Fractional Wannier Orbitals & Tight-Binding Gauge Fields
in
Kitaev Model with Flat Majorana Bands

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Overview

- Low-energy tight-binding model for "fractional" particles in the background of gauge potential

- Flat bands, Wannier orbitals, and fractional Chern Insulators for Majorana fermions

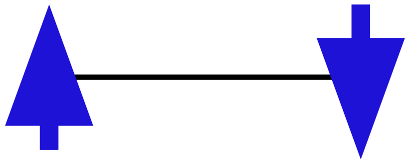
Ref: arXiv:2407.12559

with

G. Baskaran & Tanmoy Das

Introduction

$$H = J\sum_{ij} \vec{S}_i \cdot \vec{S}_j$$

For two sites: Neel State:  (Simple product state)

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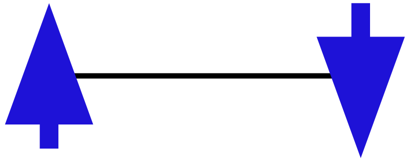
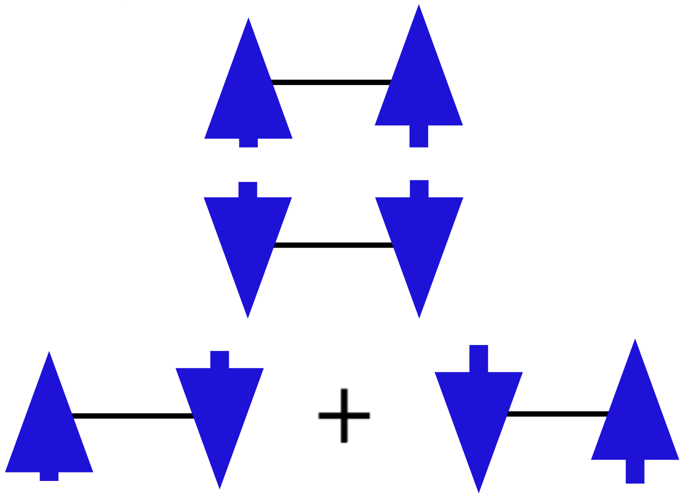
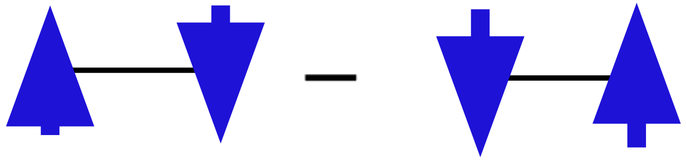


(Simple product space)

But when frustration is present (in the case of triangular lattice or geometrically frustrated models)



Triplet:



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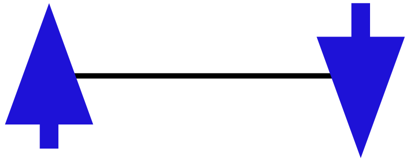

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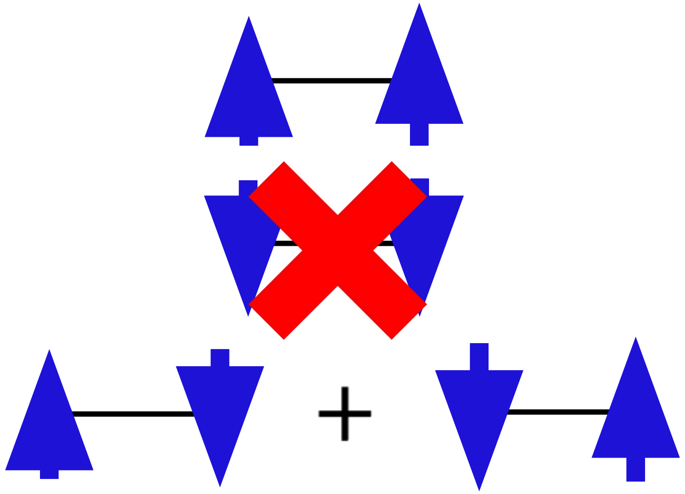
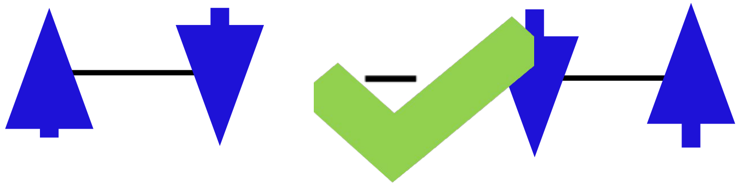


Triplet:

Low energies



Singlet:

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Baskaran, Anderson, PRB 1988

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    - The excitations have fractional statistics

K.B. Yogendra *, Tanmoy Das, Baskaran, PRB 108, 165118 (2023)*

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- The different Gauge sectors provide a platform to manipulate 'fractional' particles

  - How to construct a low-energy *'effective tight-binding model'* for these fractional particles?

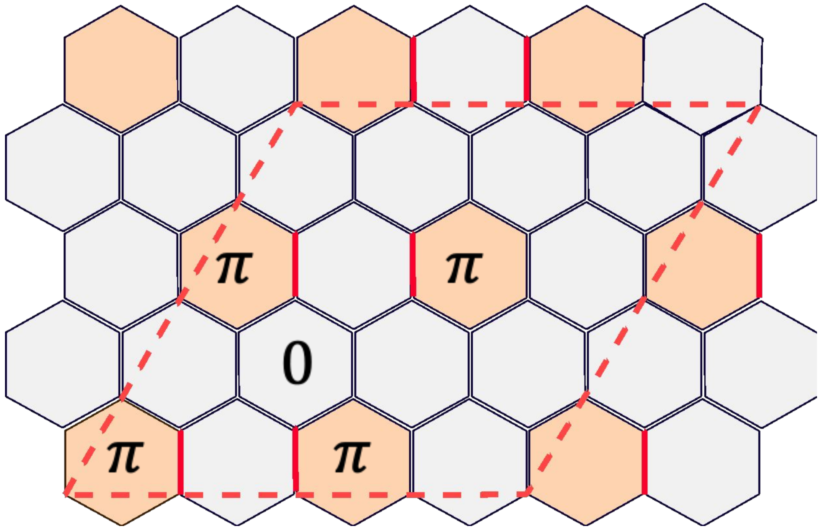
    importantly, preserving the "flux constraint" in the original model

Z_2-flux Superlattices in a Finite-field Kitaev model

$$H = i \sum_{<ij>_\alpha} J u_{ij} c_i c_j + iK \sum_{\langle\langle ik \rangle\rangle} u_{ij} u_{jk} c_i c_k$$

Z_2 – gauge operators: $u_{ij} = \pm 1$

$u_{ij} u_{jk} u_{kl} u_{lm} u_{mn} u_{no}$ = flux in the plaquette



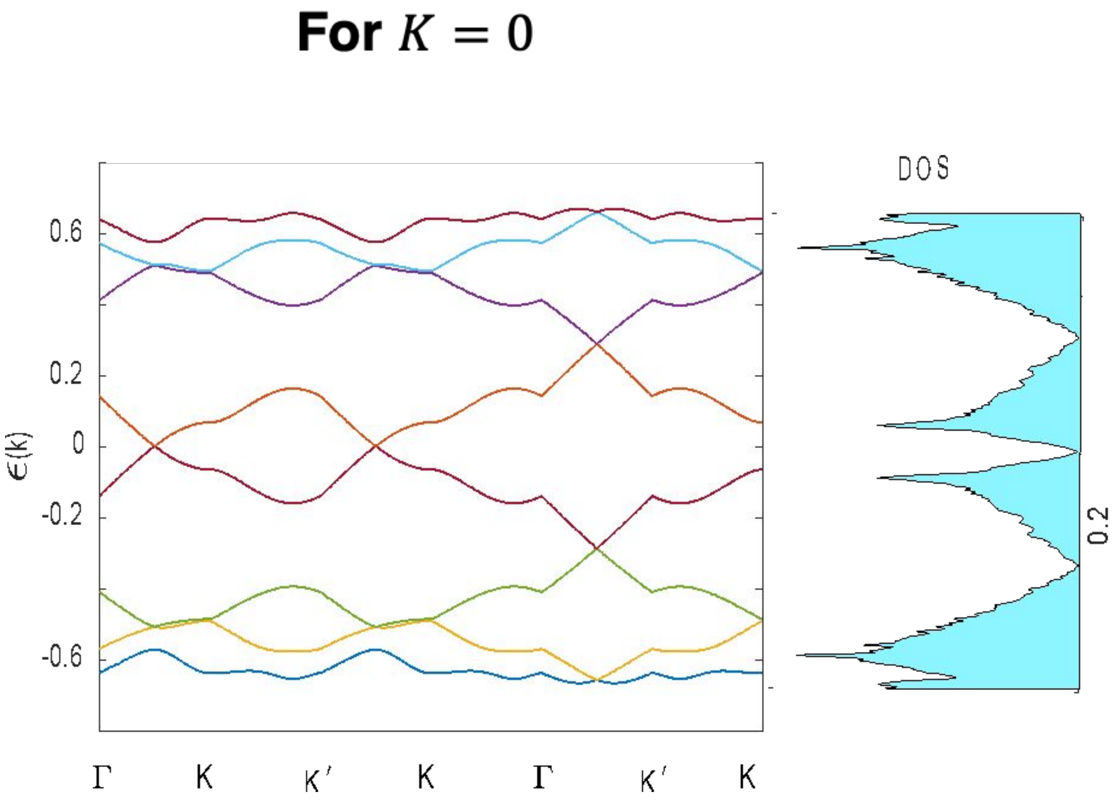
2 ×2 configuration

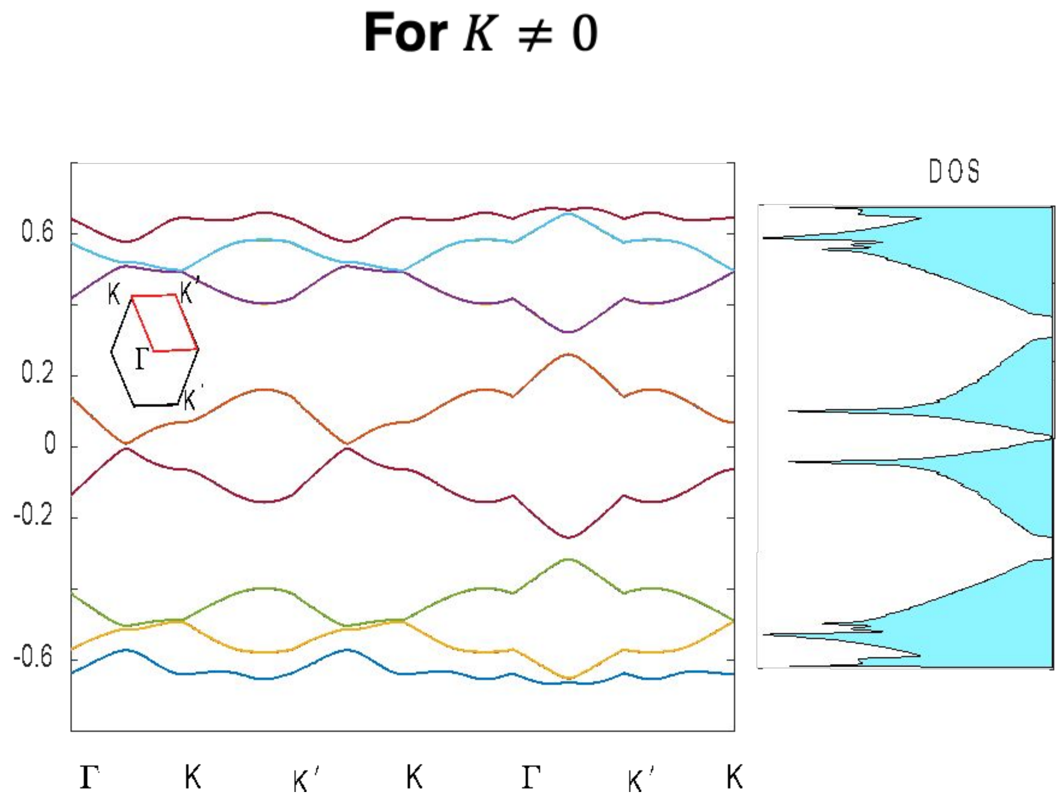
- Various periodic Z_2 - flux configurations -- denoted by d×d

K.B. Yogendra , Tanmoy Das, Baskaran, PRB 108, 165118 (2023)

- **Nearly Flat bands** for Majorana fermions -- like for electrons in Bilayer graphene at magic angles

- As d increases, the bands become more flat





For 4×4 periodic configurations

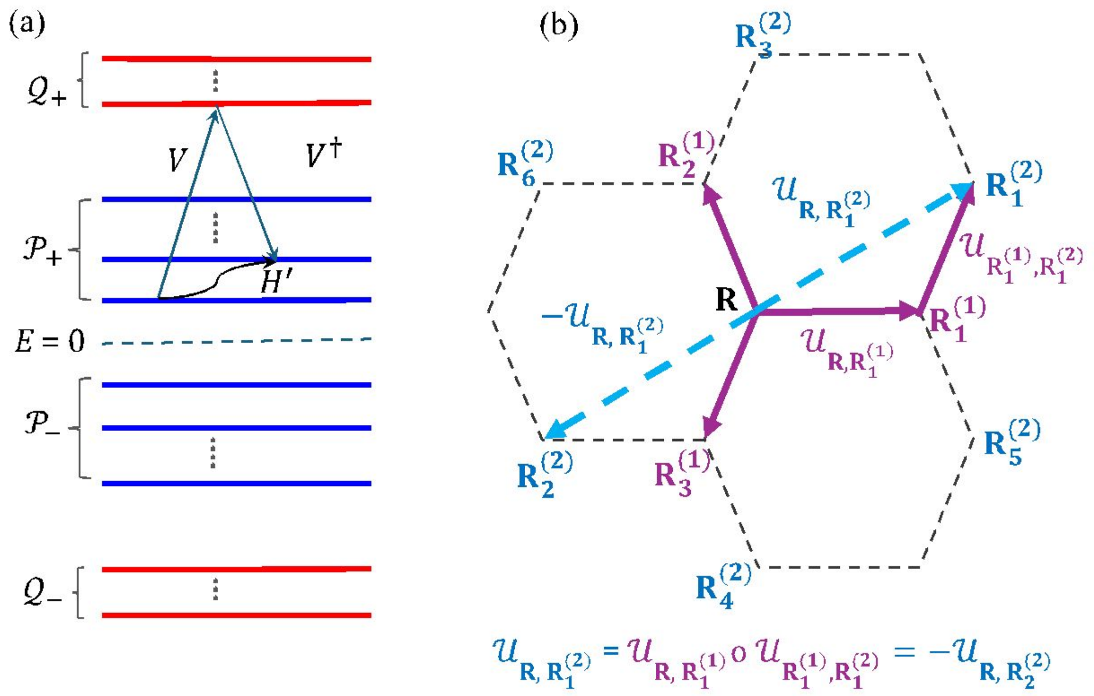
Effective Model

$$\mathcal{H}_{eff} = \wp_{\pm}(H + H')\wp_{\pm}$$

- Low-energy bands $|p\pm, k\rangle$ with projection operators $\wp_{\pm}$

H is the original Hamiltonian

H' is selt-consistence super-exchange/'gauge' potential



In the momentum space:

$$\mathcal{H}_{eff} = \sum_{n,n'} Z_n^{\dagger}(\boldsymbol{k}) T_{nn'} Z_{n'}(\boldsymbol{k})$$

where, $z_R = e^{i\,\mathbf{k}.\mathbf{r}}$ and $T_{R_n R_{n'}} = \kappa_{n-n'}{}^{-1} \frac{\partial \mathcal{H}_{eff}}{\partial \bar{z}_R \partial z_{R'}} \Big|_{z_R=0\,,z_{R'}=0}$ `

'Metric' $\sim \mathcal{G}_{nn'} \sim \mathbf{Re}\left(T_{R_n R_{n'}}\right)$

'Gauge' $\sim \mathcal{U}_{nn'} \sim \mathbf{Im}(T_{R_n R_{n'}})$

Flux - $\mathbf{Tr}\left(\prod_{nn'} \mathcal{U}_{nn'}\right)$

Fixing $T_{R_n R_{n'}}$ with flux-preserving constraint – fixes $\mathcal{H}_{eff}$

K.B. Yogendra, G. Baskaran, Tanmoy Das, arXiv: 2407.12559

Effective Model – example

- Wannier orbitals for Majorana fermions

✓ Used Maximally localized Wannier Functions (MLWFs) algorithm

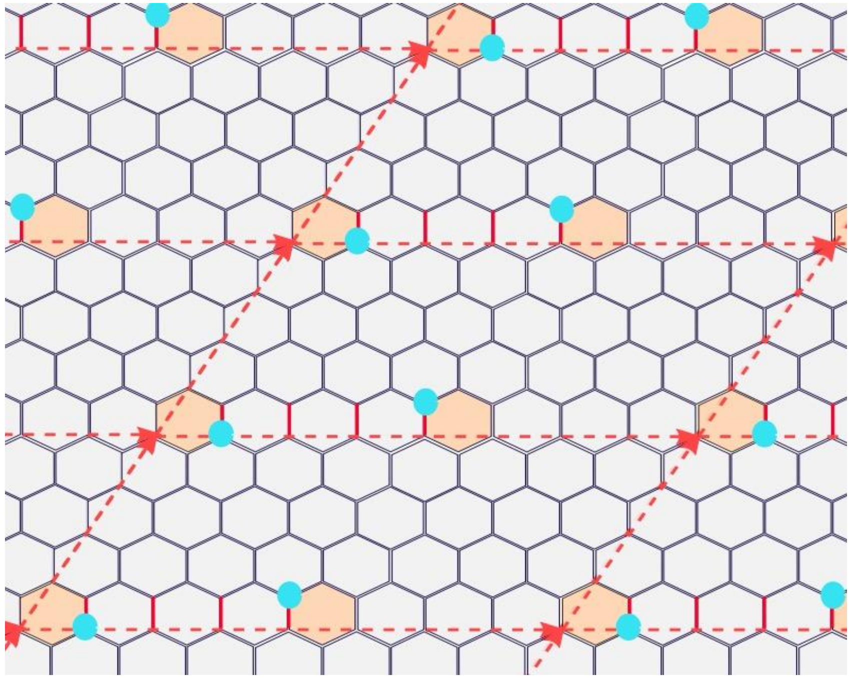
✓ particle-hole symmetry is imposed on the trail functions for Wannier Orbitals

  - on the structure of unitary matrices of eigenstates

for Majorana fermions

$$c_i^\dagger = c_i \longrightarrow c_{\boldsymbol{k}}^\dagger = c_{-\boldsymbol{k}}$$

- Majorana orbitals ~ superposition of '**electron + hole**' orbitals



4 ×4 configuration

- In $\boldsymbol{k}$-space:

Quantum metric: $\mathcal{G}_{ij,\mp}(\boldsymbol{k}) = \frac{1}{2}\mathrm{Tr}\big(P(\boldsymbol{k})\{\partial_i P_{\mp}(\boldsymbol{k}), \partial_j P_{\mp}(\boldsymbol{k})\}\big)$; $P_{\mp} = |\mp n\rangle\langle\mp n|$

Bernevig et. al, PRL 128, 087002 (2022)

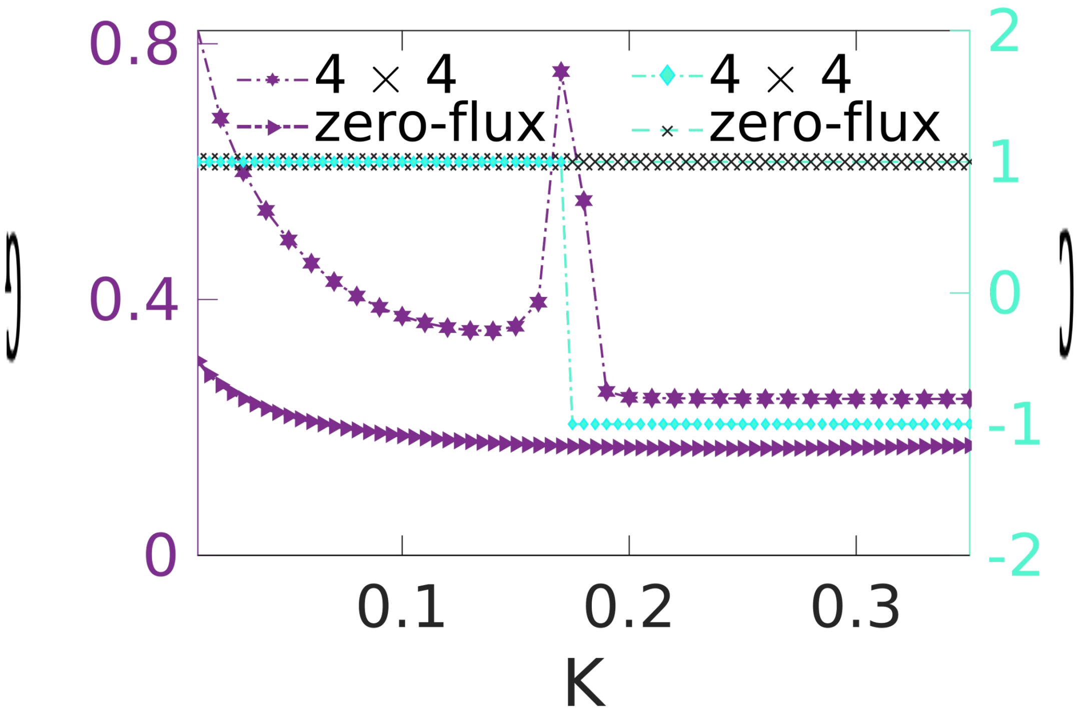
Berry Curvature: $\mathcal{U}_{ij,\mp}(\boldsymbol{k}) = \frac{-i}{2}\mathrm{Tr}\big(P(\boldsymbol{k})[\partial_i P_{\mp}(\boldsymbol{k}), \partial_j P_{\mp}(\boldsymbol{k})]\big)$

- Invariants:

from $\mathcal{G}_{ij}$: $G = \int_{\frac{BZ}{2}} \frac{dk_1 dk_2}{2\pi^2} \eta^{ij}\, \mathcal{G}_{ij}$;

from $\mathcal{U}_{ij}$: $C = \int_{\frac{BZ}{2}} \frac{dk_1 dk_2}{2\pi} \mathcal{U}_{12}$; *(Chern number)*

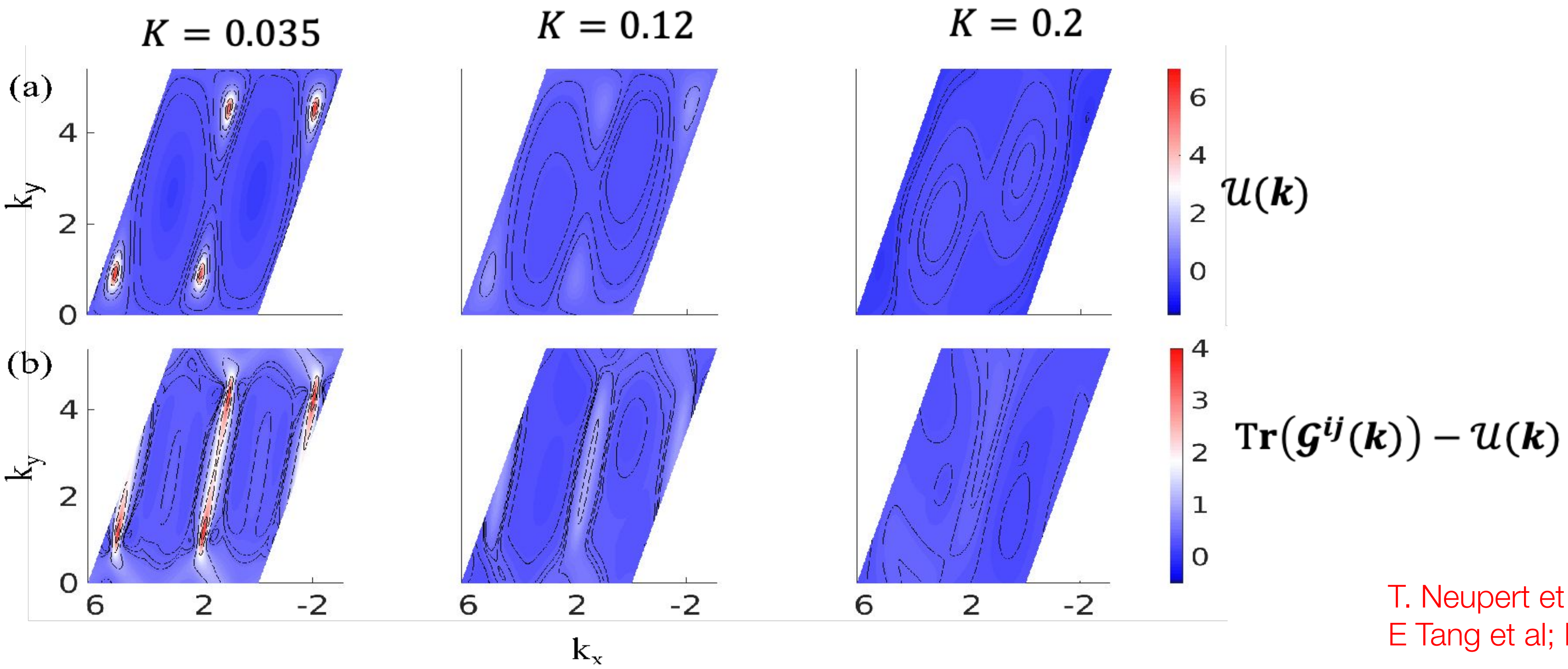
For 4×4 periodic configurations



- When the flatness ratio ($f = \frac{\delta}{\Delta}$) of the bands is low δ: bandwidth Δ: Gap

- Uniform Berry curvature $\mathcal{U}(\boldsymbol{k})$
  &
  Satisfy the "trace condition" -- $\mathbf{Tr}\left(\mathcal{G}^{ij}(\boldsymbol{k})\right) \cong \mathcal{U}(\boldsymbol{k})$

Rahul Roy, PRB 90,165139 (2014)
Daniel Parker, et al, arXiv:2209.15023



T. Neupert et al. PRL 106, 236804 (2011)
E Tang et al; PRL 106, 236802 (2011)

- As $f \rightarrow 0$, these Chern bands -- host 'fractional Chern Insulators' in the presence of interactions

Gauge-Invariant Mean-Field Theory

$$H_{\text{int}} = -i\kappa_1' \, \Sigma_{\mathbf{R,a},a'} \, i \, u_{\text{R},\text{R}_1'} \, u_{\text{R},\text{R}_2'} u_{\text{R},\text{R}_3'} \quad c_{\mathbf{a,R}} c_{\mathbf{a}',\mathbf{R_1}} \, c_{\mathbf{a}',\mathbf{R_2}} c_{\mathbf{a}',\mathbf{R_3}}$$

$$\Omega_1 = \; i \, \kappa_1' \sum_{i=1}^{3} \left\langle u_{\text{R},\text{R}_\text{i}} \; c_{\mathbf{a,R}} c_{\mathbf{a}'\mathbf{R}_\mathbf{i}'} \right\rangle$$

$$\Omega_1 = \; -i \, \kappa_1' \sum_{i \neq j=1}^{3} \langle u_{\text{R},\text{R}_\text{i}} u_{R,R_j} \; c_{\mathbf{a},\mathbf{R}_i} c_{\mathbf{a}'\mathbf{R}_j'} \rangle$$

$$\mathcal{H}_{\text{MF}} = \begin{pmatrix} \mathcal{H}_{\text{eff}}(\boldsymbol{k}) & i \begin{pmatrix} \Omega_1(\boldsymbol{Q}) & \Omega_2(\boldsymbol{Q}) \\ \Omega_2(\boldsymbol{Q})^* & \Omega_1(\boldsymbol{Q})^* \end{pmatrix} \\ \mathbf{h.\,c} & \mathcal{H}_{\text{eff}}(k+Q) \end{pmatrix} ; \quad \boldsymbol{Q} = \boldsymbol{G}_2/2$$

2 bands in $\mathcal{H}_{\text{eff}}(\boldsymbol{k})$ ⟶ 4 bands in $\mathcal{H}_{\text{MF}}(\boldsymbol{k})$

the orbital weights of 2 bands get re-distribute to 4 bands ⇒ ‘Fractional Chern number’

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Conclusions

- Construction of topologically non-trivial flat bands for Majorana fermions

- Wannier orbitals for Majorana fermions
    - Tight-binding models conserving the flux present in the plaquette

- Realization of ‘fractional Chern insulators’ for Majorana fermions in the presence of interactions
    - Analytical understanding using Mean field theory