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Nearly-flat bands with nontrivial topology

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We report the theoretical discovery of a class of 2D tight-binding models containing nearly-flat bands with nonzero Chern numbers. In contrast with previous studies, where nonlocal hoppings are usually required, the Hamiltonians of our models only require short-range hopping and have the potential to be realized in cold atomic gases. Due to the similarity with 2D continuum Landau levels, these topologically nontrivial nearly-flat bands may lead to the realization of fractional anomalous quantum Hall states and fractional topological insulators in real materials. Among the models we discover, the most interesting and practical one is a square-lattice three-band model which has only nearest-neighbor hopping. To understand better the physics underlying the topological flat band aspects, we also present the studies of a minimal two-band model on the checkerboard lattice.

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In fermionic systems, a flat band (a macroscopically degenerate manifold of single-particle states) plays an important role in the study of strongly correlated phenomena, due to the vanishing bandwidth. One way to achieve a flat band is via the destructive interference of electron hoppings, which gives rise to moderately localized single-particle eigenstates [1–9]. Landau levels, which are formed when a magnetic field is applied to a 2D electron gas (2DEG), can be considered as another type of flat bands arising in continuum rather than lattice 2D systems. Different from the examples above, a Landau level has a nontrivial topological index (the Chern number). When an integer (or certain fractional) number of Landau levels is filled, the system turns into an insulator with nontrivial topology, known as the integer (or fractional) quantum Hall effect (IQHE or FQHE) [10].

In addition to 2DEG, efforts have also been made to realize IQH and FQH effects in lattice systems without magnetic field. The first and most celebrated example is the anomalous quantum Hall state proposed by Haldane [11]. More recently, a new class of topological states, the time-reversal invariant topological insulators characterized by a \mathbb{Z}_2 topological index is discovered in various lattice systems (see the recent reviews of Refs. [12, 13] and references therein). These lattice topological states share strong similarities with the IQH states. However, the lattice counterpart of the fractional quantum Hall states has not yet been discovered. One of the key challenges to reach a fractional topological state in lattice models lies in the fact that the bandwidth of a topologically nontrivial band in these models is usually comparable or even larger than the band gap. Thus, at fractional filling, the system is expected to be a Fermi liquid while interaction effects are just subleading corrections. Therefore, a flat band with nontrivial topology is expected to be the key in realizing lattice fractional topological states similar to the FQHE. Recently, there have been some attempts to find completely flat bands with nonzero Chern numbers in 2D lattice models [14, 15]. However, it turned out that, in all examples except in the quasi-one dimensional thin torus [14], flat bands have zero Chern number.

Since a topological index remains invariant under adiabatic deformations as long as the gap is preserved, a straightforward way to form such a flat band is to use the *spectral flattening trick*, i.e., an adiabatic transformation from the original Hamiltonian to a new one with completely flat bands. This technique is used in the classification of topological insulators and superconductors [16–18]. However, such a procedure may results in longrange hopping making the Hamiltonian nonlocal [19].

In real materials, the exact flatness for a band is not a physical requirement and we can relax the constraint a little bit by allowing the band to have a nonzero bandwidth but requiring the bandwidth to remain much smaller than the band gap. Unfortunately, to the best of our knowledge, even such models have never been reported. In this letter, we propose a generic scheme to produce such kind of models based on a special class of tight-binding Hamiltonians with short-range hoppings. The band structure of these models contains nontrivial band touchings with quadratic dispersions (in contrast to the linear ones near a Dirac point), which are protected by the time-reversal and lattice point-group symmetries as well as the nontrivial topology [20, 21]. When the time-reversal symmetry is broken, a band gap opens up at the band touching point and the bands can have nonzero Chern numbers. By slightly tuning the short-range hopping strength, we find that some of the topologically nontrivial bands can become nearly-flat. We believe that this mechanism is very general and applies to any tightbinding model with quadratic band touchings. Surprisingly, in some of these models, this nearly-flat band situation is found even with only nearest-neighbor (NN) hopping. These nearly-flat bands have a strong analogy

to the Landau levels in 2DEG and thus may set the stage for exploring new fractional topological states.

Topological flat band with extremely short-range hopping: the square-lattice model — Consider a square lat-

tice with two space-inversion odd and one space-inversion even orbitals per site, e.g. the p_x , p_y and $d_{x^2-y^2}$ orbitals. This model has been demonstrated in optical lattice systems [21]. In k-space, the Hamiltonian is

$$H = \sum_{\vec{k}} \left(d^{\dagger}_{\vec{k}}, p^{\dagger}_{x,\vec{k}}, p^{\dagger}_{y,\vec{k}} \right) \left(\begin{array}{c} -2t_{dd}(\cos k_x + \cos k_y) + \\ -2it_{pd}\sin k_x \\ -2it_{pd}\sin k_y \end{array} \right)$$

δ

$$\begin{array}{ccc} 2it_{pd}\sin k_x & 2it_{pd}\sin k_y \\ 2t_{pp}\cos k_x - 2t'_{pp}\cos k_y & i\Delta \\ -i\Delta & 2t_{pp}\cos k_y - 2t'_{pp}\cos k_x \end{array} \right) \begin{pmatrix} d_{\vec{k}} \\ p_{x,\vec{k}} \\ p_{y,\vec{k}} \end{pmatrix}$$

where $d_{\vec{k}}$, $p_{x,\vec{k}}$ and $p_{y,\vec{k}}$ are the fermion annihilation operators at momentum \vec{k} and the lattice constant is set to unity. The NN hoppings between various orbitals are described by the hopping amplitudes t_{dd} , t_{pd} , t_{pp} and t'_{pp} . The δ term measures the energy difference between p and d orbitals. The term (Δ) breaks the symmetry between the states with angular momentum ± 1 ($p_x \pm ip_y$). This term breaks the time-reversal symmetry and allows the Chern number to take a nontrivial value.

At $\Delta = 0$, the time-reversal symmetry is preserved and two of the three bands cross at the center (corner) of the Brillouin zone (BZ). For $\Delta > 0$, the bands become gapped. In order to ensure the "flatness" of the top band, we require the energies are equal at the Γ point, M point and K point, which implies $\delta = -4t_{dd} + 2t_{pp} +$ $\Delta - 2t_{pp}\Delta/(4t_{pp} + \Delta)$ and $t'_{pp} = t_{pp}/(4t_{pp} + \Delta)$. For simplicity, we set $t_{dd} = t_{pd} = t_{pp} = 1$. By varying Δ , we found that the ratio of bandwidth/band gap is minimized $(\simeq 1/20)$ at $\Delta = 2.8$. Here the top and the bottom bands carry opposite Chern numbers ± 1 while the middle band has a trivial Chern number. The band structure of this model is shown in Figs. 1(b) and 1(c), where the former is computed for periodic boundary conditions (on a torus) and the latter on a cylinder with two open edges. The edge states appearing in Fig. 1(c) confirm the nontrivial Chern numbers of the system.

A two-band model on a checkerboard lattice— The model discussed above has three bands. Here we present another model with only two bands. A two-band model has the following advantages: (1) its band structure is much easier to compute analytically; and (2) the Hilbert space is much smaller than models with more bands and thus numerical studies become easier. However, here we need to allow the next-nearest-neighbor (NNN) and nextnext-nearest-neighbor (NNN) hoppings. We emphasize that single-band models can only have trivial Chern numbers and thus, a two-band model is the minimal model to have topologically nontrivial bands.

Consider a checkerboard lattice with NN (t), NNN (t'_1, t'_2) , and NNNN (t'') hoppings [Fig. 2(a)]. Here, we allow the NN hopping to carry nonzero complex phase $(\pm \phi)$, whose signs are shown by the arrows in Fig. 2(a). These



FIG. 1: (Color online) Chiral quasi-flat band in the threeband model on a square lattice. Figure (a) shows the lattice structure, where each lattice site contains three orbitals and the arrows represent the breaking of the time-reversal symmetry. By putting the system on a torus and a cylinder, the single-particle energy spectra are shown in Figs. (b) and (c). In Fig. (c), chiral edges states (thick lines) are observed.

complex hoppings break the time-reversal symmetry at $\phi \neq n\pi$ ($n \in \mathbb{Z}$). The Hamiltonian of this model is

$$H = -t \sum_{\langle i,j \rangle} e^{i\phi_{ij}} (c_i^{\dagger}c_j + h.c.) - \sum_{\langle \langle i,j \rangle \rangle} t'_{ij} (c_i^{\dagger}c_j + h.c.) - t'' \sum_{\langle \langle \langle i,j \rangle \rangle \rangle} (c_i^{\dagger}c_j + h.c.)$$
(1)

where c_i (c_i^{\dagger}) is the fermion annihilation (creation) operator at site *i*. The NN, NNN and NNNN sites are represented by $\langle i, j \rangle$, $\langle \langle i, j \rangle \rangle$ and $\langle \langle \langle i, j \rangle \rangle \rangle$. The phase factor in the NN hopping terms is $\phi_{ij} = \pm \phi$ with the sign determined by the direction of the arrows. The hopping strength between NNN sites t'_{ij} takes the value of t'_1 (t'_2) if the two sites are connected by a solid (dashed) line.



FIG. 2: (Color online) Chiral quasi-flat band on the checkerboard lattice. The lattice structure is shown in Fig.(a), with arrows and (solid and dashed) lines representing the NN and NNN hoppings respectively. The direction of the arrow shows the sign of the phase in the NN hopping terms. Two of the NNNN hoppings are shown as the dashed curve. Other convention are the same as in Fig. 1.

The checkerboard lattice has two sublattices, and thus the Hamiltonian can be written in the momentum space as $H = \sum_{\vec{k}} \psi_{\vec{k}}^{\dagger} \mathcal{H} \psi_{\vec{k}}$, where $\psi_{\vec{k}} = (a_{\vec{k}}, b_{\vec{k}})$ is a two component spinor and \mathcal{H} is a 2 × 2 matrix

$$\mathcal{H} = [(t'_1 + t'_2)(\cos k_x + \cos k_y) + 4t'' \cos k_x \cos k_y]I + 4t \cos \phi (\cos \frac{k_x}{2} \cos \frac{k_y}{2})\sigma_x + 4it \sin \phi (\cos \frac{k_x}{2} \cos \frac{k_y}{2})\sigma_y + (t'_1 - t'_2)(\cos k_x - \cos k_y)\sigma_z.$$
(2)

Here I and $\sigma_{x,y,z}$ are the identity and Pauli matrices.

At $\phi = 0$ or $n\pi$, the time-reversal symmetry is preserved and the two energy bands in this model cross at the corner of the BZ [20]. At $\phi \neq n\pi$, a gap opens up between these two bands. Due to the breaking of the time-reversal symmetry, each band can carry a nonzero Chern number. In order to reach a flat band, we require the energies of the top band are equal at at the Γ point, M point, K point and at $\vec{k} = (\pm \pi/2, \pm \pi/2)$. With t = 1 and $\phi = \pi/4$, this condition implies t = 1, $t'_1 = -t'_2 = 1/(2 + \sqrt{2}), t'' = 1/(2 + 2\sqrt{2})$. With these values, the top band becomes very flat, with bandwidth of about 1/30 of the gap [Fig. 2(b)] and each of the two bands now carries Chern number ± 1 . We further verify this conclusion via the study of the chiral edge mode [Fig. 2(c)].

Discussion— In addition to the models discussed above, similar effects can be observed in other models with quadratic touching. For example, if we allow NN and NNN hoppings, both the kagome lattice and the honeycomb lattice with the p_x and p_y orbitals [8, 22, 23] can support this type of nearly-flat bands when the timereversal symmetry is broken. Here the kagome-lattice model is a three-band one, while the other has four bands.

Here, we compare the models with quadratic band touching and those with Dirac points. Due to these fermion doubling, the Dirac points need to appear in pairs. In order to reach an insulating phase starting from a semi-metal with two Dirac points, a nonzero mass need to be introduced at each of the two Dirac points. However, depending on the relative sign of the two Dirac masses, the resulting insulator can be either topologically trivial or nontrivial [11]. Due to this uncertainty on the topological structure, the nearly-flat band from a model with Dirac points may be topologically trivial and thus irrelevant to our interests. On the contrary, for the models with quadratic band touching, the constraint of fermion doubling is absent and there is a single crossing point. This crossing point can be regarded as two Dirac points merging together, and is protected by time reversal symmetry and discrete rotational symmetry, e.g., C_4 in the checkerboard lattice model. Since two hidden Dirac cones have the same chirality [20], the energy bands will have nontrivial topological numbers once the gap is opened by breaking time reversal symmetry by complex hoppings which do not break discrete rotational symmetry [24]. Therefore, we can focus on the flatness of the band, without worrying about finding a topologicallytrivial band. This discussion is also the reason that we considered the d-orbital in the three-band square lattice model. Without the *d*-orbital, the two *p*-band have two quadratic band crossings at the center and the corner of the BZ, instead of just one. Therefore, the resulting insulator may be topologically trivial.

Although the band gap is much lager than bandwidth in these models, it is not clear whether such nearly-flat bands are equivalent to Landau levels in 2DEG. However, the Berry curvature (Fig. 3) in momentum space shows no sharp features and the only length scale is the lattice constant, in sharp contrast to the cases in which the Berry curvature has delta-function like peaks, e.g. Ref. [25]. Thus, we argue that the topological nearly-flat bands we propose are very similar to 2D Landau levels and we expect FQHE at fractional fillings when repulsive interactions are turned on. We note in this context that even 2D Landau levels have a short lattice length, typically 10-100 times smaller than the magnetic length, underlying the real physical 2DEG. A more detailed numerical study will be presented in our future work.

When spin degrees of freedom are taken into account, the discussion above can be generalized to the timereversal invariant \mathbb{Z}_2 topological index by just substituting the time-reversal symmetry breaking terms into corresponding spin-orbit couplings (where spin up and down particles break the time-reversal symmetry in the



FIG. 3: (Color online) Distributions of the Berry curvature in momentum space for the flat bands in (a) the square-lattice model and (b) the checkerboard lattice model.

opposite way and thus the time-reversal symmetry is recovered when both spin species are taken into account). In such a way, it may even be possible to realize *fractional topological insulators* [26] in these models.

Experiment realization— In the discussion above, we only provided the optimum values for the parameters at which the flatness of the band is maximized. However, the nearly-flat band does not require strictly fine-tuning to reach. In fact, even if the parameters are changed by about 10%, the band remains to be fairly flat in the models we studied [19]. Because of this stability and the simpleness of these models, we believe that experimental realizations of these models are possible in both condensed matter systems and ultra-cold atomic gases. The insulating gap in these systems can be opened via spontaneous symmetry breaking if a small amount of short-range repulsions are introduced [20, 21, 27]. The same effect can be expected via explicit symmetry breaking, e.g. by introducing a magnetic field (for charged particles) or an artificial gauge field (for charge neutral particles) [28], as well as by rotating the lattice [23]. In recent experiments, some optical lattices have been constructed whose band structures are described by the square-lattice model and the honeycomb-lattice model discussed above [29– 32. Considering the fact that hopping strength can be tuned relatively easily in cold gases via varying the optical lattices, these cold-atom systems may be the leading candidates for the realization of the topological physics predicted in our work.

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Note added.— After the completion of our work, we learned that E. Tang et al. [33] recently obtained similar topological flat-band in kagome lattices with NNN hopping and spin-orbit couplings and that T. Neupert et al. [34] have studied the flat-band limit in the context of the Haldane model. During the revising of this work, the existence of fractional quantum Hall effect in our model is confirmed by exact numerical studies as reported in Ref. [35].

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