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EXOTIC STATES EMERGED BY SPIN-ORBIT COUPLING, LATTICE MODULATION AND MAGNETIC FIELD IN LIEB NANO-RIBBONS

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Abstract. *The Lieb nano-ribbons with the spin-orbit coupling, the lattice modulation and the magnetic field are exactly studied. They are constructed from the Lieb lattice with open boundaries in a direction. The interplay between the spin-orbit coupling, the lattice modulation and the magnetic field emerges various exotic ground states. With certain conditions of the spin-orbit coupling, the lattice modulation, the magnetic field and filling the ground state becomes half metallic or half topological. In the half metallic ground state, one spin component is metallic, while the other spin component is insulating. In the half topological ground state, one spin component is topological, while the other spin component is topologically trivial. The model exhibits very rich phase diagram.*

Keywords: Lieb lattice, flat band, spin-orbit coupling, half metal, topology.

Classification numbers: 71.27.+a,71.30.+h, 75.10.-b, 73.43.Nq.

I. INTRODUCTION

The discovery of nontrivial topology in a number of materials has attracted a lot of research attention due to their extraordinary properties, for instance in topological insulators the bulk behaves like an insulator, while their boundaries exhibit conducting properties [1–3]. In the topological materials the spin-orbit coupling (SOC) plays an essential role [1–3]. It creates a gap in the electron spectra and induces a band inversion that leads to topological invariants. Without the SOC, the topological properties often disappear. On the other hand, the magnetic field and the lattice modulation break the time-reversal and the lattice symmetries that often destroy the topology. Therefore the interplay between the SOC, the magnetic field and the lattice modulation may emerge exotic states, where the topological or the insulating states are partial, i.e. a single spin component of electrons remains topological or insulating, while the other spin component becomes topologically trivial or metallic. In addition, the magnetic field usually induces a magnetization. It together with the SOC and the lattice modulation could lead the ground state to be exotically complex.

The band flatness has also attracted research attention, because in the flat band systems electron correlations become dominant over the kinetic energy, that may generate different phenomena, for instance the ferromagnetism, the fractional quantum Hall effect, or the flat-band Kondo effect [4–15]. Especially, in topological materials the band flatness may generate particle fractionalization, like in the fractional quantum Hall effect. The topological insulators can be found in a number of flat-band systems, for instance in the Lieb lattice and its higher-dimensional generation, the perovskite materials, when the SOC is included [16, 17]. In this paper we study the interplay between the SOC, the magnetic field and the lattice modulation in the Lieb lattice. The Lieb lattice is a decorated square lattice, which exhibits a flat band as well as linearly electron dispersions at low energy [4, 12–17]. These special features of the electronic structure lead to a coexistence of both the band flatness and Dirac electrons, at least in the low-energy scale. The interplay between the SOC, the lattice modulation and the magnetic field in the presence of band flatness could generate competitions between them in the formations of topology, gap, magnetization and fractionalization. By using the exact diagonalization we calculate the electronic structure of nano-ribons that are cut from the Lieb lattice in a direction. The obtained electronic structure gives both the bulk and the edge electron spectra, which allow us to monitor the gap, the magnetiztion and the topology of the ground state. By varying the model parameters, the interplay between the SOC, the lattice modulation and the magnetic field in the Lieb lattice would explicitly be realized and as a result the exotic states would emerge. The competition between the SOC and the lattice modulation has previously been reported [15]. It is found that the lattice modulation drives the ground state from a topological insulator to a band insulator [15]. However, in the previous reported results [15], the magnetic field is absent. The presence of the magnetic field would result into a rich variety of the ground state.

The present paper is organized as follows. In Sec. II we describe the tight-binding model with the SOC, the hopping modulation and the magnetic field on the Lieb lattice. The numerical results are presented in Sec. III. Finally, Sec. IV is the conclusion.

II. MODEL

We study the interplay between the SOC, lattice modulation and magnetic field in a tight-binding model, defined on the Lieb lattice. The Hamiltonian of the model reads

$$H = \sum_{\langle i,j\rangle,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + i\lambda \sum_{\langle\langle i,j\rangle\rangle,\sigma} \nu_{ij} c^{\dagger}_{i\sigma} \sigma c_{j\sigma} - \sum_{i} h_i c^{\dagger}_{i\sigma} \sigma c_{i\sigma}, \qquad (1)$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator for an electron with spin σ at lattice site i. The spin variable $\sigma = \pm 1$ denotes the spin up and down in the z-direction. 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. λ is the parameter of the SOC which is realized through the spin and direction dependent hopping between next-nearest-neighbor diagonal sites [16, 17]. The sign $v_{ij} = \pm 1$ depends on the hopping direction, and we fix its sign as shown in Fig. 1 [16, 17]. h_i is the magnetic field strength, applying to electrons at lattice site i. The magnetic field may be generated as an intrinsic effect, when a long-range magnetic ordering is present, for instance when the double exchange between conduction electrons and magnetic impurities is realized, and the resulted mean field can play as a magnetic field [18–23]. However, in this work we consider the magnetic field in general as an external field.

The Lieb lattice is a decorated square lattice with additional sites at the center of every edge (see Fig. 1). It is one of the simplest lattice structures that exhibit a band flatness for the tight-binding model. Since the discovery of the high temperature superconductors, the Lieb lattice has also attracted research attention, because it can essentially be considered as the basic structure of layered cuprate superconductors [4]. A square with three sites A, B, C, as shown in Fig. 1, can be chosen as the unit cell of the Lieb lattice. The lattice parameter is set $a = 1$ for the length unit. The hopping between nearest-neighbor sites is allowed to be modulated along the x and y axes as

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

where δ is the modulation parameter. The hopping modulation is also shown in Fig. 1 [15, 24]. Without loss of generality we take $0 \leq \delta \leq 1$. We only consider the case when the magnetic field equally applies to electrons at the sites B and C of the lattice, i.e. $h_B = h_C$. In the following $t = 1$ is used as the energy unit.

Nano-ribons are constructed by allowing the periodic boundaries in the x-axis and open boundaries in the y-axis. The open boundaries of the nano-ribons may have three different types: straight-straight, straight-zigzag and zigzag-zigzag boundaries [25]. The edge modes may depend on the type of the open boundaries [25]. However, the boundary condition does not significantly change the topological properties of the ground state [25]. In this paper we only consider the straight-straight open boundaries in the y-axis, as shown in Fig. 1. Since the nano-ribons are

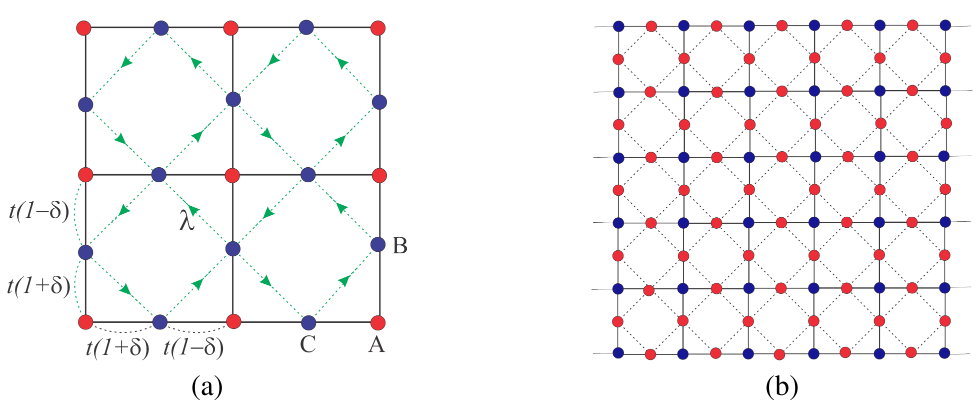

Fig. 1. (a) The Lieb lattice structure with SOC and lattice modulation. The arrows indicate the sign $v_{ij} = 1$ of the SOC. In the opposite direction $v_{ij} = -1$. (b) A nano-ribbon with straight-straight open boundaries in the y-axis and periodic boundaries in the x-axis.

periodic in the x-axis, we can perform the Fourier transform of the lattice space in the x-axis

$$c_{j_y\sigma}(k_x) = \frac{1}{\sqrt{N_x}} \sum_{j_x} c_{j_x j_y \sigma} e^{ik_x R_{j_x}}, \tag{3}$$

where j_x, j_y are the indices of the lattice cell j in the x- and y- axes, R_{j_x} is the position of the cell j in the x-axis, and N_x is the number of lattice cells in the x-axis. After making the Fourier transform, the Hamiltonian in Eq. (1) can exactly be diagonalized for a finite number N_y of the lattice cells in the y-axis. The energy spectra obtained by the exact diagonalization are the energy band and edge modes of the nano-ribons. The topology of the ground state is monitored by counting the number of the edge modes which cross the Fermi energy level. The gapless edge modes appear only when the edge modes cross the Fermi energy level and are connected to the conduction and valence bands. The number of the gapless edge modes correspondents to the topology of the bulk ground state due to the bulk-boundary correspondence [1–3]. One can notice that the main features of the nano-ribon band structure are independent on N_y. Actually, the number N_y only affects the number of the energy levels and the level spacings. Indeed, the number of the energy levels per one spin-component in the nano-ribons with the straight-straight boundaries is always equal to $3N_y + 2$, and it is independent on the model parameters. Among these energy levels, two levels come from the edges, and each N_y levels form the bulk lower, upper dispersive bands and the flat-origin band. An example of the band structure is shown in Fig. 2, where we plot the energy levels for various values of N_y. In Fig. 2, the flat band is degenerated and its degeneracy is exactly N_y. When N_y is large, the level spacings become tiny, and one can easily distinguish the bulk bands from the edge modes. In numerical calculations we use $N_y = 20$, since with this value of N_y the edge modes are clearly distinguishable from the bulk bands, as one can see in Fig. 2.

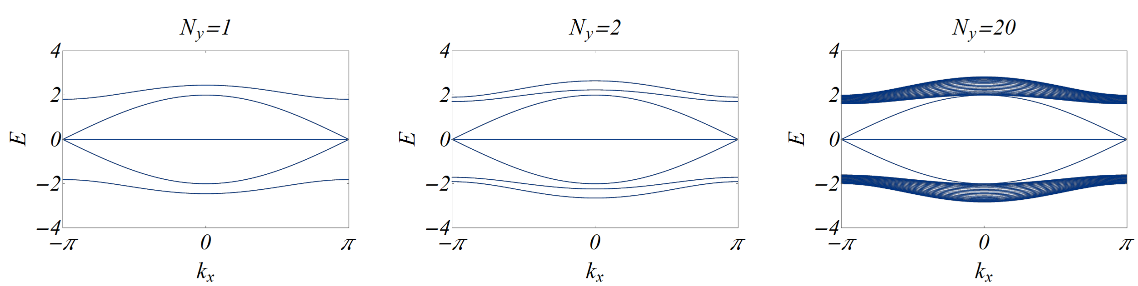

Fig. 2. (Color online) The evolution of the band structure with increasing N_y. The model parameters $\lambda = 0.4$, $\delta = 0$, $h_A = h_B = h_C = 0$ are chosen as an example.

III. NUMERICAL RESULTS

Without the SOC, the lattice modulation and the magnetic field, the tight-binding model on the Lieb lattice creates a flat band between two dispersive bands. The three bands linearly cross at the $M = (\pm\pi, \pm\pi)$ points of the Brillouin zone [4,12–17]. Both the SOC and the lattice modulation induce a gap in the band structure, that isolates the flat band from two other dispersive bands [15]. As a consequence, at half filling the system is well described by the flat band, while at third (or two thirds) filling, the ground state is insulating. At third (or two thirds) the SOC induces nontrivial topology, while the lattice modulation keeps trivial topology for the insulating state [15]. The competition between the SOC and the lattice modulation leads to a topological phase transition driven by the lattice modulation, where the ground state changes from a topological insulator to a band insulator when the lattice modulation increases [15]. This competition between the SOC and the lattice modulation has previously been reported [15]. However, when the magnetic field is present, it together with the SOC and the lattice modulation interplay each other, and as a consequence of the interplay various exotic properties may emerge.

III.1. Interplay between the spin-orbit coupling and magnetic field

In this subsection we study the interplay between the SOC and the magnetic field, when the lattice modulation is absent. Both strength and the direction of the magnetic field can vary at lattice sites A, B, and C. We will separately consider different cases of the magnetic field.

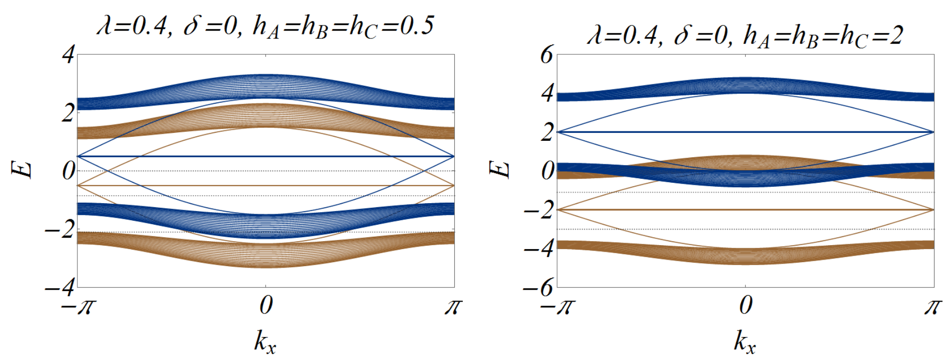

Fig. 3. (Color online) The band structure with different magnetic fields at a fixed SOC in the absence of the lattice modulation. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at half, third and sixth fillings.

First, we consider the uniform magnetic field $h_A = h_B = h_C \equiv h$. In this case the magnetic field shifts the energy bands of opposite spins in the opposite directions, as shown in Fig. 3. Actually, the flat and the dispersive bands of each spin value are exactly shifted by $\pm h$. This is purely the Zeeman effect. As a result, gaps appear at half, third (or two thirds), sixth (or five sixths) fillings. For weak magnetic fields, the ground state at half filling is ferromagnetic. There is an edge mode per spin that crosses the Fermi energy level twice. Since the considered nano-ribbon has two edges in the y-axis, hence the number of gapless modes per edge and spin is equal to 1. Based on the bulk-boundary correspondence, this reflects that the ferromagnetic insulating state is charge topological. When the magnetic field increases, the uppermost and lowermost bands of the opposite spins will cross each other (see Fig. 3), and as a consequence at half filling the ground state is metallic. With further increasing magnetic field, the bands of spin up are completely filled, while the bands of spin down are completely empty at half filling. This leads to a full ferromagnetic saturation. The ground state in this case is a band insulator. For weak magnetic fields, at third (or two thirds) filling, the ground state is paramagnetic. It is also topological because there is an edge mode per spin which crosses the Fermi energy level twice. However, when the magnetic field increases, the ground state at half filling becomes fully saturated ferromagnetic, as it is shown in

Fig. 3. It is still topological due to the twice crossing the Fermi energy level of the edge mode. At sixth (or five sixths) filling, the ground state is fully saturated ferromagnetic for strong magnetic fields. It is still topological due to the presence of the edge mode which crosses the Fermi energy level twice. However, when the magnetic field is weak, at sixth filling (or slightly larger than sixth filling) the ground state is half metallic, because the spin-up component is insulating while the spin-down component is metallic. The spin-up component is topological due to its edge mode which crosses the Fermi energy level twice.

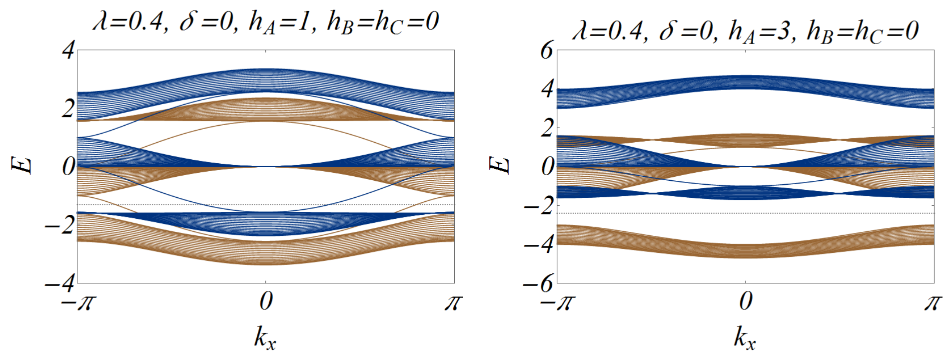

Fig. 4. (Color online) The band structure with different magnetic fields $h_A = 0$, $h_B = h_C \neq 0$ at fixed SOC in the absence of the lattice modulation. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at third filling (left panel) and at sixth filling (right panel).

When the magnetic field is non-uniform, the flat band does not exist anymore. An example of the band structure is shown in Fig. 4. The magnetic field induces two effects. First, it broadens the flat band, and second, it shifts the bands of opposite spins in the opposite directions like in the Zeeman effect. Depending on the magnetic field non-uniform, at half filling the ground state may be metallic or insulating, except for very strong magnetic field, when it fully polarizes the ground state. Since the metallic state does not exhibit the topological properties, we discard this case from the further consideration. However, the gap may also be opened at other fillings. In the case $h_A \neq 0$, $h_B = h_C = 0$, i.e. the magnetic field only applies to electrons at the corner sites, at a particular filling the ground state may become insulating, providing the magnetic field is not strong enough. Examples are shown in Fig. 4. When the magnetic field is weak, a gap is opened at third (or two thirds) filling. There is an edge mode per spin that crosses the Fermi energy level twice. Therefore, the ground state is a charge topological insulator. Although, the magnetic field is present, the ground state is still paramagnetic. With stronger magnetic field, the ground state becomes insulating at sixth (or five sixths) filling, as it is shown in Fig. 4. However, this ground state is ferromagnetic and topologically trivial due to the absence of edge modes crossing the Fermi energy level. In this ferromagnetic ground state, the lowest band of the spin-up component is fully occupied.

In the opposite case $h_A = 0$ and $h_B = h_C \neq 0$, the flat band is also broadened by the interference between the magnetic field and the SOC. For weak magnetic fields, the ground state is a paramagnetic insulator at third (or two thirds) filling, as it is shown in Fig. 5. It is also nontrivially

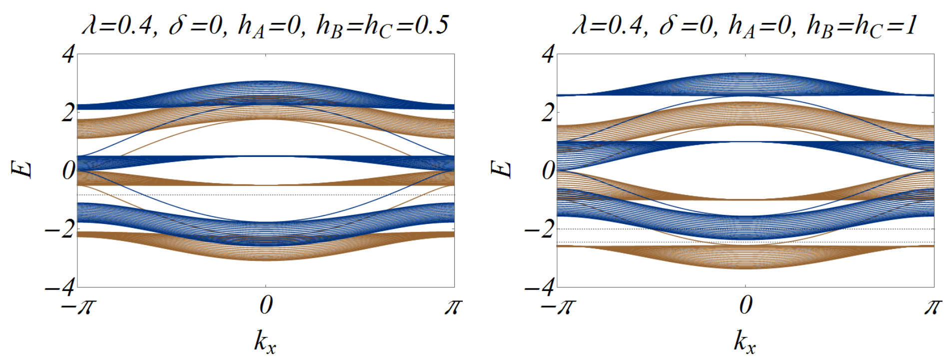

Fig. 5. (Color online) The band structure with different magnetic fields $h_A = 0$, $h_B = h_C \neq 0$ at fixed SOC in the absence of the lattice modulation. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at third filling (left panel) and at sixth and slightly larger sixth fillings (right panel).

topological, because there is an edge mode per spin that crosses the Fermi energy level twice. With further increasing the magnetic field, the ground state becomes insulator at sixth (or five sixths) filling, similar to the previous case $h_A \neq 0$, $h_B = h_C = 0$. In contrast to the previous case $h_A \neq 0$, $h_B = h_C = 0$, there is an edge mode that crosses the Fermi energy level twice. However, in this case, only the spin-up component exhibits the edge mode that crosses the Fermi energy level. This indicates that the spin-up component becomes topological, while the bands of the spin-down component are completely empty. However, at fillings which are slightly larger than sixth, the spin-down component band is partially filled. As a consequence, the spin-up component is still topological insulator, while the spin-down component is metallic. This reflects the ground state is half metallic, half topological insulator and ferromagnetic, similar to the previous case where the magnetic field is uniform and weak. The exotic ground state is due to the interplay between the SOC, the magnetic field and the lattice structure.

Next, we consider the case $0 < h_A < h_B = h_C$. In Fig. 6 we plot the band structure at a fixed h_A and increasing $h_B = h_C > h_A$. For weak magnetic fields $h_B = h_C > h_A$, gaps are opened at half and at sixth (or five sixths) fillings. At half filling there is an edge mode per spin which crosses the Fermi energy level twice. This indicates that the ground state is charge topological insulator. It is also a ferromagnetic. At sixth filling, the spin-down component is completely empty, while the lowest energy band of the spin-up component is fully filled. In this case the spin-up component is topological insulator. When the lowest energy band of the spin-down component is partially filled, the spin-down component becomes metallic, while the spin-up component still remains topologically insulating. This case is similar to the previous case $h_A = 0$, $h_B = h_C \neq 0$. When the magnetic field $h_B = h_C$ increases, the gap at half filling is closed, as it is shown in Fig. 6. In this case the ground state becomes metallic. However, at sixth filling, the spin-up component is still a topological insulator, while the spin-down component is completely empty.

In the opposite case $0 < h_B = h_C < h_A$, the ground state has properties similar to the ones of the previous case $0 < h_A < h_B = h_C$. In Fig. 7 we plot the band structure in this case. For small values of the magnetic field h_A, but still $h_A > h_B = h_C$, the gap is opened at half and at sixth (or

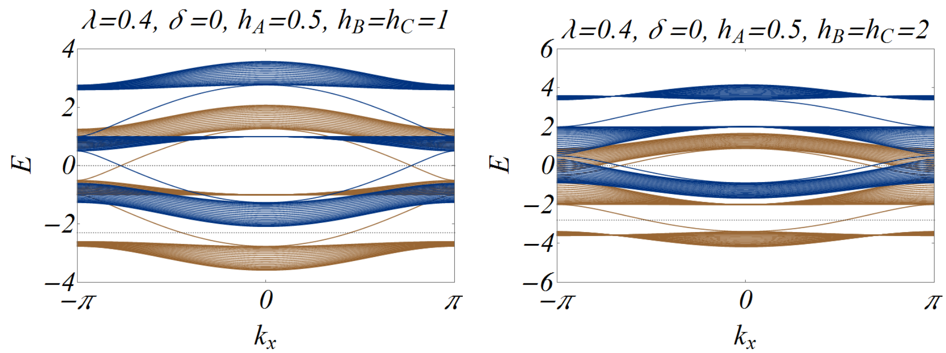

Fig. 6. (Color online) The band structure with different magnetic fields $0 < h_A < h_B = h_C$ at fixed SOC in the absence of the lattice modulation. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at half and sixth fillings.

five sixths) fillings. At half filling the ground state is a paramagnetic topological insulator, while at sixth (or five sixths) filling it is a saturated ferromagnetic topological insulator. However, when the magnetic field h_A increases, an additional gap is opened at third (or two thirds) filling, but the gap at half filling tends to be closed. Both at third and sixth fillings the ground state is saturated ferromagnetic. However, it is topological at third filling, and topologically trivial at sixth filling due to the edge modes, as they are shown in Fig. 7. For slightly doping from third filling, the lowest band of the spin-down component is partially filled that leads the ground state to be half metallic and half topological.

When the magnetic field has the opposite directions at site A and B, C, i.e. $h_B = h_C < 0 < h_A$, or $h_A < 0 < h_B = h_C$, the gap at half filling is closed, as shown in Fig. 8. Actually, the case $h_A < 0 < h_B = h_C$ is equivalent to the case $-h_A > 0 > -h_B = -h_C$, because the up and down

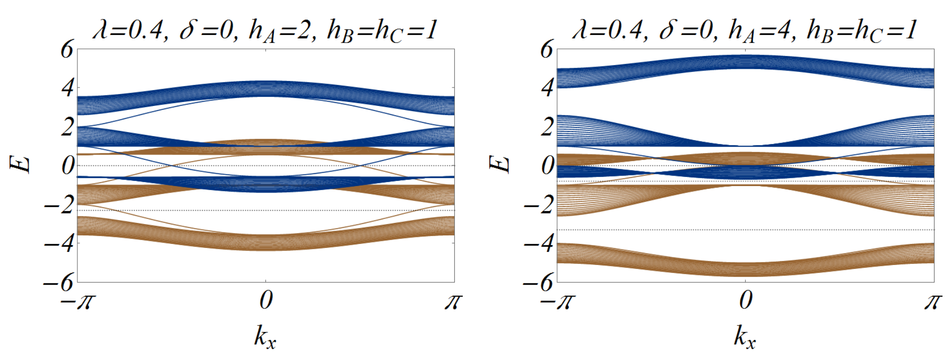

Fig. 7. (Color online) The band structure with different magnetic fields $h_B = h_C < 0 < h_A$ at fixed SOC in the absence of the lattice modulation. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at half filling and at sixth filling.

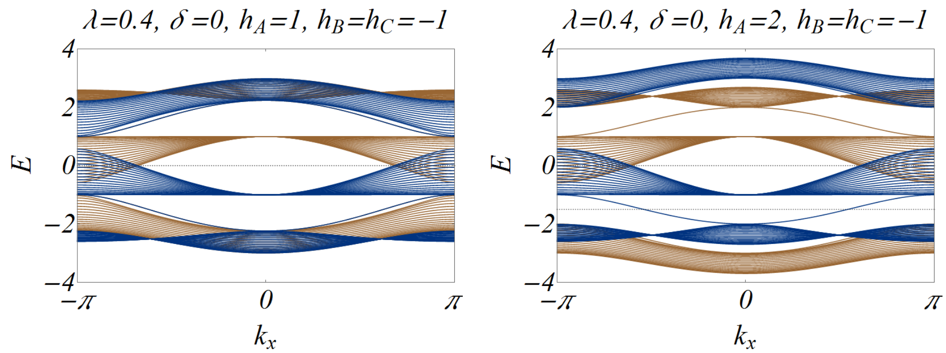

Fig. 8. (Color online) The band structure with different magnetic fields $0 < h_A < h_B = h_C$ at fixed SOC in the absence of the lattice modulation. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at half and third fillings.

directions of the magnetic field are equivalent. When h_A is larger a certain value, a gap at third (or two thirds) filling is opened. Although the magnetic field is present, the ground state at third (or two thirds) filling is paramagnetic. In Fig. 8, however, one can see there is only one edge mode of the spin-down component that crosses the Fermi energy level twice, while the edge mode of the spin-up component is completely below the Fermi energy level. This indicates that the spin-down component is topological insulating, while the spin-up component is a band insulator. Although the ground state is paramagnetic, the symmetry between the spin-up and spin-down components is broken. The ground state yields half topological. Especially, in this half topology both spin components are insulating.

III.2. Effect of the lattice modulation

When the lattice modulation is present, it interplays with the SOC and the magnetic field. In the absence of the magnetic field, the lattice modulation broadens the flat band, and it drives the ground state from a charge topological insulator to a band insulator [15]. The interplay between the SOC, the lattice modulation and the magnetic field becomes complex. First, we consider the case of uniform magnetic field. The magnetic field strength distinguishes two regimes: weak and strong magnetic fields, as we have showed in the previous subsection. In Fig. 9 we plot the band structure of nano-ribons with different lattice modulations at a fixed SOC and uniform weak magnetic field $h_A = h_B = h_C$. When both the SOC and the lattice modulation are present, they broaden the flat band [15]. For weak lattice modulations, gaps are opened at half and sixth (or five sixth) fillings, as shown in Fig. 9. At these fillings the ground state is ferromagnetic. At half filling it is topological because there is an edge mode per spin that crosses the Fermi energy level twice. However, at sixth filling, only the spin-up component is topological, since the spin-down component is empty. However, when the lattice modulation increases, the gap at half filling decreases, and at a certain value it is closed. When the gap at half filling is closed, despite of the gap opening at sixth (or five sixth) filling, the ground state is s only a band insulator, because the edge mode is isolated, as it is shown in Fig. 9. This indicates a topological transition driven by the lattice modulation at sixth (or five sixths) filling. When the uniform magnetic field is strong, the gap at half filling is closed, as it is shown in Fig. 10. At half filling the ground state is metallic. However, gaps are still opened at third (or two thirds) and sixth (or five sixths) fillings. At these filling the ground state is fully saturated ferromagnetic. When the lattice modulation is weak, the ground state at third (or two thirds) and sixth (or five sixths) fillings is topological. However, when the lattice modulation is strong, it becomes topologically trivial, because the edge modes are isolated in the gaps.

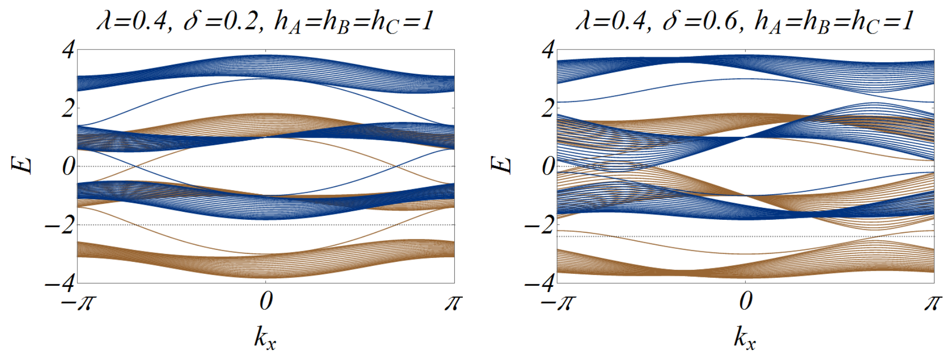

Fig. 9. (Color online) The band structure with different lattice modulations δ at fixed SOC and weak $h_A = h_B = h_C$. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at half and sixth fillings.

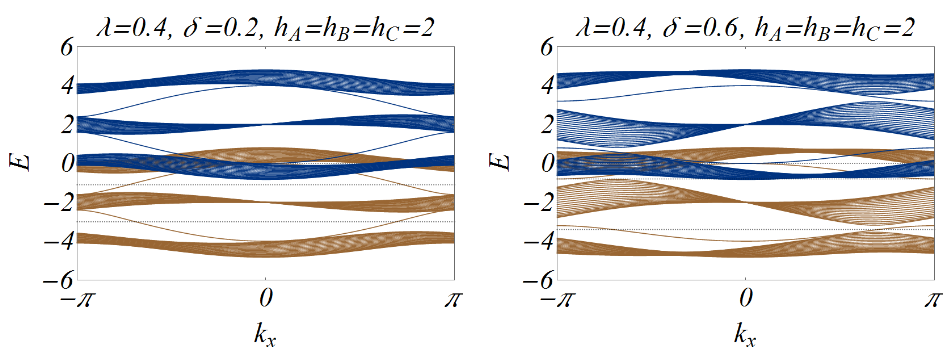

Fig. 10. (Color online) The band structure with different lattice modulations δ at fixed SOC and strong $h_A = h_B = h_C$. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at half, third and sixth fillings.

In general, we have observed the lattice modulation drives the ground state from a topological insulator to a band insulator, similar to the case when the magnetic field is absent [15]. However, when the ground state is half topology, i.e. when one spin component is a topological insulator while the other spin component is a band insulator, the topology of the ground state is robust again the lattice modulation. In Fig. 11 we plot this case. It shows the ground state remains

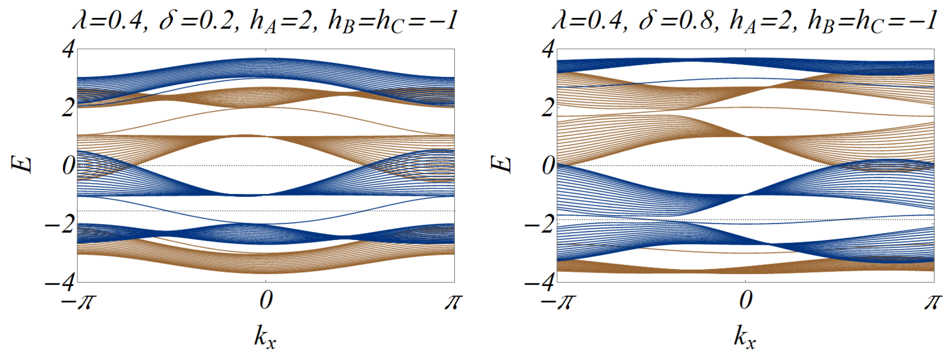

Fig. 11. (Color online) The band structure with different lattice modulations δ at fixed SOC and $h_A > 0 > h_B = h_C$. Brown (blue) color represents the band structure for the spin up (down) component. The dotted lines show a position of the chemical potential at half and third fillings.

half topology at third filling until strong lattice modulation. Only in the extreme case $\delta \to 1$, the topology is destroyed.

IV. CONCLUSION

We have studied the interplay between the SOC, the lattice modulation and the magnetic field in nano-ribons on the Lieb lattice. The interplay emerges various exotic states. Depending on the filling and the model parameters, the ground state may vary from band or topological insulating to half metallic and half topology. In the half metallic state one spin component is metallic and the other spin component is insulating. Half topology is characterized by the fact that one spin component becomes topological, while the other spin component still remains topologically trivial. The lattice modulation may drive the ground state from a topological insulator to a band insulator. However, the half topology is robust again the lattice modulation. The interplay between the SOC and the magnetic field broadens the flat band and leads to a complex Zeeman effect. In certain conditions of the SOC and the magnetic field, the ground state is paramagnetic even when the magnetic field is present. In this work we have only considered the nano-ribons with straight-straight open boundaries. The nano-ribons with other open boundaries will separately be studied in further works.

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