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High temperature fractional quantum Hall states

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We show that a suitable combination of geometric frustration, ferromagnetism and spin-orbit interactions can give rise to nearly flat bands with a large bandgap and non-zero Chern number. Partial filling of the flat band can give rise to fractional quantum Hall states at high temperatures (maybe even room temperature). While the identification of material candidates with suitable parameters remains open, our work indicates intriguing directions for exploration and synthesis.

Landau symmetry breaking[1, 2] has been the standard theoretical concept in the classification of phases and transitions between them. However, this theory turned out insufficient when the fractional quantum Hall (FQH) state[3, 4] was discovered. These highly-entangled quantum states are not distinguished by symmetries but characterized by new topological quantum numbers such as robust ground state degeneracy[5, 6] and robust non-Abelian Berry's phases[7] of the ground states[8]. The new kind of order revealed in these topological quantum numbers is named topological order.[8, 9] Recently it was realized that topological order can be interpreted as patterns of long-range quantum entanglement[10–12]. This entanglement has important applications for topological quantum computation: the robust ground state degeneracy can be used as quantum memory[13]. Fractional defects from the entangled states which carry fractional charges[4] and fractional statistics[14–16] (or non-Abelian statistics[17, 18]) can be used to perform fault tolerant quantum computation[19, 20].

Presently, highly entangled gapped phases in FQH systems[3, 4] are only realized at very low temperatures. Here we present a proposal to realize these states at high temperatures (even room temperature). The ideal is to combine spin-orbit coupling, ferromagnetism, and geometric frustration. Both spin-orbit coupling and ferromagnetism can have high energy scales and can appear at room temperature. In some cases, combining them leads to energy bands with non-zero Chern numbers and filling such an energy band will give rise to integer quantum Hall states. Further, in geometrically frustrated systems — lattices on which hopping is frustrated — some of these topologically non-trivial energy bands can be very flat[21, 22]. These would mimic Landau levels in free space. When such a flat band with a non-zero Chern number is partially filled (such as 1/3 or 1/2 filled), FQH states can appear. Here we study a simple example of this idea on the geometrically frustrated kagome lattice.

Several aspects of these ideas have been active in recent research. Spin-orbit coupling can lead to a topological insulator in various geometrically frustrated systems,[23–26] and non-collinear magnetic order can lead to integer quantum Hall states.[24, 27] Alternatively, interactions in geometrically frustrated systems can break time-reversal symmetry[28–36] which again can give rise to integer quantum Hall states. Here we show that an extension of these ideas may set the stage for FQH states and other highly entangled states with fractional statistics and fractional charges — possibly even at room temperature.

Nearly flat band; non-zero Chern number We consider nearest and next-nearest neighbor hopping on a kagome

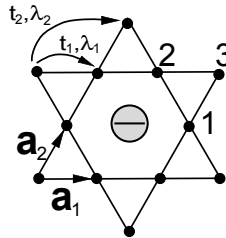


FIG. 1: The kagome lattice is a triangular Bravais lattice with a 3-point basis labelled $l = 1, 2, 3$; $\mathbf{a}_1 = \hat{x}$ and $\mathbf{a}_2 = (\hat{x} + \sqrt{3}\hat{y})/2$ are the basis vectors. In the metallic kagome lattice Fe_3Sn_2 , spin-orbit coupling arises from the electric field due to the Sn ion at the center of the hexagon.

lattice with spin-orbit interactions in the Hamiltonian

$$\begin{aligned}
H = & -t_1 \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda_1 \sum_{\langle ij \rangle \alpha \beta} (\mathbf{E}_{ij} \times \mathbf{R}_{ij}) \cdot \boldsymbol{\sigma}_{\alpha\beta} c_{i\alpha}^\dagger c_{j\beta} \\
& -t_2 \sum_{\langle\langle ij \rangle\rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda_2 \sum_{\langle\langle ij \rangle\rangle \alpha \beta} (\mathbf{E}_{ij} \times \mathbf{R}_{ij}) \cdot \boldsymbol{\sigma}_{\alpha\beta} c_{i\alpha}^\dagger c_{j\beta}
\end{aligned} \tag{1}$$

where $c_{i\sigma}^\dagger$ creates an electron with spin σ on site \mathbf{r}_i . Here $\langle ij \rangle$ denotes nearest neighbors and $\langle\langle ij \rangle\rangle$ next-nearest neighbors. The second and fourth terms are time-reversal invariant and describe spin-orbit interactions. \mathbf{R}_{ij} is the distance vector between sites i and j and \mathbf{E}_{ij} the electric field from neighboring ions experienced along \mathbf{R}_{ij} .

To obtain FQH states we need to break time-reversal symmetry. This is likely to happen spontaneously from exchange effects in the flat band that cause ferromagnetism[28–30]. Alternatively, one can apply an external magnetic field or couple the system to a ferromagnet. In the extreme limit the electron spins are totally polarized within the partially filled band — the case we examine here. Hence we consider spin-orbit coupling that also conserves S_z , i.e. the electric field on each site is in the 2D plane. First studying just nearest-neighbor hopping ($t_2 = \lambda_2 = 0$), in momentum-space Eq. 1 is

$$\begin{aligned}
H_{\mathbf{k}} = & -2t_1 \begin{pmatrix} 0 & \cos k_1 & \cos k_2 \\ \cos k_1 & 0 & \cos k_3 \\ \cos k_2 & \cos k_3 & 0 \end{pmatrix} \\
& \pm i2\lambda_1 \begin{pmatrix} 0 & \cos k_1 & -\cos k_2 \\ -\cos k_1 & 0 & \cos k_3 \\ \cos k_2 & -\cos k_3 & 0 \end{pmatrix}
\end{aligned} \tag{2}$$

where $\mathbf{a}_1 = \hat{x}$, $\mathbf{a}_2 = (\hat{x} + \sqrt{3}\hat{y})/2$, $\mathbf{a}_3 = \mathbf{a}_2 - \mathbf{a}_1$ and $k_n = \mathbf{k} \cdot \mathbf{a}_n$. We use units where the hopping parameter $t_1 = 1$. The $+$ ($-$) sign refers to spin up (down) electrons; from here we focus on just the spin up electrons.

The spectrum consists of three energy bands and is gapless at $\lambda_1 = 0, \pm\sqrt{3}$. At all other points the spectrum is gapped and the top and bottom bands have unit Chern number with opposite sign while the middle band has zero Chern number. The Chern number is defined as[37]

$$c = \frac{1}{2\pi} \int_{BZ} d^2k F_{12}(k) \tag{3}$$

where $F_{12}(k)$ is the associated field strength given by $F_{12}(k) = \frac{\partial}{\partial k_1} A_2(k) - \frac{\partial}{\partial k_2} A_1(k)$ with the Berry connection $A_\mu(k) = -i\langle n_{\mathbf{k}} | \frac{\partial}{\partial k_\mu} | n_{\mathbf{k}} \rangle$. In the above $|n_{\mathbf{k}}\rangle$ is a normalized wave function of the respective band.

Focusing on the lowest band which has a non-zero Chern number, we look for where this band is very flat compared to the bandgap and the energy scale of interactions. We denote W as the maximum bandwidth of the lowest band, Δ_{12} as the minimum bandgap between the two lowest bands and U as the strength of electron-electron interactions. When $U \gg W$, interaction effects dominate kinetic energy and partially filling the flat band would favor the Laughlin state.[4] Since band mixing could destroy band flatness, ideally $\Delta_{12} \gg U$. Hence we aim to maximize the ratio Δ_{12}/W in order to obtain FQH states. As the middle band has zero Chern number, any mixing between only two of the bands would not change the Chern number of the lowest band. If the lowest band remains flat even with mixing then Δ_{13} , the minimum bandgap between the lowest and highest bands, (and consequently the ratio Δ_{13}/W) is also of interest.

We find that $W \geq \Delta_{12}$ always — as the bandwidth vanishes so does the bandgap between the two lower bands (topological symmetry in real-space[38]), see Fig. 2. Here we show the band structure for $\lambda_1 = 1$ where $W = 1.3$ and $\Delta_{13}/W = 3.7$. As $\Delta_{12}/W \leq 1$ always, the spectrum does not have a clear separation of energy scales. When interactions are on the order of W , the bands will mix. This scenario is quite different from Landau levels in free space that are flat and well-separated, which could be due to limitations of this simplest model.

For a more realistic scenario we include second-nearest neighbor hopping which adds terms in the Hamiltonian

$$\begin{aligned}
H_{\mathbf{k}} = & -2t_2 \begin{pmatrix} 0 & \cos(k_2 + k_3) & \cos(k_3 - k_1) \\ & 0 & \cos(k_1 + k_2) \\ & & 0 \end{pmatrix} \\
& + i2\lambda_2 \begin{pmatrix} 0 & -\cos(k_2 + k_3) & \cos(k_3 - k_1) \\ & 0 & -\cos(k_1 + k_2) \\ & & 0 \end{pmatrix}
\end{aligned} \tag{4}$$

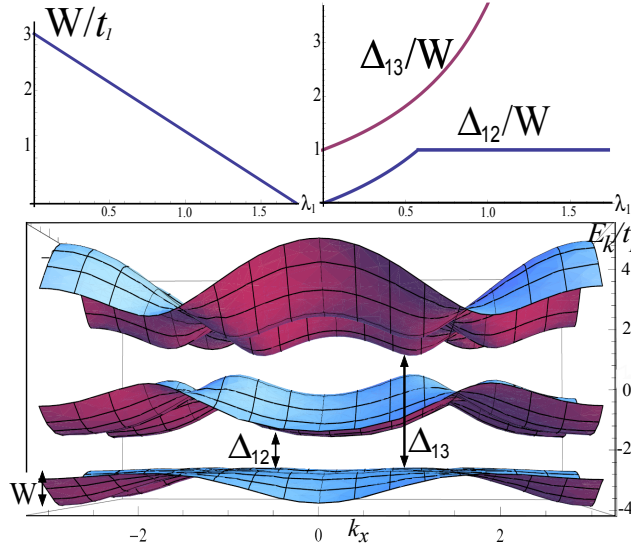


FIG. 2: (Color online) Results for nearest neighbor hopping as a function of λ_1 (nearest neighbor spin-orbit coupling). The bandwidth of the lowest band W vanishes at $\lambda_1 = \sqrt{3}$; however $W \geq \Delta_{12}$ always where Δ_{12} is the bandgap between the two lowest bands. Here we show the band structure for $\lambda_1 = 1$ where $W = 1.3$ and $\Delta_{13}/W = 3.7$. The spectrum does not have a clear separation of energy scales between Δ_{12} , W and U , the interaction strength, which could be due to limitations of the nearest neighbor hopping model.

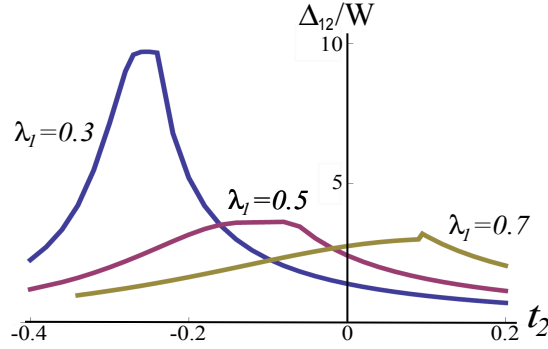


FIG. 3: (Color online) With the inclusion of next-nearest neighbor hopping, we obtain much higher bandgap to bandwidth ratios. We choose three values of $\lambda_1 = \lambda_2 = 0.3, 0.5$ and 0.7 , and sweep Δ_{12}/W with t_2 . For lower values of spin-orbit coupling, the ratio peaks at negative t_2 ; for relatively higher values of spin-orbit coupling the converse is true.

In this larger parameter space the band maxima and minima are no longer fixed at the same symmetry points. We find that the largest values of Δ_{12}/W (and Δ_{13}/W) occur when λ_1 and λ_2 are of the same sign – in which case the results are symmetric under changing signs of both λ 's in this spin polarized case. In Fig. 3, Δ_{12}/W is plotted as a function of t_2 for three values of $\lambda_1 = \lambda_2$. We see that at negative values of t_2 a lower spin-orbit coupling is needed; while for positive values of t_2 higher values of spin-orbit coupling would maximize the bandgap to bandwidth ratio.

We present two examples where Δ_{12}/W and Δ_{13}/W reach high values at $t_2 = -0.3$. In Case 1, setting $t_2 = -0.3$, $\lambda_1 = 0.28$ and $\lambda_2 = 0.2$, we obtain a very flat lowest band separated from the two higher bands by a large gap (see Fig. 4). The values of Δ_{12}/W and Δ_{13}/W are 52 and 99 respectively. In another example, all three bands are fairly flat (particularly the lowest one) and mutually well-separated. The parameters used are $t_2 = -0.3$, $\lambda_1 = 0.6$ and $\lambda_2 = 0$. In Case 2, we obtain $\Delta_{12}/W = 8.7$ and $\Delta_{13}/W = 24$ respectively (see Fig. 5).

Calculating the Chern number c of the lowest flat band in these two cases, we find it is 1. This is expected as slowly turning off t_2 and λ_2 does not close the bandgap — and we have previously seen that in the absence of next nearest-neighbor hopping, the lowest band always has unit Chern number. When $\Delta \gg U \gg W$ is satisfied, partial filling of this flat band would favor the FQH state.

The distribution of the field strength $F_{12}(k)$ in the Brillouin zone is plotted in Fig. 6. We observe there are no

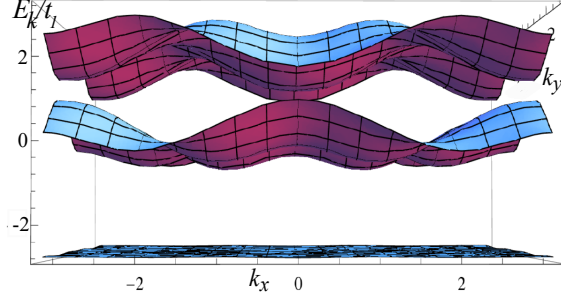


FIG. 4: (Color online) A very flat lowest band — well-separated from the two higher bands — is obtained with the parameters $t_2 = -0.3$, $\lambda_1 = 0.28$ and $\lambda_2 = 0.2$ (Case 1). The bandgap to bandwidth ratios are high: $\Delta_{12}/W = 52$ and $\Delta_{13}/W = 99$ respectively.

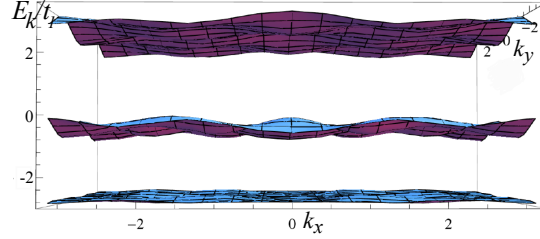


FIG. 5: (Color online) Three fairly flat bands are mutually well-separated with bandgap to bandwidth ratios of $\Delta_{12}/W = 8.7$ and $\Delta_{13}/W = 24$. Parameters used are $t_2 = -0.3$, $\lambda_1 = 0.6$ and $\lambda_2 = 0$ (Case 2).

singularities or very sharp features but $F_{12}(k)$ varies fairly smoothly especially in the first case with the flatter band. The presence of singularities — e.g. localized at the Dirac point — would have signalled a new (and much larger) length scale in the system. In our case, both the magnetic length scale (arising from spin-orbit interactions) and the variation of field strength $F_{12}(k)$ are on the order of the lattice constant a .

Thus the interaction energy scale is generated from the lattice constant a : $U \sim e^2/\epsilon a$ where ϵ is the dielectric constant. For a $1/3$ filled flat band, analogous to results from FQH states in semiconductor-based systems[39] the gap for this $\nu = 1/3$ state is roughly $0.09e^2/\epsilon a = 500\text{K}$. (We choose $\epsilon = 3$ and $a = 10\text{\AA}$; a is defined as the square root of the unit cell area). As the interaction energy scale is a hundred times larger than in semiconductors, we may see the FQH effect at room temperature. As band gaps Δ_{12} and Δ_{13} are easily much higher than room temperature, a fully filled band could give the integer quantum Hall state at unusually high temperatures too.

Materials realization We see that a suitable combination of geometric frustration, ferromagnetism and spin-orbit interactions can give rise to nearly flat bands with a large bandgap and non-zero Chern number. The ferromagnetism can arise from an external magnetic field, a ferromagnetic substrate for a thin film sample, and/or exchange effects. If the flat band is close to the Fermi energy, partial filling of the flat band can be controlled by doping and give rise

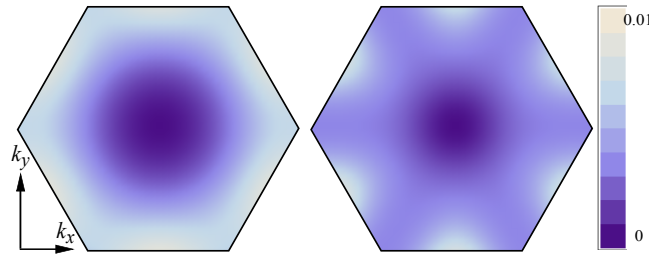


FIG. 6: (Color online) Distribution of the field strength $F_{12}(k)$ (Eq. 3) in the Brillouin zone for the flat bands in Cases 1 and 2 discussed above. They do not contain sharp features — especially Case 1 with the flatter band — hence the magnetic length scale remains on the order of the lattice constant a .

to FQH states at high temperatures.

The choice of parameters in our calculations is based on known values of spin-orbit coupling. For example, in Herbertsmithite (a common copper-based 2D kagome lattice) the spin-orbit interaction is 8% of the kinetic energy.[40] Other compounds with 4d or 5d orbitals (instead of 3d as in Cu) may experience a larger spin-orbit interaction. For instance, the strength of spin-orbit coupling in Iridium-based kagome compounds can be on the order of magnitude of the kinetic energy, hence the substitution with 4d or 5d atoms in metallic kagome lattices could result in hopping parameters similar to the ones used in our work. Alternatively, making thin films of frustrated lattices with 4d or 5d atoms may lead to a flat band with strong spin-orbit coupling, where exchange effects in this flat band could cause ferromagnetism.

Most existing kagome compounds are Cu-based insulators. Some 2D kagome lattices show metallic behavior, for instance Fe_3Sn_2 [41, 42] which shows ferromagnetism along the c -axis above 60K and in the kagome plane below 60K. Also, as spin-orbit interactions can be simulated in cold atom systems,[43, 44] it is possible to realize our hopping model in such systems. This would provide a method to obtain FQH states in cold atom systems.

In short, flat bands with non-zero Chern number arise in the examples we have given and in other geometrically frustrated systems with suitable levels of spin orbit interaction. By partially filling these bands e.g. via doping, one can expect the emergence of FQH states at high temperatures. While the identification of exact material candidates remains open, our work indicates intriguing directions for synthesis and development.

After completion of this paper, we learned that T. Neupert et. al[45] also discussed the possibility of the FQH effect in interacting two-band lattice systems, while K. Sun et. al[46] found flat bands with non-zero Chern numbers on various lattices (including the kagome lattice) after including some complex hopping. This research is supported by NSF Grant No. DMR-1005541.

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