Nearly flat band with Chern number $C = 2$ on the dice lattice

Fa Wang$^1$ and Ying Ran$^2$

$^1$Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
$^2$Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA

(Dated: March 21, 2012)

We point out the possibility of a nearly flat band with Chern number $C = 2$ on the dice lattice in a simple nearest-neighbor tightbinding model. This lattice can be naturally formed by three adjacent (111) layers of cubic lattice, which may be realized in certain thin films or artificial heterostructures, such as the SrTiO$_3$/SrIrO$_3$/SrTiO$_3$ trilayer heterostructure grown along the (111) direction. The flatness of two bands is protected by the bipartite nature of the lattice. Including the Rashba spin-orbit coupling on nearest-neighbor bonds separate the flat bands from the others but maintains their flatness. Repulsive interaction will drive spontaneous ferromagnetism on the Kramer pair of the flat bands and split them into two nearly flat bands with Chern number $C = \pm 2$. We thus propose that this may be a route to the quantum anomalous Hall effect and further conjecture that the partial filling of the $C = 2$ band may realize exotic fractional quantum Hall effects.

PACS numbers: 71.10.Fd,73.43.Cd,73.20.At

A few years after the experimental discovery of integer quantum hall effect (IQHE)\cite{Haldane88}, Haldane wrote down a tight-binding model on the honeycomb lattice with IQHE\cite{Haldane88}, explicitly showing that the essence of IQHE is not the external magnetic field. However, it takes more than two decades for people to show that the similar statement is also true for fractional quantum Hall effect (FQHE). Recently several groups have proposed to realize FQHE without Landau levels\cite{Haldane04,Heinrich08}. The basic idea is to engineer a nearly flat band in two dimensions (2D) with nonzero Chern number. Electron interaction in this partially filled band may realize fractional quantum Hall effect, as suggested by exact diagonalization studies\cite{Kato08,Long09,Chen10}.

In these proposals nearly flat bands are obtained by fine-tuning ratios between nearest-neighbor (NN), next-nearest-neighbor (NNN), and even further neighbor tight-binding parameters. In this paper we point out a route to get completely flat bands without this fine-tuning by employing a bipartite lattice with unequal number of two subsets of sites\cite{Wang12}. As a concrete example we consider the dice lattice as shown in Fig. 1. It is bipartite with unequal number of two subsets of sites (the coordination-number-3 sites are twice as many as the coordination-number-6 sites). This system is inversion symmetric with respect to the coordination-number-6 sites. We consider a single s-orbital with spin-1/2 degrees of freedom (DOF) on every site, and mainly focus on systems close to half-filling, i.e., one electron per site. The NN tight-binding model, including the Rashba-type spin-orbit coupling (SOC) consistent with lattice symmetry, will produce two completely flat bands separated from the other bands. Because the two flat bands are half-filled, ferromagnetism is a natural consequence of correlation\cite{Wang12,Mitra06,Yang07}, which gives rise to a Zeeman field on the mean-field level. We demonstrate the spontaneous ferromagnetism by a variational wave function study of Hubbard interactions.

As a nice feature of the current model system, even a small Zeeman field can split this Kramer pair of flat bands and produce two separated nearly flat bands with Chern number $C = \pm 2$. Filling one of them will then produce quantized anomalous Hall (QAH) effect with $\sigma_{xy} = 2e^2/h$. This Zeeman field could also be extrinsic, e.g., growing the system on a ferromagnetic substrate. Note that in a usual ferromagnetic system, a realistic Zeeman splitting would not completely separate the two bands with opposite spin polarizations, and a ferromagnetic metal results. This is partially why the QAH insulator, which needs to be a ferromagnetic insulator, has not been realized experimentally so far. The main advantage of the presently studied system is the existence of the half-filled flat bands, which naturally support well-separated bands by a realistic Zeeman splitting.

Material realizations: This model Hamiltonian may actually be relevant to some real systems. Heterostructures of transition metal oxide (TMO) perovskites, whose crystal structures are cubic, are becoming available owing to the recent development\cite{Hruza11,Dowben12} in the fields of oxide superlattices and oxide electronics (for a review, see\cite{Wang12}). In particular, layered structures of TMO heterostructures can now be prepared with atomic precision, thus offering a high degree of control over important material properties, such as lattice constant, carrier concentration, spin-orbit coupling, and correlation strength.

TMO heterostructures grown along the (111) direction have been synthesized experimentally (e.g., Ref.\cite{Hruza11,Heinrich08}). Recently it was pointed out that TMO (111) bilayer heterostructures are promising candidates hosting various topological phases of matter\cite{Wang12}. The dice lattice here can be formed by three adjacent (111) layers of cubic lattice, each of which is a triangular lattice (Fig. 1). Although we considered only simple s-orbital on every site here, the result should be valid if the active orbital is a one dimensional representation of the $D_{3h}$ group. Some examples are the $p_{Z}$-orbital ($p_{x} + p_{y} + p_{z}$), and the $a_{1g}$ orbital $(d_{yz} + d_{zx} + d_{xy})$ of $d$-electrons under cubic and trigonal crystal potential.

A particularly relevant example is the transition metal oxide SrTiO$_3$/SrIrO$_3$/SrTiO$_3$ trilayer heterostructure.
Note that although the crystal structure of the bulk SrIrO$_3$ is a monoclinic distortion of the hexagonal BaTiO$_3$ structure, thin films of perovskite SrIrO$_3$ have been synthesized on substrates, which are reported to be metallic. This indicates that an itinerant electronic model could be a good starting point of describing the SrTiO$_3$/SrIrO$_3$/SrTiO$_3$ trilayer heterostructure. Due to the strong spin-orbit coupling on the Ir$^{4+}$ ion, together with the octahedral crystal field, the active orbital is a half-filled effective orbital with the octahedral crystal field, the active orbital is a half-filled effective orbital.

Therefore we think that our proposal is a promising route to realize QAH effect. In the same spirit of previous works on the FQHE without Landau levels, we conjecture that fractional filling of these bands might produce exotic fractional quantum hall (FQH) states. The nature of these FQH states remains unclear and we leave it as a subject of future research. But it is worth pointing out that, in a nearly flat band with Chern number $C = 2$, the natural candidate ground states for $\nu = 1/m$ (m is odd integer) filling fractions are non-abelian states described by SU($m$)$_2$ Chern-Simons effective theory.

**NN model without SOC.** The dice lattice and coordination system are defined in Fig. 1. Label the three sublattices by V$_{1,2,3}$ respectively. Consider a single s-orbital with spin-1/2 DOF on every site. As a warmup consider NN spin-independent hopping only:

$$H_0 = -\sum_{\langle ij \rangle, \alpha} (t c^\dagger_{i\alpha} c_{j\alpha} + h.c.) - \sum_{i \in V_3} \epsilon n_i,$$

where $\alpha = \uparrow, \downarrow$ labels spin, $i, j$ label sites, $n_i = \sum_{\alpha} c^\dagger_{i\alpha} c_{i\alpha}$ is the electron density on site $i$. Note that sublattice-3 (V$_3$) has an onsite energy difference $\epsilon$ from the other two sublattices, as is allowed by symmetry. In this section the spin DOF will be omitted.

In momentum space the hamiltonian reads

$$H_0(k) = -\begin{pmatrix} 0 & 0 & t \gamma_k^* \\ 0 & 0 & t \gamma_k \\ t \gamma_k & t \gamma_k & \epsilon \end{pmatrix},$$

where $\gamma_k = 1 + e^{ik_1} + e^{ik_2}, \epsilon = \sqrt{-1}, k_{1,2} = k \cdot e_{1,2}$ respectively, and the basis is $(c_{1k}, c_{2k}, c_{3k})$. This model has three bands with dispersions $E_1 = -\epsilon/2 - \sqrt{\epsilon^2/4 + 2t^2|\gamma_k|^2}$, $E_2 = 0$, and $E_3 = -\epsilon/2 + \sqrt{\epsilon^2/4 + 2t^2|\gamma_k|^2}$, as illustrated in Fig. 2(a).

The flat band has Bloch wavefunction $(\gamma_k^*, -\gamma_k, 0)$ on the three sublattices. It has local Wannier functions residing on the six neighbors of a coordination-number-6 site (sublattice-3) with opposite amplitudes between sublattice-1 and sublattice-2.

**NN model with Rashba SOC.** Rashba SOC induced by electric fields can be included as

$$H_{0,SO} = H_0 - \sum_{\langle ij \rangle, \alpha, \beta} [i \lambda c^\dagger_{i\alpha} (\mathbf{D}_{ij} \cdot \sigma)_{\alpha\beta} c_{j\beta} + h.c.],$$

where $\sigma$ are spin Pauli matrices, $\mathbf{D}_{ij}$ is the unit vector along the direction of the cross product $\mathbf{E}_{ij} \times \mathbf{r}_{ij}$ of elec-
tric field $E_{ij}$ and displacement $r_{ij}$ for bond $ij$, $\lambda$ is the strength of SOC and is uniform on all NN bonds as required by translation and $D_{3d}$ symmetry of the tri-layer. The $D_{3d}$ symmetry further restricts the direction of $E_{ij}$ to be within the vertical [perpendicular to the (111) layers] plane containing bond $ij$. Therefore $\mathbf{D}_{ij}$ are all parallel to the (111) layers. Their directions are illustrated in Fig. 1. In momentum space the hamiltonian reads

$$H_{0, SOC}(\mathbf{k}) = H_{0}(\mathbf{k}) \otimes 1_{2 \times 2} - i \lambda \begin{pmatrix} 0 & 0 & 0 & 0 & \gamma_{k+}^* & 0 \\ 0 & 0 & 0 & 0 & \gamma_{k-}^* & 0 \\ 0 & 0 & 0 & 0 & \gamma_{k-}^* & 0 \\ 0 & 0 & 0 & 0 & \gamma_{k+}^* & 0 \\ -\gamma_{k-} & 0 & -\gamma_{k+} & 0 & 0 & 0 \\ -\gamma_{k+} & 0 & -\gamma_{k-} & 0 & 0 & 0 \end{pmatrix},$$

(5)

where $\gamma_{k+} = 1 + e^{i(kz+2\pi/3)} + e^{i(kz+4\pi/3)}$, and the basis is $(c_{1k1}, c_{1k1}, c_{2k1}, c_{2k1}, c_{3k1}, c_{3k1})$. It has three doubly degenerate bands with dispersions $E_1 = -\epsilon/2 - \sqrt{\epsilon^2/4 + 2t^2|\gamma_{k+}|^2 + \lambda^2(|\gamma_{k-}|^2 + |\gamma_{k+}|^2)}$, $E_2 = 0$, $E_3 = -\epsilon/2 + \sqrt{\epsilon^2/4 + 2t^2|\gamma_{k+}|^2 + \lambda^2(|\gamma_{k-}|^2 + |\gamma_{k+}|^2)}$. If $\lambda < \epsilon$, the effective four-band hamiltonian at the original band touching point $\pm K$ is

$$\frac{3t^2}{4\epsilon} \begin{pmatrix} |\delta k|^2 & \delta k_+^2 \\ \delta k_+^2 & |\delta k|^2 \end{pmatrix} \otimes 1_{2 \times 2} + \frac{3\sqrt{3}\lambda t}{2\epsilon} \begin{pmatrix} 0 & k_+ \\ k_- & 0 \end{pmatrix} + \frac{9\lambda^2}{2\epsilon} \begin{pmatrix} 1_{4 \times 4} \pm \tau^z \otimes \sigma^z \\ O(\lambda^2 \delta k) + O(\delta k^4), \end{pmatrix}$$

(6)

where Pauli matrix $\tau^z$ acts on the sublattices-1,2 space. The mass term $\tau^z \otimes \sigma^z$ has opposite sign between the two band touching points $\pm K$, similar to the Haldane model. The dispersions are illustrated in Fig. 2(b). There are still two completely flat band dictated by the hamiltonian structure.

The flat bands have Bloch wavefunctions $(t \gamma_{k+}^* \Gamma_k \cdot \pi \lambda \gamma_{k-}^* \Gamma_k \cdot -t \gamma_{k+} \Gamma_k \cdot -\pi \lambda \gamma_{k-} \Gamma_k \cdot 0, 0)$ and its Kramer pair, where $\Gamma_k = \gamma_{k+} \gamma_{k-} - \gamma_{k-}^* \gamma_{k+}$. Therefore these flat bands also have local Wannier functions. One of the Wannier functions is illustrated in Fig. 3. The other Wannier functions can be produced by translation and time-reversal. Note that the spin-up component of the illustrated Wannier function acquires a phase $2\pi/3$ under six-fold rotation around its “guiding center”, similar to the cyclotron orbit in Landau levels except that the phase here is twice as large, suggesting Chern number $C = 2$. The Wannier functions is illustrated in Fig. 3. The other Wannier functions can be produced by translation and time-reversal. Note that the spin-up component of the illustrated Wannier function acquires a phase $2\pi/3$ under six-fold rotation around its “guiding center”, similar to the cyclotron orbit in Landau levels except that the phase here is twice as large, suggesting Chern number $C = 2$. The previous double-degeneracy of the flat bands is protected by time-reversal symmetry. Consider magnetic field effect,

$$H_{0, SOC + B} = H_{0, SOC} - g \sum_i B_i \cdot S_i$$

(7)

where $S_i = (1/2) \sum_{\alpha, \beta} \delta_{\alpha \beta}^4 c_{\alpha i} \sigma_{\alpha \beta} c_{\beta i}$ is electron spin, the Bohr magneton $\mu_B$ is omitted, and $g = 2$ ($g = -2$ for the $J_{eff} = 1/2$ states of Ir$^{4+}$ ion) is assumed hereafter. The field on sublattice-1, 2 may be different from that on sublattice-3. For illustration purpose we draw the band structure with uniform field $B_i = 0.2t$ along (111) direction (Z direction) in Fig. 2(c). As expected the Kramer pair of flat bands split into two nearly flat bands. Direct
computation of Chern numbers shows that they carry Chern number $C = \pm 2$ [Fig. 2(c)].

There is a simple physical argument that proves the $C = \pm 2$ for the two nearly flat bands. Let us turn off the Rashba-type spin-orbit coupling $\lambda$ for the moment. Note that the sublattice-1,2 form a honeycomb lattice by themselves. We could turn on another artificial $\lambda \sigma \cdot (1,1,1)$ spin-orbit coupling between the second-neighbors on these two sublattices only, with the same signs as the Kane-Mele model\cite{Kanemele2005}. In this $\lambda_1$-only model, spin rotation along (111) direction is not the free fermion wavefunction by half-filling this mean field hamiltonian with magnetic field. We hope these results could encourage experimental syntheses and characterization of the material proposed here, as well as future theoretical investigations on the nature of the possible FQH states.

The edge state on a cylindrical geometry is also shown in Fig. 4. The three occupied mean field bands have total Chern number $C = 2$ and exhibit anomalous quantum Hall effect. The edge state on a cylindrical geometry is also shown in Fig. 4.

**Conclusion.** In this paper we discuss a model with spin-orbit coupling on the dice-lattice and the correlation physics in it. A transition metal oxide SrTiO$_3$/SrIrO$_3$/SrTiO$_3$ trilayer heterostructure grown along the (111) direction, where this model may be realized, is proposed. In this system, two degenerate flat bands at half-filling are found. Stoner’s instability naturally leads to ferromagnetism and split the two bands, which gives rise two nearly flat bands with Chern number $\pm 2$. This indicate a promising route to realize QAHE. We further speculate that further doping into the nearly flat Chern bands could lead to FQHE without an external magnetic field. We hope these results could encourage experimental syntheses and characterization of the material proposed here, as well as future theoretical investigations on the nature of the possible FQH states.

FW thanks the Institute for Advanced Study at Tsinghua University for hospitality where part of this work was finished. YR is supported by the startup fund at Boston College.

---

1. K. v. Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. 45, 494 (1980).
2. F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
3. Evelyn Tang, Jia-Wei Mei, and Xiao-Gang Wen, Phys. Rev. Lett. 106, 236802 (2011).
4. Kai Sun, Zhengcheng Gu, Hosho Katsura, and S. Das Sarma, Phys. Rev. Lett. 106, 236803 (2011).
5. Titus Neupert, Luiz Santos, Claudio Chamon, and
Christopher Mudry, Phys. Rev. Lett. 106, 236804 (2011).
6 D.N. Sheng, Z.C. Gu, K. Sun, and L. Sheng, Nature Commun. 2, 389 (2011).
7 X. Hu, M. Kargarian, G. A. Fiete, Phys. Rev. B 84, 155116 (2011).
8 N. Regnault, B. A. Bernevig, arXiv:1105.4867 (unpublished).
9 E. H. Lieb, Phys. Rev. Lett. 62, 1201 (1989).
10 A. Mielke, J. Phys. A 24, 3311 (1991).
11 H. Tasaki, Phys. Rev. Lett. 69, 1608 (1992).
12 E. C. Stoner, Phil. Mag. 15, 1018 (1933).
13 M. Izumi, Y. Ogimoto, Y. Konishi, T. Manako, M. Kawasaki, and Y. Tokura. Materials Science and Engineering B, 84, 53 (2001).
14 A. Ohtomo, D. A. Muller, J. L. Grazul, and H. Y. Hwang. Nature, 419, 378 (2002).
15 A. Ohtomo, and H. Y. Hwang. Nature, 427, 423 (2004).
16 J. Mannhart, and D. G. Schlom. Science, 327, 1607 (2010).
17 S. Chakraverty, A. Ohtomo, and M. Kawasaki. Applied Physics Letters, 97, 243107 (2010).
18 Benjamin Gray, Ho Nyung Lee, Jian Liu, J. Chakhalian, and J. W. Freeland. Applied Physics Letters, 97, 013105 (2010).
19 Di Xiao, Wenguang Zhu, Ying Ran, Naoto Nagaosa, and Satoshi Okamoto. arXiv:1106.4296 (unpublished).
20 J. M. Longo, J. A. Kafalas, and R. J. Arnott, J. Solid State Chem. 3, 174 (1971).
21 S. J. Moon, H. Jin, K.W. Kim, W. S. Choi, Y. S. Lee, J. Yu, G. Cao, A. Sumi, H. Funakubo, C. Bernhard, and T.W. Noh, Phys. Rev. Lett. 101, 226402 (2008).
22 Y.K. Kim, A. Sumi, K. Takahashi, S. Yokoyama, S. Ito, T. Watanabe, K. Akiyama, S. Kaneko, K. Saito, and H. Funakubo, Jpn. J. Appl. Phys. 45, L36 (2005); A. Sumi, Y.K. Kim, N. Oshima, K. Akiyama, K. Saito, H. Funakubo, Thin Solid Films 486, 182 (2005).
23 Yuan-Ming Lu, and Ying Ran, arXiv:1105.0226 (unpublished).
24 E. McCann, and V. I. Falko, Phys. Rev. Lett. 96, 086805 (2006).
25 D. L. Bergman, C. Wu, and L. Balents, Phys. Rev. B 78, 125104 (2008).
26 B. Bleaney, and M. C. M. O’Brien, Proc. Phys. Soc. B 69, 1216 (1956).
27 C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).