The Chern states on the honeycomb and Lieb lattices

Igor N. Karnaukhov and Igor O. Slieptsov

1G.V. Kurdyumov Institute for Metal Physics, 36 Vernadsky Boulevard, 03142 Kiev, Ukraine

The Haldane model of the Chern insulator is considered on the Lieb and honeycomb lattices. We provide a detailed analysis of the model’s ground-state phase diagram and demonstrate a scenario of the topological phase transitions in the system with a single-particle spectrum that includes flat and dispersion bands, that is realized on the Lieb lattice. We find that the Chern number of the flat band is non-zero, depending on the parameters of the model. We define the topological metal state as an intermediate state between topological insulator and trivial metal. The phase transition between topological insulator and topological metal states is accompanied by continuous changing of the Chern number, a jump of the surface charge or spin current defines the point of the topological metal-trivial metal phase transition. The results have been illustrated with numerical calculations of the model.

INTRODUCTION

The Haldane model [1] is a key model for understanding the topological states of 2D fermion systems— the Chern insulators. The Chern number C is well defined in insulator state, being an integer. The Berry curvature is a gauge-invariant for both insulator and metal phases, in metal phase it defines a Chern number as an integral over the Fermi surface (in contrast to insulator phase, where an integral is defined over the Brillouin zone). The topological state in the metal state may be characterized by the charge or spin Chern numbers, which define the surface charge or spin currents that have a topological nature in the metal state. We will study the Chern state in insulator and metal phases in the framework of the Haldane model defined on two different 2D lattices in order to investigate the peculiarities of their behavior.

Models of strongly correlated electrons in decorated 2D lattices (such as the Lieb lattice) are extensively studied, motivated by the search for metallic (flat-band) ferromagnetism [2]. Phase diagrams of such models include different phases with spin, charge and spin-charge orderings. The topological and nematic phases are realized on the Lieb lattice for single fermion states forming a flat band [3,4]. Traditionally, the topological insulator’s (TI) behavior derives from the dispersive bands that have nontrivial Chern numbers or \( Z_2 \) indices. The systems with dispersionless (flat) bands can be topologically non-trivial, e.g. flat Landau levels for particles in a magnetic field, where the fractional quantum Hall effect is the result of nontrivial correlated physics [5]. A 2D electron gas in transverse magnetic field, known as the Hofstadter model [6], represents various quantum Hall states, each one is characterized by a quantum number— the Chern number [7]. The Chern insulator state where the bulk-edge correspondence accompanies the topological insulator state is realized in the Hofstadter model [6,8] (see also ref. [9]).

A model of TI on the Lieb lattice in 2D and its 3D counterpart the perovskite or edge centered cubic lattice that takes in account a spin-orbit interaction term has been presented in ref. [8]. The next-nearest neighbor spin-orbit-induced interaction opens a gap in the M point and the system is TI at 1/3 and 2/3 band filling with \( Z_2 \) index equals to 1 for two dispersive bands and 0 for topologically trivial flat band. In ref. [4] the authors have considered a variant of the tight-binding model on the Lieb lattice that takes into account a staggered potential, nearest-neighbor (NN) and next-nearest-neighbor (NNN) hoppings of fermions. They have shown that the point of band crossing is not topologically non-trivial, but also only weak interaction can induce the TI phase. As a rule, the Chern number of the flat bands is \( C_{flat} = 0 \), therefore (opposed to Landau levels) we get no quantized Hall conductance for these particular flat bands.

We consider topological phase transitions in the framework of the Haldane model [1] on the honeycomb and Lieb lattices. The studied model is a variant of the Haldane model realizing on the Lieb lattice — the tight-binding model of TI with the NN and NNN hoppings. The orbitals on the different sites of unit cell in the cubic lattice have different energies. The phase diagram of the model also depends on the filling of the fermion bands, the TI phases are realized at 1/3 and 2/3 filling when the Fermi level is positioned within a forbidden band between flat and neighboring dispersing bands. At the point of the topological phase transition (TPT) the flat band and a neighboring dispersing band touch at the Dirac point. Breaking the time-reversal symmetry (TRS) leads to topological states that are fundamentally different from traditional insulator phases. In the studied model an inversion symmetry is conserved, the system exhibits a topological Chern insulator.

The purpose of this paper is to understand the topological state of the fermion system with different spectrum (namely band and flat band spectrum), to calculate the Chern numbers in both insulator and metal phases. We will shown also that the flat band is isolated in the TI phase due to breaking TRS, therefore the flat band can be viewed as critical point at TPT. In other words, we correlate the topological nature of the flat band and...
We will investigate the ground-state phase diagram in a one-particle excitations is a spatial inversion symmetric. TPT from which emerges a reincarnation of the quantum Hall conductivity. We will show that the Chern number of the flat band is changed from zero to one depending on parameters of the model. The Chern state exhibits the chiral gapless edge modes that define the surface charge or spin currents in metal and insulator phases.

THE STUDIED 2D MODEL OF THE CHERN INSULATOR

We will analyze the tight-binding model of the TI defined on the honeycomb and Lieb lattices, that describes an influence of a magnetic field. In the real space the Hamiltonian of the model is

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j - \tau \sum_{\langle i,j \rangle} \epsilon \phi_{ij} a_i^\dagger a_j + \epsilon \sum_{j=1}^{n_{\text{bands}}} a_j^\dagger a_j,$$  \hspace{1cm} (1)

where $a_i$ and $a_j^\dagger$ are the spinless fermion operators with the usual anticommutation relations. The first term represents NN hopping with a magnitude $t$, the second term is NNN hopping with a hopping parameter $\tau$ and a Peierls phase $\phi_{ij}$, the last term represents a staggered potential with a value $\epsilon$. The unit cell of the Lieb lattice consists of three sites for the lattice denoted as $A$, $B$, $C$ and two sites $A$ and $B$ for the honeycomb lattice (see fig. 1). The homogeneous Peierls phase $\phi_{ij}$ (denoted as $\pm \phi$ the clockwise (anticlockwise) NNN hopping relatively to a cell) is considered as the parameter of the model. The model defined on the honeycomb lattice has been introduced by Haldane. The phase state of the model on the Lieb lattice for two different complex phases $\phi = \pi/4$ and $\phi = \pi/2$ at filling 1/3 has been investigated recently in ref. [11].

The NNN hoppings in (1) breaks TRS which is crucial in obtaining the TI phase. The staggered potential does not break inversion symmetry, the spectrum of one-particle excitations is a spatial inversion symmetric. We will investigate the ground-state phase diagram in a low filling region at $0 < n \leq 1/2$. Using the particle-hole transformation $a_i^\dagger (a_j) \rightarrow a_i (a_j)^\dagger$ for the Hamiltonian (1), one may obtain the phase diagram at filling $1/2 < n \leq 1$, as $\mathcal{H}(t, \tau, \phi, \epsilon, n) \rightarrow \mathcal{H}(t, -\tau, \phi, -\epsilon, 1 - n)$. The model can be considered as the Haldane model defined on the Lieb and honeycomb lattices.

THE HONEYCOMB LATTICE

The phase diagram of the Haldane model has a rich structure for different values of $t$ and $\tau$ [11], in the case $t \gg \tau$ the system is in the insulator state at half-filling $n=1$. For arbitrary values of the parameters of the Hamiltonian the phase diagram consists of insulator, TI and metal phases at $n=1$. A traditional Haldane diagram $\epsilon = -3\sqrt{3} \tau \sin \phi$ (brown lines in fig. 2) that separates insulator and TI phases is realized in the $\tau < t$ limit. At $t < 5\tau$ the phase diagram contains a metal phase which is shown in fig. 2 for different values of $t$, this region decreases with increasing $t$.

The phase of TI is defined by the Haldane diagram at $t \gg \tau$, the spectrum of excitations has a traditional form for TI (see in fig. 3), where two bulk fermion subbands are connected via edge chiral modes. The Chern number and chiral edge modes define the state of the Chern insulator. In the system with zero-net magnetic field $C_{\gamma}$ yields a Hall surface conductance $\sigma_H = C_{\gamma} e^2/h$. The Chern number is a topological invariant which can be easily defined for a band isolated from all other bands by...
The phase transition to insulator phase can be realized at filling $n = 1/3$ ($n = 2/3$). In fig. 2, the phase diagram describes the phase transition between metal (or bad metal) and insulator phase states at $n = 1/3$. The Haldane-like diagram $\Delta_{\pm} = 0 \iff \epsilon = \pm 4\pi \sin \phi$ separates the phases of topological and trivial insulators for $\pi/4 < \phi < 7\pi/4$, the Chern number calculated according to (2) in the TI phase is equal to the signum of $\phi$. for $n \neq 1$ for a wide region of the Fermi energies (a grey region in fig 4). In other words, the topological metal state is characterized by a surface chiral edge current and $0 < C < 1$.

FIG. 3. Energy levels of the Haldane model on the honeycomb lattice calculated on a cylinder with open boundary conditions for a zig-zag boundary (a) in the (topologically trivial) insulator state at $\tau = 10\tau_2$, $\phi = \pi/2$, $\epsilon = 6\tau$ and (b) in TI state at $\tau = 10\tau_2$, $\phi = \pi/2$, $\epsilon = 2\tau$. The wave vector $k$ is along the boundary.

The phase transition to insulator phase can be realized at filling $n = 1/3$ ($n = 2/3$). In fig. 2, the phase diagram describes the phase transition between metal (or bad metal) and insulator phase states at $n = 1/3$. The Haldane-like diagram $\Delta_{\pm} = 0 \iff \epsilon = \pm 4\pi \sin \phi$ separates the phases of topological and trivial insulators for $\pi/4 < \phi < 7\pi/4$, the Chern number calculated according to (2) in the TI phase is equal to the signum of $\phi$. for $n \neq 1$ for a wide region of the Fermi energies (a grey region in fig 4). In other words, the topological metal state is characterized by a surface chiral edge current and $0 < C < 1$.

FIG. 4. The Chern number of the Haldane model as function of the Fermi energy $E_F$ calculated at (a) $\tau = 10\tau$, $\phi = \pi/2$, $\epsilon = 6\tau$ and (b) $\tau = 10\tau$, $\phi = \pi/2$, $\epsilon = 2\tau$ (the same parameters as in fig. 3), upper (red) dashed line stands for an upper subband, lower (blue) dashed line is for lower subband, a solid black line is for the total Chern number.
FIG. 5. Dispersion curves $E(k)$ ($k$ is the wave vector along the boundary) and Chern numbers $C$ of each band of the Lieb lattice finite in $y$-direction for different values of parameters, $t = 10\tau$, (a) $\epsilon = \tau$, $\phi = \pi/6$, (b) $\epsilon = 2\tau$, $\phi = \pi/6$, (c) $\epsilon = 4\tau$, $\phi = \pi/6$, (d) $\epsilon = 2\tau$, $\phi = \pi/3$, (e) $\epsilon = 6\tau$, $\phi = \pi/3$. Fermi levels for $n = 1/3$ and $n = 2/3$ are marked with red dashed lines.

The metal phase is realized only when $-\pi/4 < \phi < \pi/4$, a curve $\epsilon = -4\tau \cos \phi$ separates this phase from the trivial insulator state. The region of metal phase depends on the ration of $t/\tau$ and reduces to a stripe in the infinite $t$-limit; it shrinks with $t/\tau$ decreasing. Most TIs are narrow band gap semiconductors, thus $\tau/t \ll 1$ in practical situations. The Haldane-like diagram is defined by the TPT with the Dirac-like one-particle spectrum at the point $M$. Figs 3 demonstrate the one-particle spectrum of a finite 2D lattice and calculations of the Chern number of the subbands for different points of the phase diagram Fig. 2. The one-particle spectrum has gaps in topologically trivial and nontrivial insulator phases and a “quasiflat” band touches dispersing band at a Dirac-like point. The insulating phase state is defined by the Chern number of each subband of spinless fermions below the Fermi level. The sign of the Chern number determines the chirality of the edge modes on the Fermi level. As we have mentioned, the middle and upper bands acquire Chern numbers plus and minus one in trivial insulator phase at $n = 1/3$, while the lower one has $C = 0$. Moreover, the flatness and the Chern number of the middle (“quasiflat”) band $C_{\text{flat}}$ depend on the values of $\tau$, $\epsilon$ and $\phi$ and defined as

$$C_{\text{flat}} = \begin{cases} 0, & |\epsilon| < 4|\tau \sin \phi|, \\ \text{sgn}(\tau \sin \phi), & |\epsilon| > 4|\tau \sin \phi|. \end{cases}$$

In other words, the Haldane-like diagram is also strongly connected with the changing of the flat band’s topology.

The edge states are symmetric, when fermions on the boundary interact with fermions along the boundary. We compare the calculations of the Chern number and the number edge modes that cross the Fermi surface for given filling of the system. Such approach gives possibility to find “bulk-edge correspondence in metallic phase” in the model with a flat band. The behavior of the Chern number calculated on the Lieb lattice (figs 6) for different $E_F$ is similar to the case of the honeycomb lattice (figs 4). Calculations of the Chern number for topologically trivial and nontrivial flat bands are shown in figs 6. The phase transition from TI state with $C = -1$ at $E_F = 0$ to the trivial metal state is realized via an intermediate topological metal phase.

The calculations of the Chern number in the framework of the Haldane and Lieb models show that the topological metal state is realized as an intermediate state between TI and metal states at doping of system. According to figs 4 and figs 6 this topological state is characterized by both $0 < |C| < 1$ and one or two edge mode(s). In other words, the topological order $C \neq 0$ and the chiral edge mode(s) that take place in the metal phase give us possibility to consider this metal state as topological.

**CONCLUSIONS**

Let us consider the spin variant of the model [1] with different sings of the hopping integrals $\tau_\sigma = \sigma_2 \tau$ [12]. The system is the sum of two decoupled subsystems of $\sigma = \uparrow, \downarrow$ and their Chern numbers $C_\sigma$ are topologi-
FIG. 6. The Chern number as function of the Fermi energy $E_F$ numerically calculated on the Lieb lattice for (a) topologically trivial ($\epsilon = 2\tau$) and (b) topologically nontrivial ($\epsilon = 6\tau$) flat band, $t = 10\tau$, $\phi = \pi/3$. Dashed lines stand for Chern number of each subband, while a solid line is a total.

cal indices. Their sum (total Chern number) and the half of their difference (the spin Chern number) define the topological states of such system. A spin current $J = (\hbar/2e)(J_F - J_L)$ is characterized by a quantized spin Hall conductivity. The edge spin current defines a topological metal state of system, because it is equal to zero in the topologically trivial metal state. The Chern number in the topological metal state is less than one and nonequal to zero, it defines the topological phase transition from TI state (with $C = 1$) to the topological metal state (with $0 < C < 1$). The phase transition from the topological metal state to the trivial metal state is realized for $C \neq 0$, in this case the jump of the edge charge or spin currents defines the point of topological metal–trivial metal phase transition.

We have show that the topological insulator states in the Lieb lattice are realized at one third and two third band filling when the Fermi level separates narrow (nearly dispersionless) and neighboring dispersing bands of spinless fermions. The Chern number of the flat band depends on the parameters of the model, its value is changed at the point of the topological phase transition.

[1] F.D.M. Haldane, Phys. Rev. Lett., 61, 2015 (1988).
[2] J.D. Gouveia and R.G. Dias, Journal of Magnetism and Magnetic Materials, 382, 312 (2015); K. Noda, K. Inaba, and M. Yamashita, Phys. Rev. A, 90, 043624 (2014); J.D. Gouveia and R.G. Dias, Solid State Communications, 185, 21 (2014); J.D. Gouveia and R.G. Dias, Spin and charge density waves in the Lieb lattice, arXiv:1505.01656v1 [cond-mat.str-el]; K. Noda, K. Inaba and M. Yamashita Magnetism in the three-dimensional layered Lieb lattice: Enhanced transition temperature via flat-band and Van Hove singularities, arXiv:1505.06591.
[3] C. Weeks and M. Franz, Phys. Rev. B 85, 041104R (2012).
[4] W.-F. Tsai, C. Fang, H. Yao and J. Hu, New J. Phys. 17, 055016 (2015).
[5] S.A. Parameswaran, R. Roy and S.L. Sondhi, Comptes Rendus Physique, 14, 816 (2013); S.A. Parameswaran, R. Roy and S.L. Sondhi, Phys. Rev. B 85, 241308R (2012).
[6] D. Hofstadter, Phys Rev B 14, 2239 (1976).
[7] D.J. Thouless, M. Kohmoto, M.P. Nightingale, M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
[8] G.Naumis and I.I.Satija Topological Map of the Hofstadter Butterfly Macroscopic Chern Annihilations and Van Hove Singularities, arXiv:1507.08130v1 [cond-mat.other] 29 Jul 2015.
[9] Y.Zhang, D.Bulmash, A.V. Maharaj, C.-M. Jian, and S.A. Kivelson The almost mobility edge in the almost Mathieu equation, arXiv:1504.05205v2 [cond-mat.mes-hall] 25 Jun 2015.
[10] B. Jaworowski, A. Manolescu and P. Potasz, Fractional Chern Insulator phase at the transition between checkerboard and Lieb lattice arXiv:1508.04399 [cond-mat.str-el] 2015.
[11] I.N. Karnaukhov and I.O. Sliptsov, Eur.Phys.J. B, 87, 230 (2014).
[12] C.L. Kane and E.J. Mele, Phys. Rev. Lett. 95, 146802 (2005).