Flat bands with non-trivial topology in three dimensions

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We construct a simple model for electrons in a three-dimensional crystal where a combination of short-range hopping and spin-orbit coupling results in nearly flat bands characterized by a non-trivial $Z_2$ topological index. The flat band is separated from other bands by a bandgap $\Delta$ much larger than the bandwidth $W$. When the flat band is partially filled we show that the system remains non-magnetic for a significant range of repulsive interactions. In this regime we conjecture that the true many-body ground state may become a three-dimensional fractional topological insulator.

Introduction. – When single-particle states of bosons or fermions comprise a flat band, the effect of interactions is generically non-perturbative and can lead to new states of quantum matter. For 2D electrons in a strong perpendicular magnetic field the flatness of Landau levels combined with non-zero Chern numbers leads to the spectacular fractional quantum Hall (FQH) effect, and other exotic states such as the Wigner crystal. Recently, models for spinless fermions moving in two-dimensional lattices have been constructed that exhibit nearly-flat bands with non-zero Chern numbers, but remarkably in zero external magnetic field. It has been proposed, on the basis of heuristic arguments and numerical simulations, that at partial filling repulsive interactions may drive these systems into the zero-field FQH states. Although it is not clear apriori how to experimentally realize the above situation in a physical system, the prospect of engineering systems that can support fractional excitations without involving a magnetic field has led to significant interest recently in flat or nearly flat bands in various lattice models.

In this Communication we ask whether it is possible to achieve a flat band with non-trivial topology in a system of electrons in three spatial dimensions. It is well known that the concept of the first Chern number (and the FQH physics) does not generalize to three dimensions. However, recent advances in the theory of time-reversal invariant band insulators have established a uniquely three-dimensional $Z_2$-valued topological invariant, called $\nu_0$ which, as we argue below, can play a similar role. Taking a specific example of electrons moving in the 3D edge-centered cubic (perovskite) lattice we show that a suitable combination of short-range hoppings and spin-orbit coupling (SOC) terms can give rise to a nearly flat band with a non-trivial $Z_2$ index $\nu_0 = 1$. With the chemical potential inside the bandgap such crystal would be a strong topological insulator with an odd number of topologically protected gapless states associated with all of its surfaces. At partial filling and in the presence of repulsive interactions we argue that the system may become a three-dimensional ‘fractional’ topological insulator.

Many lattice models are known to support completely flat bands. In 2D these include $p$-orbitals in the honeycomb lattice as well as $s$-orbitals in the kagome, dice and Lieb lattices. 3D examples include the pyrochlore and the perovskite lattice. In their simplest form however the above tight-binding models do not constitute a platform suitable for the study of exotic correlated phases for at least two reasons. First, in all cases the flat bands touch other dispersing bands, usually in a quadratic fashion. The interactions are thus bound to mix states from adjacent bands and this is clearly detrimental to the emergence of correlated phases. Second, even when the Hamiltonian is modified to open a gap, e.g. by adding SOC as in Ref. the resulting flat (or nearly-flat) bands are in all known cases topologically trivial. In such topologically trivial flat bands the eigenstates can be chosen as exponentially localized around lattice sites and, at partial filling, interactions will typically select a crystalline ground state with broken translational symmetry and not an exotic featureless liquid that underlies the FQH effect. As already argued in Refs. a natural place to seek such exotic phases is in a flat band that is topologically non-trivial.

It is well known that in 2D a non-zero Chern number represents a topological obstruction to the formation of exponentially localized Wannier states. It is precisely this obstruction that tilts the balance in favor of FQH states in partially filled Landau levels (although Wigner crystal phases are still known to arise at very low filling fractions). For $Z_2$-odd phases of $\mathcal{T}$-invariant band insulators in 2D and 3D a similar topological obstruction exists if one insists on Wannier states that respect $\mathcal{T}$. This consideration suggests that interacting electrons partially filling a flat band with a non-trivial $Z_2$ index in a 3D crystal could either (i) spontaneously break $\mathcal{T}$ and form a Wigner crystal, or (ii) remain $\mathcal{T}$-invariant and form one of the proposed 3D fractional topological insulators characterized either by spin-charge separation or by fractional magneto-electric effect controlled by fractional values of the axion parameter accompanied by ground state degeneracy.

In the following we lay groundwork for future investigations of these 3D exotic phases by constructing a simple tight-binding model whose spectrum has a flat band characterized by $\nu_0 = 1$ and is separated from other bands by a large gap. We remark that constructing a flat band with non-trivial topology in a 3D crystal is mathematically more constrained problem than in 2D and it is by no means obvious that this can be achieved with short-range hoppings only.
The model. — As a first step in the program outlined above we study a simple tight-binding model with intrinsic SOC terms on the 2D Lieb lattice, seen in Fig. 1a, and the 3D perovskite lattice seen in Fig. 2a. The relevant Hamiltonian reads

$$H = -\sum_{\langle ij \rangle} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} - \delta \sum_{i \text{ corner}} c_{i\alpha}^\dagger c_{i\alpha} + i\lambda \sum_{\langle\langle ij\rangle\rangle} (d_{ij}^1 \times d_{ij}^2) \cdot \sigma_{\alpha\beta} c_{i\alpha}^\dagger c_{j\beta},$$

(1)

where $c_{i\alpha}^\dagger$ creates an electron of spin $\alpha$ on site $i$ of the lattice, $t_{ij}$ are the hopping amplitudes which we take equal to $t_1$, $t_2$, and $t_3$ for the first, second and third nearest neighbor sites respectively, and $\delta$ is an onsite energy for the corner sites (indicated as filled circles in Figs. 1a and 2a). Lastly, $\lambda$ represents the amplitude for the next-nearest neighbour SOC where $d_{ij}^1$ and $d_{ij}^2$ are the two unit vectors along the nearest neighbour bonds connecting site $i$ to its next-nearest neighbour $j$ and $\sigma$ is the vector of Pauli spin matrices.

In Ref. [20] we showed that for nearest neighbor hopping ($t_1$ only) and non-zero $\lambda$ both Lieb and perovskite lattices became topological insulators possessing a non-trivial $\mathbb{Z}_2$ invariant. In both cases the bands carrying non-trivial invariants were strongly dispersing. From here then, our goal is to flatten out these bands by tuning the hopping strengths $t_2$, $t_3$, $\lambda$ and the onsite energy $\delta$ without leaving the topological phase. Also, we want the flat band to be separated from all other bands by a large gap $\Delta$ so that interactions do not mix states from different bands. The relevant figure of merit, then, is the ratio of the flat-band width $W$ to the bandgap $\Delta$.

Lieb lattice. — As a warm-up exercise we first consider the valence band in the 2D Lieb lattice. Going over to momentum space and diagonalizing the Hamiltonian $\mathcal{H}_k$ that follows from Eq. (1), the result of the tuning procedure can be seen in Fig. 1b.

The procedure used for the tuning was the simplest available, namely introducing the parameters one by one and modifying the values by hand until the band was as flat as we could achieve. For the following set of values: $t_1 = 1$, $t_2 = -0.17$, $t_3 = -0.114$, $\lambda = 0.303$ and $\delta = -0.725$, the ratio of the bandwidth to the bandgap, $\Delta/W \approx 40.45$. A systematic numerical minimization technique could probably improve upon our result, but comparing to previous results on the kagome, honeycomb, square, checkerboard and ruby lattices, this value is already quite respectable.

To show that the system has not migrated away from the topological phase during the parameter tuning stage, we first solve the system in a strip geometry numerically using the same parameters as above. This verifies that the spin-filtered gapless edge states, seen in Fig. 1c, indeed persist. We also consider the Hamiltonian

$$H'(x) = (1-x)H_0 + xH,$$

(2)

where $H_0$ includes only $t_1$ and $\lambda$ and is known to support the topological phase. The result for $\Delta/W$, starting at $\lambda = 0.1$ ($t_1 = 1$) then adiabatically tuning $x$ from 0 to 1, for the same final set of parameters in $H$, can be seen in Fig. 1d. The ratio increases from its initial value $\Delta/W \approx 0.17$ to its largest value 40.45 at $x = 1$, without closing the gap. The system is seen to remain in the topological phase.

What can one say about the fate of the ground state in the presence of repulsive interactions when the flat band is partially filled? Close to half filling, since the spin up and down electrons are decoupled, one expects the Stoner instability towards the ferromagnetic state. If we parametrize the interaction by the usual on-site Hubbard $U$ then a gap $\sim U$ should open between the majority and minority bands when $W < U < \Delta$. For large enough $U$ one can focus on the spin-polarized electrons in the majority band. In the presence of sufficiently strong residual interactions (e.g. nearest-neighbor repulsion $V$) and at fractional filling, this problem becomes similar to that considered in Refs. [14] with spinless fermions. Analogous arguments then suggest the emergence of FQH states under favorable conditions. Another possibility is the formation of a $\mathcal{T}$-invariant fractional topological insulator which can be pictured as two decoupled FQH states for the two spin species. Such a state might be...
FIG. 2: (Color online) (a) Perovskite lattice showing 4 sites in unit cell along with basis vectors. Second and third neighbor hoppings are indicated by red and green dotted lines, respectively. (b) High symmetry points in the Brillouin zone. (c) Bandstructure inside bulk along path of high symmetry for $H_k$ with finely tuned parameter set. (d) Semi-Log plot showing the evolution of the gap as one moves between a known topological insulating phase and the final set of finely tuned parameters.

Perovskite Lattice. – We now approach the main objective of this work: constructing flat bands with a non-trivial $\mathbb{Z}_2$ index in a 3D lattice. Our starting point is again the Hamiltonian given in Eq. (1) but now on the perovskite lattice, shown in Fig. 2(a). In Ref. [20] we showed that for nearest-neighbor hopping and $\lambda > 0$ the system becomes a $\Gamma_5 \Lambda$ strong topological insulator when the lowest doubly degenerate band is filled. In an analogous fashion to the two dimensional case then, we aim to flatten out the lowest energy band by means of including additional parameters $t_2$, $t_3$ and $\delta$. The bandstructure for the set of parameters that maximize the bandgap to bandwidth ratio is shown in Fig. 2(c), over a path of high symmetry in the Brillouin zone illustrated in Fig. 2. The following set of values: $t_1 = 1$, $t_2 = -0.416$, $t_3 = -0.047$, $\lambda = -0.331$ and $\delta = 1.318$, yielded the ratio $\Delta/W \approx 17.56$. We remark that the ratio was calculated over the entire Brillouin zone and in Fig. 2(c) we have simply chosen one possible path here to illustrate the result. Including additional parameters in $H$, such as longer range hoppings, could no doubt further improve the above figure of merit but we do not pursue this here.

To ensure that the system remains in the topological phase, we adiabatically tune the parameter $x$ from 0 to 1 in the Hamiltonian $H'(x)$ defined in Eq. (4). The result of this procedure can be seen in Fig. 2(d). The ratio, again, remains finite across the entire range from its initial value $\Delta/W \approx 0.15$ to its largest value 17.56 at $x = 1$. We conclude that the flat-band carries $\mathbb{Z}_2$ index $\langle 1;111 \rangle$.

Now imagine that the (doubly degenerate) flat band is partially filled and consider the effect of repulsive interactions. Unlike the 2D case discussed above where the residual $U(1)$ spin symmetry is preserved despite the presence of SOC, in the 3D strong topological insulator the SU(2) spin symmetry is completely broken. In this situation it is not clear what the leading instability might be. In a similar flat-band setting describing Ir-based pyrochlore $Y_2Ir_2O_7$ Pesin and Balents argued for an exotic $T$-invariant spin-charge separated topological Mott insulator while others found more conventional magnetic phases. Below, we investigate the magnetic instabilities of our model in the simplest case with on-site repulsion and at exact half filling of the flat bands. We show that the system remains non-magnetic when interaction strength is below the critical value which is large compared to the bandwidth $W$. In this regime, therefore, the true many-body ground state could become a $T$-invariant fractional topological insulator.

Magnetic Instabilities. – We extend the Hamiltonian
We have established that it is possible to engineer nearly flat bands characterized by non-trivial interaction strengths.

The key observation to be made here is that both dressing the nature of the many-body ground state that makes these findings potentially broadly relevant is that to the best of our knowledge completely novel. What ble of producing this behavior, whereas the 3D result is

denotes the basis sites in the lattice, Figs. 1a and 2a. We use the following decoupling

and define the magnetization \( m_i^{(l)} = \langle n_i^{(l)} \rangle - \langle n_i^{(l)} \rangle ^{\dagger} \) and occupation number \( \tilde{n}_i^{(l)} = \langle n_i^{(l)} \rangle + \langle n_i^{(l)} \rangle ^{\dagger} \). Furthermore, we focus on uniform magnetic phases, such that \( m_i^{(l)} = m^{(l)} \)

independent of the site index \( i \).

To map out the phase diagram, we minimize the ground state energy with respect to \( m^{(l)} \). The result for half filling of the flat bands can be seen in Figures 3a

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