

MIT Open Access Articles

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

The MIT Faculty has made this article openly available. **Please share** how this access benefits you. Your story matters.

Citation: Wang, Fa, and Ying Ran. "Nearly Flat Band with Chern Number $C=2$ on the Dice Lattice." *Physical Review B* 84.24 (2011): n. pag. Web. 8 Mar. 2012. © 2011 American Physical Society

As Published: <http://dx.doi.org/10.1103/PhysRevB.84.241103>

Publisher: American Physical Society (APS)

Persistent URL: <http://hdl.handle.net/1721.1/69601>

Version: Final published version: final published article, as it appeared in a journal, conference proceedings, or other formally published context

Terms of Use: Article is made available in accordance with the publisher's policy and may be subject to US copyright law. Please refer to the publisher's site for terms of use.



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

Fa Wang¹ and Ying Ran²

¹*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

²*Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA*

(Received 2 September 2011; published 1 December 2011)

We point out the possibility of a nearly flat band with Chern number $C = 2$ on the dice lattice in a simple nearest-neighbor tight-binding 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 SrTiO₃/SrIrO₃/SrTiO₃ 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 causes the flat bands to separate from the others but maintain 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.

DOI: 10.1103/PhysRevB.84.241103

PACS number(s): 71.10.Fd, 73.43.Cd, 73.20.At

A few years after the experimental discovery of the integer quantum hall effect (IQHE),¹ Haldane wrote a tight-binding model on the honeycomb lattice with IQHE,² explicitly showing that the essence of IQHE is *not* the external magnetic field. However, it took more than two decades for people to show that a similar statement is also true for the fractional quantum Hall effect (FQHE). Recently several groups have proposed to realize FQHE without Landau levels.^{3–7} The basic idea is to engineer a nearly flat band in two dimensions (2D) with a nonzero Chern number. Electron interaction in this partially filled band may realize a fractional quantum Hall effect, as suggested by exact diagonalization studies.^{4,5,7}

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 Rapid Communication, 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.⁸ As a concrete example, we consider the dice lattice as shown in Fig. 1. It is bipartite with an 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- $\frac{1}{2}$ degrees of freedom (DOFs) on every site and mainly focus on systems close to half-filling, that is, 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,^{8–11} 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 a quantized anomalous Hall (QAH) effect with $\sigma_{xy} = 2\frac{e^2}{h}$. This Zeeman field could also be extrinsic, for example, 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 recent developments^{12–14} in the fields of oxide superlattices and oxide electronics (for a review, see Ref. 15). 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., Refs. 16 and 17). Recently it was pointed out that TMO (111) bilayer heterostructures are promising candidates for hosting various topological phases of matter.¹⁸ 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 a simple s -orbital on every site here, the result should be valid if the active orbital is a one-dimensional representation of the D_{3d} 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 potentials.

A particularly relevant example is the transition-metal oxide SrTiO₃/SrIrO₃/SrTiO₃ trilayer heterostructure. Note that although the crystal structure of the bulk SrIrO₃ is a monoclinic distortion of the hexagonal BaTiO₃ structure,¹⁹ thin films of perovskite SrIrO₃ have been synthesized on substrates,²⁰ which are reported to be metallic.²¹ This indicates that an itinerant electronic model could be a good starting point for describing the SrTiO₃/SrIrO₃/SrTiO₃ trilayer heterostructure. Due to the strong spin-orbit coupling on the Ir⁴⁺ ion,

together with the octahedral crystal field, the active orbital is a half-filled effective $J_{\text{eff}} = \frac{1}{2}$ doublet.²¹ The explicit form of these doublet in the presence of cubic symmetry is $|J_z = \frac{1}{2}\rangle = \frac{1}{\sqrt{3}}(+i|xy, \uparrow\rangle - |xz, \downarrow\rangle + i|yz, \downarrow\rangle)$, and $|J_z = -\frac{1}{2}\rangle$ is its time-reversal partner. These half-filled orbitals hop around the dice lattice and contribute to states close to the Fermi level, indicating the correlation in the bulk system is intermediate. In a (111) heterostructure, cubic symmetry is reduced to trigonal symmetry. Nevertheless, to the leading order with respect to trigonal distortion, the nearest-neighbor hoppings between these $J = \frac{1}{2}$ orbitals are identical to the hoppings of the s orbitals, which form the model Hamiltonian considered here.

Therefore, we think that our proposal is a promising route to realize the 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. However, 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.²²

NN model without SOC. The dice lattice and coordination system are defined in Fig. 1. Label the three sublattices by

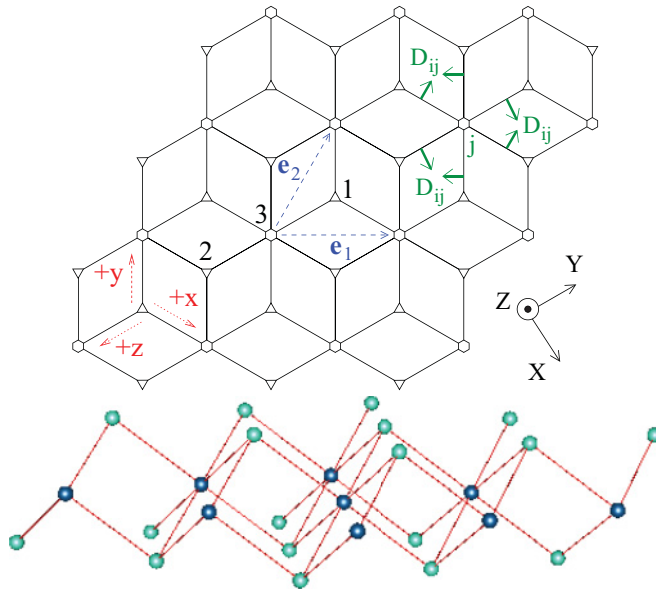


FIG. 1. (Color online) Top: The dice lattice. Small upward triangles (bottom layer), downward triangles (top layer), and hexagons (middle layer) indicate the three sublattices. Numbers 1, 2, and 3 label the three basis sites in the unit cell at origin. Coordination-number-3 sites (1 and 2) and coordination-number-6 sites (3) are the two subsets of this bipartite lattice. Blue dashed arrows labeled by \mathbf{e}_1 and \mathbf{e}_2 indicate the two translations of the dice lattice. Thick green arrows labeled as D_{ij} indicate the Rashba SOC directions on those bonds ij , with coordination-number-6 site j . Red dotted arrows with the labels $+x$, $+y$, and $+z$ indicate of the projection of the cubic lattice axis. Capital letters X , Y , and Z are axes for spin space in Rashba SOC. Z is the original (111) direction. Bottom: Perspective view of three adjacent (111) layers of the cubic lattice. The middle layer has a different color for easy recognition. The top view of this trilayer is the dice lattice.

$\mathcal{V}_{1,2,3}$ respectively. Consider a single s orbital with spin- $\frac{1}{2}$ DOF on every site. As a warmup, consider NN spin-independent hopping only:

$$H_0 = - \sum_{(ij), \alpha} (t c_{i\alpha}^\dagger c_{j\alpha} + \text{H.c.}) - \sum_{i \in \mathcal{V}_3} \epsilon n_i, \quad (1)$$

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

In momentum space, the Hamiltonian reads

$$H_0(\mathbf{k}) = - \begin{pmatrix} 0 & 0 & t \gamma_{\mathbf{k}}^* \\ 0 & 0 & t \gamma_{\mathbf{k}} \\ t \gamma_{\mathbf{k}} & t \gamma_{\mathbf{k}}^* & \epsilon \end{pmatrix}, \quad (2)$$

where $\gamma_{\mathbf{k}} = 1 + e^{i k_1} + e^{i k_2}$, $i = \sqrt{-1}$, $k_{1,2} = \mathbf{k} \cdot \mathbf{e}_{1,2}$ respectively, and the basis is $(c_{1\mathbf{k}}, c_{2\mathbf{k}}, c_{3\mathbf{k}})$. This model has three bands with dispersions $E_1 = -\epsilon/2 - \sqrt{\epsilon^2/4 + 2t^2|\gamma_{\mathbf{k}}|^2}$, $E_2 = 0$, and $E_3 = -\epsilon/2 + \sqrt{\epsilon^2/4 + 2t^2|\gamma_{\mathbf{k}}|^2}$, as illustrated in Fig. 2(a).

The middle band is completely flat as required by the bipartiteness. However, the top band touches the flat bands quadratically at the Brillouin zone corners $\pm \mathbf{K} = \pm(k_1 = 4\pi/3, k_2 = 2\pi/3)$, similar to double-layer graphene²³ or certain other models with flat bands.²⁴ The effective two-band Hamiltonian at the band touching point $\pm \mathbf{K}$ is

$$\frac{3t^2}{4\epsilon} \begin{pmatrix} |\delta \mathbf{k}|^2 & \delta k_{\pm}^2 \\ \delta k_{\mp}^2 & |\delta \mathbf{k}|^2 \end{pmatrix} + O(\delta \mathbf{k}^4), \quad (3)$$

where $\delta \mathbf{k} = \mathbf{k} \mp \mathbf{K}$, $\delta k_{\pm} = e^{i\pi/3}(\delta k_x + i \delta k_y)$, and $\delta k_{-} = (\delta k_{+})^*$.

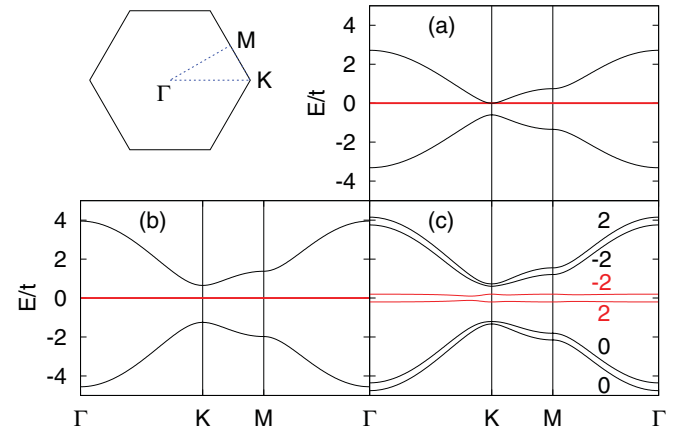


FIG. 2. (Color online) Dispersions of NN tight-binding models on dice lattice along high-symmetry directions. Parameters used are $\epsilon = 0.6t$, $\lambda = 0.3t$, and $B = 0.2t$. The bands marked as red in the middle are the (nearly) flat bands. Top left corner is the Brillouin zone with the high-symmetry lines indicated by dashed blue lines. (a) Spin-independent hoppings only. (b) Spin-independent hoppings plus Rashba SOC λ . (c) Spin-independent hoppings plus Rashba SOC λ and magnetic field B along the Z (111) direction. The Chern number of each band is indicated.

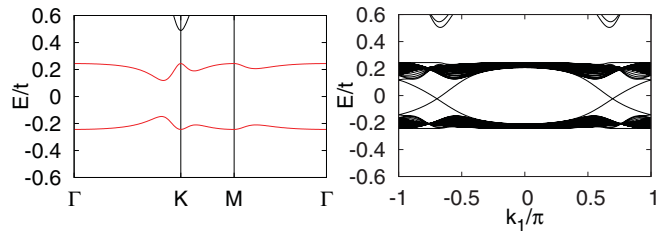


FIG. 4. (Color online) Left: The two nearly flat bands (red) with Chern numbers $C = \pm 2$. Parameters are $\epsilon = 0.6t$, $\lambda = 0.3t$, $B_1 = 0.2440t$, and $B_3 = -0.0162t$. Right: Dispersion of a cylinder with 32-unit-cell open boundary condition along \mathbf{e}_2 and periodic boundary condition along \mathbf{e}_1 , showing the edge states between the nearly flat bands.

\mathbf{B} along (111) split the $C = \pm 2$ bands, and clearly, the resulting bands and their Chern numbers must be very similar to those of the λ -only model [see Fig. 2(c)]. By fixing a Zeeman field \mathbf{B} , it turns out that one can adiabatically connect the λ_1 -only model with the λ -only model by interpolation while keeping all the six bands isolated from one another. This adiabatic evolution preserves the Chern numbers of each bands. We thus prove the Chern numbers in Fig. 2(c).

Spontaneous ferromagnetism. The flat band is half-filled if the entire system is at half-filling. Add onsite Hubbard interactions in the Hamiltonian,

$$H_{\text{int}} = H_{0,\text{SOC}} + \sum_i U n_{i\uparrow} n_{i\downarrow}. \quad (8)$$

If SOC $\lambda = 0$, by Lieb's theorem⁸ the ground state is ferromagnetic with total spin $S = (\frac{1}{2})[(N_1 + N_2) - N_3] = (\frac{1}{2})N_{\text{cell}}$ ($N_{1,2,3}$ is the number of sites on sublattices 1, 2, and 3 respectively and equals the number of unit cells N_{cell}). With Rashba λ there is no known proof of ferromagnetism. We use a variational (mean-field) treatment of this problem.

The ferromagnetic “mean-field” Hamiltonian is just the free fermion Hamiltonian with magnetic field $H_{0,\text{SOC}+B}$. By inversion symmetry we assume fields on sublattices 1 and

2 are the same, $\mathbf{B}_2 = \mathbf{B}_1$, but may be different from that on sublattice 3, \mathbf{B}_3 . The variational wave function is the free fermion wave function by half-filling this mean-field Hamiltonian. We then evaluate the energy expectation value of the Hubbard model H_{int} and try to minimize it with respect to the variational parameters \mathbf{B}_1 and \mathbf{B}_3 . From preliminary numerical results, the system is unstable to spontaneous ferromagnetism for infinitesimal repulsive U , consistent with the Stoner criterion.¹¹ However, the energy gain is very insensitive to the field directions. For $\epsilon = 0.6t$, $\lambda = 0.3t$, $U = t$, and the field directions along (111) (Z direction), the field strength is $B_1 = 0.2440t$ on sublattices 1 and 2 and $B_3 = -0.0162t$ on sublattice 3. The mean-field band structure is very similar to Fig. 2(c) where a uniform $B = 0.2t$ is used. The two nearly flat mean-field bands are drawn 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 Rapid Communication, we discuss a model with spin-orbit coupling on the dice lattice and the correlation physics in it. A transition-metal oxide SrTiO₃/SrIrO₃/SrTiO₃ 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 splits the two bands, which give rise two nearly flat bands with Chern number ± 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.

Acknowledgments. F.W. thanks the Institute for Advanced Study at Tsinghua University, where part of this work was finished. Y.R. is supported by the startup fund at Boston College.

¹K. v. Klitzing, G. Dorda, and M. Pepper, *Phys. Rev. Lett.* **45**, 494 (1980).

²F. D. M. Haldane, *Phys. Rev. Lett.* **61**, 2015 (1988).

³E. Tang, J.-W. Mei, and X.-G. Wen, *Phys. Rev. Lett.* **106**, 236802 (2011).

⁴K. Sun, Z. Gu, H. Katsura, and S. Das Sarma, *Phys. Rev. Lett.* **106**, 236803 (2011).

⁵T. Neupert, L. Santos, C. Chamon, and C. Mudry, *Phys. Rev. Lett.* **106**, 236804 (2011).

⁶X. Hu, M. Kargarian, and G. A. Fiete, *Phys. Rev. B* **84**, 155116 (2011).

⁷N. Regnault and B. A. Bernevig, e-print arXiv:1105.4867 (unpublished).

⁸E. H. Lieb, *Phys. Rev. Lett.* **62**, 1201 (1989).

⁹A. Mielke, *J. Phys. A* **24**, 3311 (1991).

¹⁰H. Tasaki, *Phys. Rev. Lett.* **69**, 1608 (1992).

¹¹E. C. Stoner, *Phil. Mag.* **15**, 1018 (1933).

¹²M. Izumi, Y. Ogimoto, Y. Konishi, T. Manako, M. Kawasaki, and Y. Tokura, *Mater. Sci. Eng. B* **84**, 53 (2001).

¹³A. Ohtomo, D. A. Muller, J. L. Grazul, and H. Y. Hwang, *Nature (London)* **419**, 378 (2002).

¹⁴A. Ohtomo, and H. Y. Hwang, *Nature (London)* **427**, 423 (2004).

¹⁵J. Mannhart and D. G. Schlom, *Science* **327**, 1607 (2010).

¹⁶S. Chakraverty, A. Ohtomo, and M. Kawasaki, *Appl. Phys. Lett.* **97**, 243107 (2010).

¹⁷B. Gray, H. N. Lee, J. Liu, J. Chakhalian, and J. W. Freeland, *Appl. Phys. Lett.* **97**, 013105 (2010).

¹⁸D. Xiao, W. Zhu, Y. Ran, N. Nagaosa, and S. Okamoto, e-print arXiv:1106.4296 (unpublished).

¹⁹J. M. Longo, J. A. Kafalas, and R. J. Arnott, *J. Solid State Chem.* **3**, 174 (1971).

²⁰Y. 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, and H. Funakubo, *Thin Solid Films* **486**, 182 (2005).

- ²¹S. 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).
- ²²Y.-M. Lu and Y. Ran, e-print arXiv:1109.0226 (unpublished).
- ²³E. McCann and V. I. Falko, *Phys. Rev. Lett.* **96**, 086805 (2006).
- ²⁴D. L. Bergman, C. Wu, and L. Balents, *Phys. Rev. B* **78**, 125104 (2008).
- ²⁵B. Bleaney and M. C. M. O'Brien, *Proc. Phys. Soc. B* **69**, 1216 (1956).
- ²⁶C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 146802 (2005).