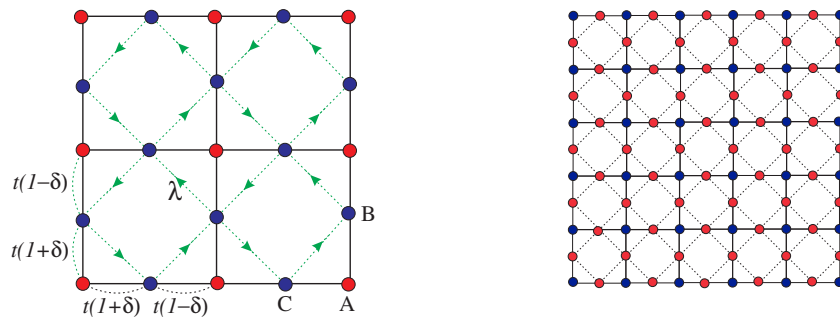

Figure 1. Left panel: The Lieb lattice structure with SOC and lattice modulation. The arrows indicate the hopping direction with $\nu_{ij} = 1$. In the opposite hopping direction $\nu_{ij} = -1$. Right panel: a ribbon with straight open boundaries.
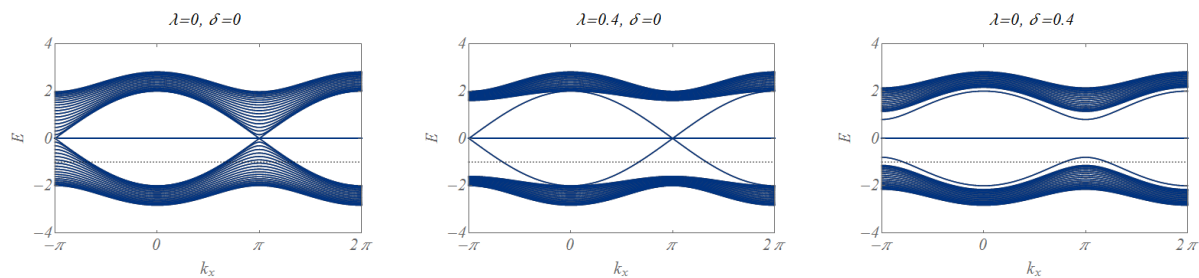
Figure 2. Band structure of ribbon with different SOC and lattice modulations. The dotted lines show a position of the chemical potential at third filling

3. Numerical results

In this section we calculate the band structure for ribbon with the size in the y axis $N_y = 20$. A large size in the x axis is chosen that the spectra can be considered as continuous in momenta in the x axis. Without the SOC ($\lambda = 0$) and the lattice modulation ($\delta = 0$), Hamiltonian in Eq. (1) just describes the standard tight-binding model on the Lieb lattice. This model exhibits a flat band and two linearly dispersive bands [1]. In Fig. 2 we plot the band structure for $\lambda = 0$ and $\delta = 0$. It indeed shows two linearly dispersive bands crossing the flat band at $k_x = \pm\pi$. In this case any edge mode is absent. Figure 2 shows that the ground state is always metallic. For other open boundaries a gap may be opened at half filling [20]. When the SOC is present ($\lambda \neq 0$), but the lattice modulation is still absent ($\delta = 0$), the flat band is isolated from two dispersive bands, separated by a gap, as it is also shown in Fig. 2. In addition, two edge modes appear in the gap. These edge modes is linear in momenta at $k_x = \pm\pi$. They also cross the flat band at $k_x = \pm\pi$. At half filling, the chemical potential is positioned at the flat band. However, at third (or two thirds) filling the chemical potential lies in the gap between the dispersive and the flat bands. In this case the ground state is insulating. However, there is one edge mode per one edge that crosses one time the Fermi level in the gap. Therefore the insulating state is topological. When the lattice modulation is present ($\delta \neq 0$), but the SOC is absent ($\lambda = 0$), the flat band is also isolated from the dispersive bands, like the previous case. However, the edge mode is also isolated in the gap. As a consequence, at third (or two thirds) filling, the ground state is insulating, but topologically trivial. Actually, these properties were already previously reported [14, 20]. However, there is a lack of study when both the SOC and the lattice modulation are present.

When both the SOC and the lattice modulation are present, the band structures for different
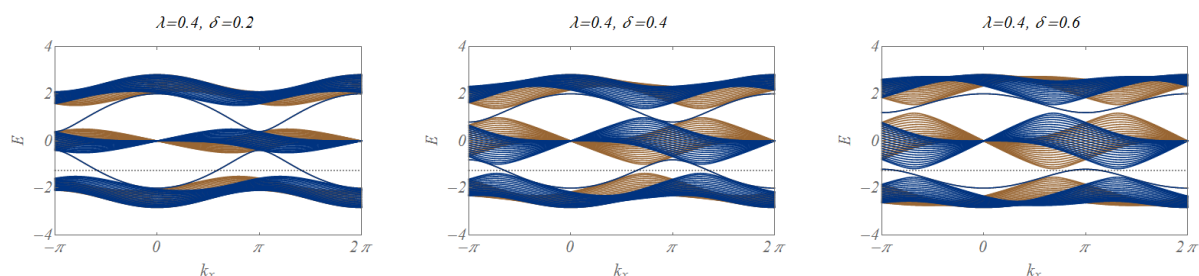

Figure 3. Band structure of ribbon with different SOC and lattice modulations. Different colors represent the band structure for different spin components. The dotted lines show a position of the chemical potential at third filling.

spin components become different, although the system is still paramagnetic. They are shown in Fig. 3. In contrast to the previous cases, the flat band does not longer exist. The SOC together with the lattice modulation already broaden the flat band. However, gaps are still opened between the dispersive and broadened flat bands. In the gaps the edge modes always exist. However, they never cross each other as in the previous cases, plotted in Fig. 2. When the lattice modulation is small ($\delta < 0.5$), there is one edge mode per one edge that crosses one time the Fermi level at third (or two thirds) filling. Therefore at third (or two thirds) filling the insulating ground state is topological. When the lattice modulation increases, the edge modes have a tendency of leaving from the broadened flat band. With large lattice modulation ($\delta > 0.5$) they are completely isolated from the broadened flat band, as it is shown in Fig. 3. In the strong lattice modulation case, the edge modes are equivalent to completely isolated edge modes. Therefore, the insulating ground state at third (or two thirds) filling is topologically trivial. In the presence of SOC, the lattice modulation drives the insulating ground state from topological to non-topological one.

4. Conclusion
We have studied the interplay between the SOC and the lattice modulation in the Lieb lattice. When both the SOC and the lattice modulation are present, they broaden the flat band. However, at third (or two thirds) filling the ground state is still insulating. By monitoring the edge modes, we determine the topology of the ground state at third (or two thirds) filling. In the presence of SOC, the lattice modulation drives the system to topological insulator to topologically trivial one. However, in this paper we have only reported the results obtained with straight open boundaries. The results with other open boundaries as well as the effect of external magnetic field on the ground state topology will be published somewhere else.

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