## Self-Trapped Polarons and Topological Defects in a Topological Mott Insulator

Alexandre Dauphin
KITP Program: Interacting Topological Matter: Atomic, Molecular and Optical Systems 19 July 2021


## ICFO - The institute of Photonic Sciences

I am currently working as a la Caixa Junior Leader fellow at ICFO (Barcelona, Spain). of Photonic Sciences
$\overline{" l a C a i x a " ~ F o u n d a t i o n ~}$


Self-Trapped Polarons and Topological Defects in a Topological Mott Insulator
Sergi Julià-Farré@, ${ }^{1,{ }^{*}}$ Markus Müller®, ${ }^{2,3}$ Maciej Lewenstein®, ${ }^{1,4}$ and Alexandre Dauphin $\odot^{1, \dagger}$


Sergi Julià-Farré ICFO


Maciej Lewenstein ICFO


Markus Müller Aachen /Jülich (Germany)

Outline

## Outline

1. Introduction


## Outline

1. Introduction


## 2. Topological Mott insulator in the checkerboard lattice



## Outline

1. Introduction


## 2. Topological Mott insulator in the checkerboard lattice



## 3. Beyond half filling



## Outline

1. Introduction


## 2. Topological Mott insulator in the checkerboard lattice


4. Conclusions and Outlook


## 1. Introduction



## Topological Insulators



- Magnetic field $\longrightarrow$ Time reversal symmetry breaking
- Quantized conductivity
- Robust conductivity against disorder and interactions

- TKNN formula $\longrightarrow$ Link with the topological invariant
- Characterized by a global topological property

Thouless et al., Phys. Rev. Lett. 49, 405(1982).

- Topological insulators
- Time reversal symmetry conserved
- Bulk insulators $\longrightarrow$ gap in the energy spectrum
- Non trivial topological invariant $\longrightarrow$ quantized conductivity
- In geometry with border, conducting edge states protected by the topology.


## Realization of Topological Insulators : Solid State Physics

-2D topological insulators

## Quantum Spin Hall effect

Theoretically proposed in graphene:
C. L. Kane and E. J. Mele,

Phys. Rev. Lett. 95, 226801 (2005)
Conjecture: spin-orbit coupling converts graphene into a Q. spin Hall insulator

... effect turned out to be too small.
-3D topological insulators
Natural generalization of the Quantum spin Hall effect in 3D.

Theoretical proposal in $\mathrm{CdTe} / \mathrm{HgTe}$ nanowell structure
B. A. Bernevig, T. A. Hughes, and S. C. Zhang, Science 314, 1757 (2006)


Insulator



Experiment M. König, et al., Science 318, 766 (2007)

Top. Insulator



Qi and Zhang, Physics Today 63, 33 (2010).

Theoretically predicted in real materials :
Fu and Kane, Phys. Rev. B 76, 045302 (2007).

1st experiment reported:
7 Hsieh et al., Nature 452, 970 (2008)

## Realization of Topological Insulators : Quantum Simulation



Laser Assisted tunneling [M. Aidelsburger et al.,Phys. Rev. Lett. 2013]

lattice shaking
[G. Jotzu et al., Nature (2014)]


Synthetic dimensions
[Mancini et al., Science (2015)]

M.C.Rechtsman et al., Nature (2013)
Array of wave guides
[M.C.Rechtsman et al., Nature (2013)]


Quantum walk of twisted photons
[A D'errico et al., Optica (2020)]

## Classification and Beyond

- Classification of topological insulators in terms of the discrete symmetries they break, the celebrated periodic table of topological insulators and superconductors.

Chiu et al., Rev. Mod. Phys. 88, 035005 (2017).

- Beyond the periodic table: crystalline topological insulators, Weyl semimetals, topological Mott insulator, Floquet topological insulators, HOTIs, etc.


## Classification and Beyond

- Classification of topological insulators in terms of the discrete symmetries they break, the celebrated periodic table of topological insulators and superconductors.

Chiu et al., Rev. Mod. Phys. 88, 035005 (2017).

- Beyond the periodic table: crystalline topological insulators, Weyl semimetals, topological Mott insulator, Floquet topological insulators, HOTIs, etc.


## Interactions in Chern Insulators

- Interactions can destroy topological phases.
- They can induce a fractional QAH effect.
T. Neupert et al. PRL 106, 236804 (2011)
- Even more, they can even induce the topology.
S. Raghu et al. ,PRL 100, 156401 (2008)


Chern insulators due to spontaneous breaking of time-reversal symmetry driven by interactions

Review: S. Rachel, Rep. Prog. Phys. 81, 116501 (2018)

## Chern Insulators VS SSB Chern insulators

| Time reversal <br> symmetry breaking? | Sponge field <br> breaking |  |
| :---: | :---: | :---: |
| Topology mechanism | Externally induced | From system interactions |
| Local order |  |  |
| parameter? |  |  |

## 2. Topological Mott insulator in the checkerboard lattice



## Topological Mott Insulator on the Checkerboard lattice

- Extended Fermi-Hubbard model of spinless fermions on the checkerboard lattice with a pi-flux.
K. Sun et al. PRL 103, 046811 (2009)

$$
\hat{H}=\sum_{i j} t_{i j} \hat{c}_{i}^{\dagger} \hat{c}_{j}
$$



## Topological Mott Insulator on the Checkerboard lattice

- Extended Fermi-Hubbard model of spinless fermions on the checkerboard lattice with a pi-flux.
K. Sun et al. PRL 103, 046811 (2009)

$$
\hat{H}=\sum_{i j} t_{i j} \hat{c}_{i}^{\dagger} \hat{c}_{j}+V_{1} \sum_{\langle i j\rangle} \hat{n}_{i} \hat{n}_{j}+V_{2} \sum_{\langle\langle i j\rangle\rangle} \hat{n}_{i} \hat{n}_{j}
$$



## Topological Mott Insulator on the Checkerboard lattice

- Extended Fermi-Hubbard model of spinless fermions on the checkerboard lattice with a pi-flux.
K. Sun et al. PRL 103, 046811 (2009)

$$
\hat{H}=\sum_{i j} t_{i j} \hat{c}_{i}^{\dagger} \hat{c}_{j}+V_{1} \sum_{\langle i j\rangle} \hat{n}_{i} \hat{n}_{j}+V_{2} \sum_{\langle\langle i j\rangle\rangle} \hat{n}_{i} \hat{n}_{j} \hat{n}_{i} \hat{n}_{j} \simeq-\left\langle\left\langle\hat{c}_{i}^{\dagger} \hat{c}_{j}\right\rangle\right\rangle_{c}^{\dagger} \hat{c}_{i}-\left\langle\hat{c}_{\hat{c}}^{\dagger} \hat{c}_{i} \hat{c}_{i}^{\dagger} \hat{c}_{i}^{\dagger} \hat{c}_{j},+\left\langle\hat{n}_{i} \hat{n}_{j}+\left\langle\hat{n}_{j}\right\rangle+\ldots\right\rangle\right\rangle\langle\ldots\rangle
$$



## Topological Mott Insulator on the Checkerboard lattice

- Extended Fermi-Hubbard model of spinless fermions on the checkerboard lattice with a pi-flux.
K. Sun et al. PRL 103, 046811 (2009)

$$
\hat{H}=\sum_{i j} t_{i j} \hat{c}_{i}^{\dagger} \hat{c}_{j}+V_{1} \sum_{\langle i j\rangle} \hat{n}_{i} \hat{n}_{j}+V_{2} \sum_{\langle\langle i j\rangle\rangle \begin{array}{c}
\hat{n}_{i} \hat{n}_{j} \simeq-\left\langle\hat{c}_{i}^{\dagger} \hat{c}_{j}\right\rangle \hat{c}_{j}^{\dagger} \hat{c}_{i}-\left\langle\hat{c}_{j}^{\dagger} \hat{c}_{i} \hat{c}_{i}^{\dagger} \hat{c}_{j}\right. \\
+\left\langle\hat{n}_{i}\right\rangle \hat{n}_{j}+\left\langle\hat{n}_{j}\right\rangle+\langle\ldots\rangle\langle\ldots\rangle
\end{array}}^{\substack{\text { mimicks Haldane's } \\
\text { imaginary hoping }}} \hat{n}_{j}
$$



## Topological Mott Insulator on the Checkerboard lattice

- Extended Fermi-Hubbard model of spinless fermions on the checkerboard lattice with a pi-flux.
K. Sun et al. PRL 103, 046811 (2009)



## Phase diagram at half filling

- Quantum Anomalous Hall phase (two ground states)



$$
\begin{aligned}
\hat{n}_{i} \hat{n}_{j} \simeq & -\left\langle\hat{c}_{i}^{\dagger} \hat{c}_{j}\right\rangle \hat{c}_{j}^{\dagger} \hat{c}_{i}-\left\langle\hat{c}_{j}^{\dagger} \hat{c}_{i}\right\rangle \hat{c}_{i}^{\dagger} \hat{c}_{j} \\
& +\left\langle\hat{n}_{i}\right\rangle \hat{n}_{j}+\left\langle\hat{n}_{j}\right\rangle+\langle\ldots\rangle\langle\ldots\rangle
\end{aligned}
$$

translationally invariant ansatz

## Quantum Anomalous Hall phase and Chern number

- The QAH can salo be captured with a two-atom unit cell ansatz

$$
H_{\mathrm{eff}}=\alpha(k) 1+\vec{v}(k) \cdot \vec{\sigma}
$$

- One can show that the system is actually gapped in the QAH
- This phase is not insulating (gap) but also topological.

$$
E(\mathbf{k})
$$

- Topological invariant: Chern number

$$
\vec{n}=\frac{\vec{v}}{|\vec{v}|} \quad C=\frac{1}{4 \pi} \int_{\mathrm{BZ}} \vec{n} \cdot\left(\partial_{k x} \vec{n} \times \partial_{k y} \vec{n}\right)
$$

Qi et al., Phys. Rev. B 78, 195424 (2008)

## Quantum Anomalous Hall phase and Chern number

- The QAH can salo be captured with a two-atom unit cell ansatz

$$
H_{\mathrm{eff}}=\alpha(k) 1+\vec{v}(k) \cdot \vec{\sigma}
$$

- One can show that the system is actually gapped in the QAH
- This phase is not insulating (gap) but also topological.

$$
E_{i n t}(\mathbf{k})
$$

- Topological invariant: Chern number

$$
\vec{n}=\frac{\vec{v}}{|\vec{v}|} \quad C=\frac{1}{4 \pi} \int_{\mathrm{BZ}} \vec{n} \cdot\left(\partial_{k x} \vec{n} \times \partial_{k y} \vec{n}\right)
$$



Qi et al., Phys. Rev. B 78, 195424 (2008)

## Quantum Anomalous Hall phase and Chern number

- The two SSB ground states have an opposite Chern number



## Quantum Anomalous Hall phase and Chern number

- The two SSB ground states have an opposite Chern number



## Quantum Anomalous Hall phase and Chern number

- The two SSB ground states have an opposite Chern number



## Fate of the TMI beyond mean field

- Recent Density Renormalization group studies.
- The authors also found the QAH phase.
npj $\mid$ Quantum Materials
www.nature.com/npjquantmats

ARTICLE OPEN
Tuning topological phase and quantum anomalous Hall effect by interaction in quadratic band touching systems
Tian-Sheng Zeng $\mathbb{( 0}^{1}$, Wei Zhu ${ }^{2,3}$ and Donna Sheng ${ }^{4}$

PHYSICAL REVIEW B 98, 125144 (2018)

Quantum anomalous Hall insulator stabilized by competing interactions
Shouvik Sur, ${ }^{1}$ Shou-Shu Gong, ${ }^{2,3,{ }^{*}}$ Kun Yang, ${ }^{1}$ and Oskar Vafek ${ }^{1, \dagger}$


## 3. Beyond half filling



## Phases beyond half filling

- We fix $\mathrm{V} 1 / \mathrm{t}=2.5, \mathrm{~V} 2 / \mathrm{t}=1.5$.
-What is the behavior with particle doping?
- Two possibilities:

(Rigid band scenario)


## Phases beyond half filling

- We fix $\mathrm{V} 1 / \mathrm{t}=2.5, \mathrm{~V} 2 / \mathrm{t}=1.5$.
-What is the behavior with particle doping?
- Two possibilities:



## Phases beyond half filling

- We fix $\mathrm{V} 1 / \mathrm{t}=2.5, \mathrm{~V} 2 / \mathrm{t}=1.5$.
-What is the behavior with particle doping?
- Two possibilities:

s

(Interacting band scenario)

## Phases beyond half filling

- We fix $\mathrm{V} 1 / \mathrm{t}=2.5, \mathrm{~V} 2 / \mathrm{t}=1.5$.
- What is the behavior with particle doping?
- Two possibilities:

(Interacting band scenario)
- Localized solutions inside the gap break also translational invariance

$$
\begin{aligned}
\hat{n}_{i} \hat{n}_{j} \simeq & -\left\langle\left\langle\hat{c}_{i}^{\dagger} \hat{c}_{j}\right\rangle \hat{c}_{j}^{\dagger} \hat{c}_{i}-\left\langle\hat{c}_{j}^{\dagger} \hat{c}_{i}\right\rangle \hat{c}_{i}^{\dagger} \hat{c}_{j}\right. \\
& +\left\langle\hat{n}_{i}\right\rangle \hat{n}_{j}+\left\langle\hat{n}_{j}\right\rangle+\langle\ldots\rangle\langle\ldots\rangle
\end{aligned}
$$

- How do we study the topology in this case?


## Local Chern number

- The definition of the Chern number relies on some kind of boundary conditions (periodic or twisted) giving a notion of $k$-space.
- But the single-particle insulating ground state is characterized by
$P=\sum_{i \in \text { occ }}\left|\Phi_{i}\right\rangle\left\langle\Phi_{i}\right| \quad P\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \sim e^{-\alpha\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}$


$$
\Longrightarrow C(\mathbf{R})=\frac{1}{A} \sum_{\mathbf{r}} \mathcal{C}(\mathbf{r})
$$

R. Bianco and R. Resta, Phys. Rev. B 84, 241106(R) (2011)

## Local Chern number

- Extremely useful in non-homogeneous phases, to detect different topological regions.

R. Bianco and R. Resta, Phys. Rev. B 84, 241106(R) (2011)
- Local order parameter of the time reversal symmetry breaking
$\left\langle\hat{C}_{i}^{\dagger} \hat{C}_{j}\right\rangle \equiv \xi_{i j}^{R}+i \xi_{i j}^{I}$ ( $\sim$ Haldane's imaginary hopping)
- Local Chern number (not a local order parameter, identifies global topology)

$$
C(\mathbf{R})=\frac{1}{A} \sum_{\mathbf{r}} \mathcal{C}(\mathbf{r})
$$

## One extra particle: Self-trapped polaron

- State localized in the gap
- Density cloud in real space
- Reduction of the local order parameter
- Even sign inversion (change of the SSB sector)
- Local Chern number not quantized inside


Similar behavior in self-trapped polarons in 2D fermi-hubbard model (but no topology).
J. A. Verges et al., Phys. Rev. B 43, 6099 (1991)

## Two Extra Particles: Bi-Polaron States

- Separated polarons are metastable solutions.
- There is a collapse radius.
- Bipolaron state.

(b)

(c)



## Eight Extra Particles: Ring Domain Walls

- Single domain wall.
- Bulk solution (independent of boundaries)

- Coexistence of the two ground states
- Appearance of chiral edge states.


## Eight Extra Particles: Ring Domain Walls

- Single domain wall.
- Bulk solution (independent of boundaries)
- Coexistence of the two ground states
- Appearance of chiral edge states.



## Eight Extra Particles: Ring Domain Walls

- Single domain wall.
- Bulk solution (independent of boundaries)

- Coexistence of the two ground states
- Appearance of chiral edge states.


## Eight Extra Particles: Ring Domain Walls

- Single domain wall.
- Bulk solution (independent of boundaries)

- Coexistence of the two ground states
- Appearance of chiral edge states.



## Eight Extra Particles: Metastable State

## LINEAR DOMAIN WALLS

- Density accumulation in linear regions (DW).
- Appearance of chiral edge states.



## Quantum simulation with Dressed Rydberg atoms

- Simulation Topological Mott insulator in other lattices:
A. Dauphin et al, Phys. Rev. A 86, 053618 (2012)
A. Dauphin et al, Phys. Rev. A 93, 043611 (2016)
- pi-flux can be achieved with laser assisted tunneling.
- V1 and V2 interactions ~ t can be achieved with dressed Rydberg atoms due to a far detuned laser field.



## Quantum simulation with Dressed Rydberg atoms

- Simulation Topological Mott insulator in other lattices:
A. Dauphin et al, Phys. Rev. A 86, 053618 (2012)
A. Dauphin et al, Phys. Rev. A 93, 043611 (2016)
- pi-flux can be achieved with laser assisted tunneling.
- V1 and V2 interactions ~ t can be achieved with dressed Rydberg atoms due to a far detuned laser field.




## The implementation scheme

- off-resonant laser coupling to the Rydberg state + vdW- Rydberg-Rydberg interactions



## The implementation scheme

- off-resonant laser coupling to the Rydberg state + vdW- Rydberg-Rydberg interactions

- Perturbation theory up to the fourth order in small parameter $\Omega / \Delta \ll 1$. note: treatment is non-perturbative in the interaction strength $V_{i j}$

$$
(\Delta E)_{|g g\rangle}=2 \frac{\Omega^{4}}{\Delta^{3}}\left[1+\frac{2 \Delta}{V_{i j}}\right]^{-1}
$$

## The implementation scheme

- off-resonant laser coupling to the Rydberg state + vdW- Rydberg-Rydberg interactions
a) single-atom laser dressing


- Perturbation theory up to the fourth order in small parameter $\Omega / \Delta \ll 1$. note: treatment is non-perturbative in the interaction strength $V_{i j}$

$$
\begin{gathered}
(\Delta E)_{|g g\rangle}=2 \frac{\Omega^{4}}{\Delta^{3}}\left[1+\frac{2 \Delta}{V_{i j}}\right]^{-1} \int_{28} \text { critical Rydberg blockade radius: } 2 \Delta \approx V_{i j} \\
r_{c}=\left(C_{\alpha} / 2 \Delta\right)^{1 / \alpha}
\end{gathered}
$$

## Choice of the parameters

effective 2-body 4th order pert. theory


$\Delta$ interactions tunable completely independently from hopping $t$

$$
(\Delta E)_{|g g\rangle}=2 \frac{\Omega^{4}}{\Delta^{3}}\left[1+\frac{2 \Delta}{V_{i j}}\right]^{-1}
$$

## Choice of the parameters

effective 2-body interactions


## Choice of the parameters

effective 2-body interactions
$\Delta$ interactions tunable completely independently from hopping $t$
$\triangleright$ strong and almost equally large $V_{1}$ and $V_{2}$ interactions
$\Delta$ significantly weaker long-range interactions $V_{3}, V_{4}, \ldots$


## 4. Conclusions and Outlook

## Conclusions and Outlook

- Interaction-induced topological insulators are richer than topological insulators with external gauge fields.
- Away from half filling, the system prefer to deform the lattice and create in gap states than becoming metallic.
- Interplay SSB and topology leads to interaction induced domain walls (Edge states in the bulk)

- Effect of the temperature
- More realistic treatment of the truncation of the interactions.
- Beyond Mean field study: DMRG?



## Beyond Mean Field: Configuration Interaction

- The polaron solution spontaneously breaks translational invariance.
- Configuration interaction (CI) method:

One hybridizes all the polaron solutions to restore translational invariance and decrease the ground state energy.

$$
\left|\Psi^{C I}\right\rangle=\sum_{\alpha} \alpha\left|\psi_{\text {polaron }}(\alpha)\right\rangle
$$

Polaron band structure


