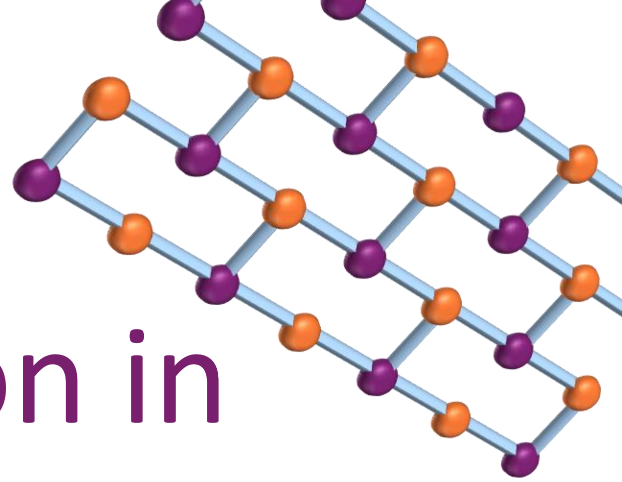
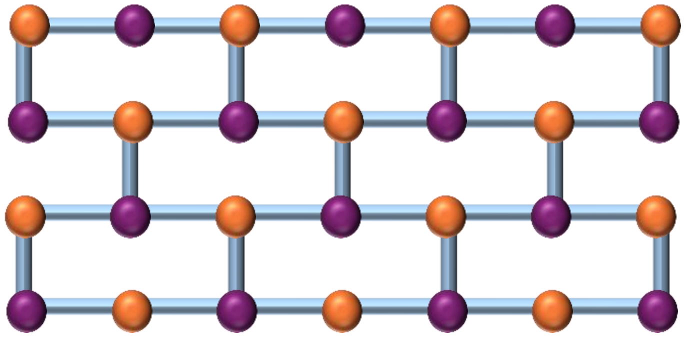


Topological phase transition in quantum materials: brickwall lattice with a defect

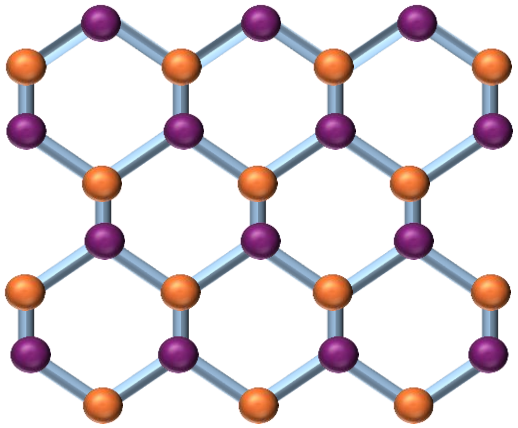
Anna Hassine
Advisor: Prof. Eric Akkermans

Physics retreat 04.03.2025

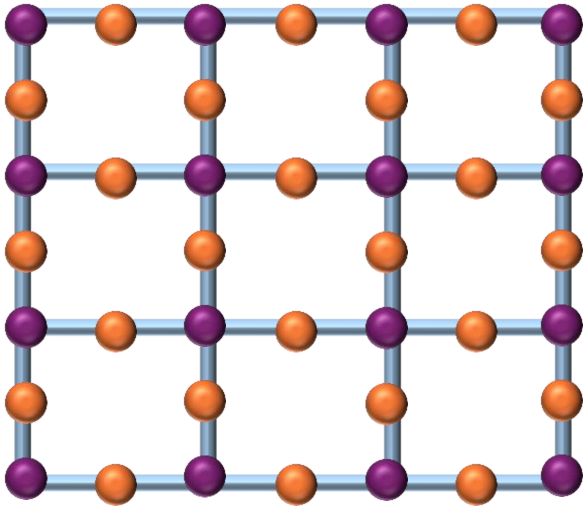
2D lattices



Brickwall lattice



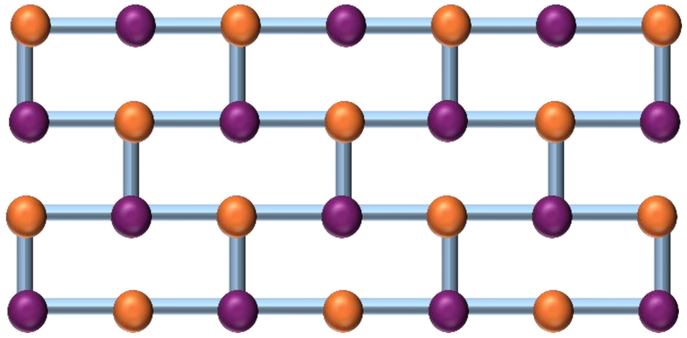
Honeycomb lattice

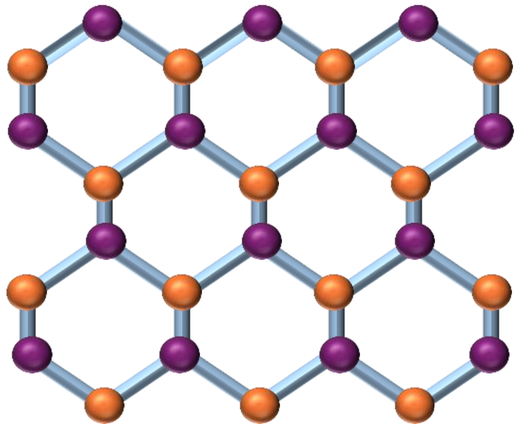


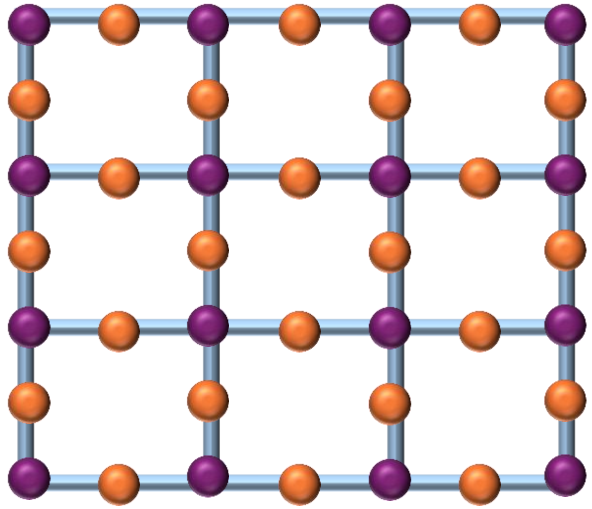
Lieb lattice

2D lattices

Interlaid lattices
Orange and Purple:
"bi-partite"


Brickwall lattice


Honeycomb lattice


Lieb lattice

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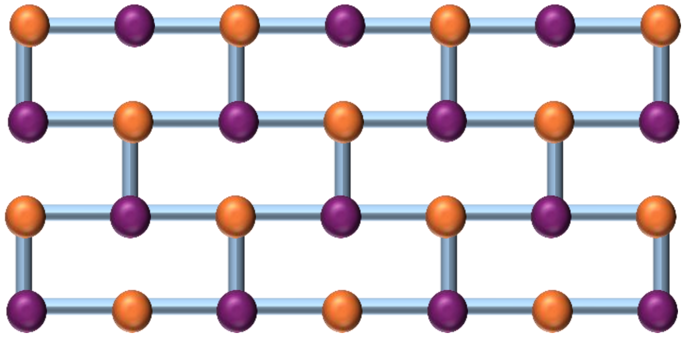
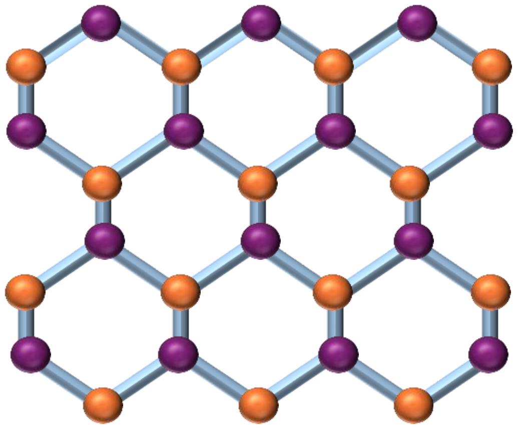
+

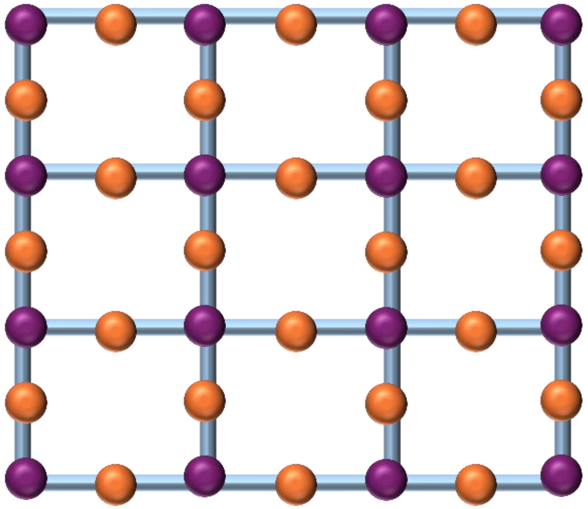
Tight binding model
Nearest neighbors



Brickwall lattice



Honeycomb lattice



Lieb lattice

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Tight binding model
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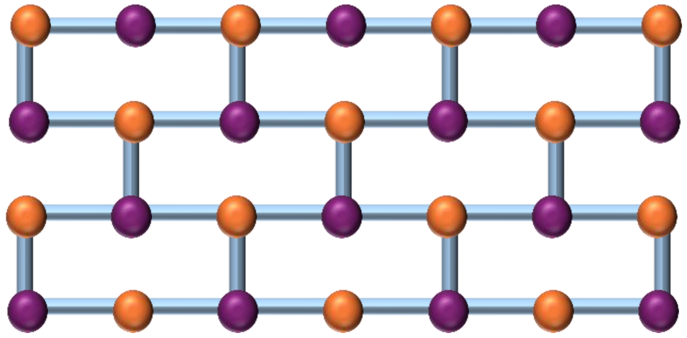
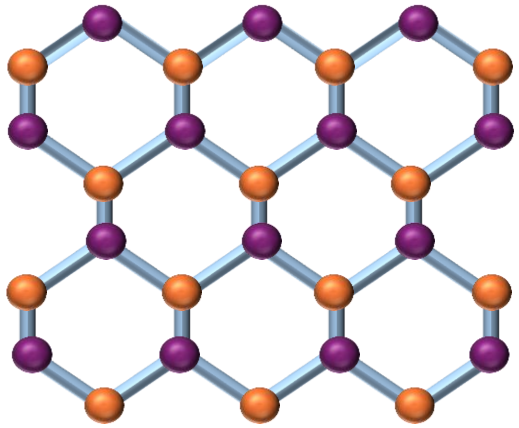
=

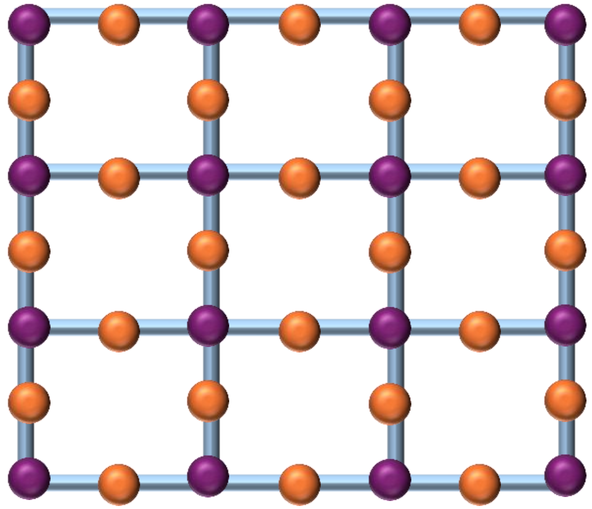
Hopping between
different colors only!



Brickwall lattice



Honeycomb lattice



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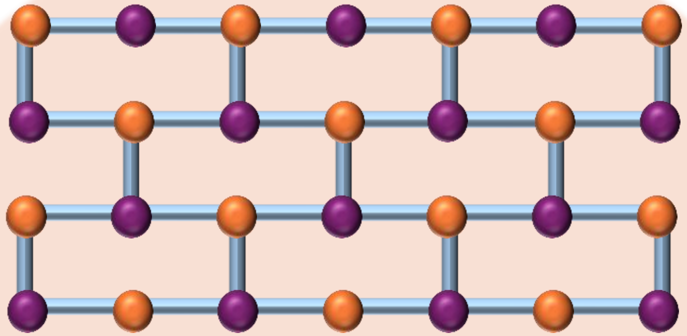
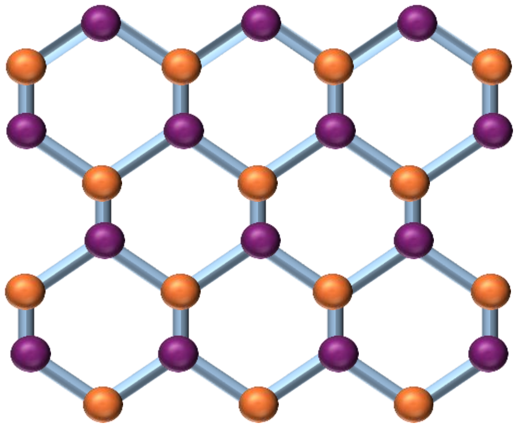
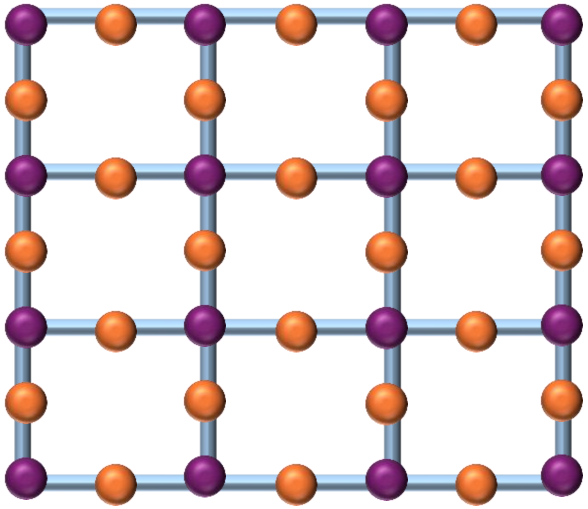


Brickwall lattice

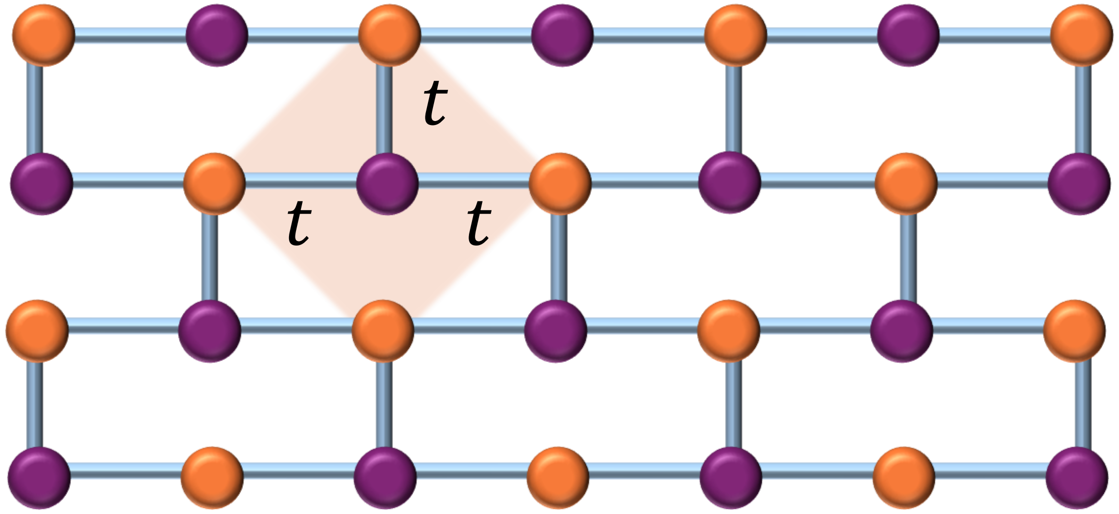


Honeycomb lattice



Lieb lattice

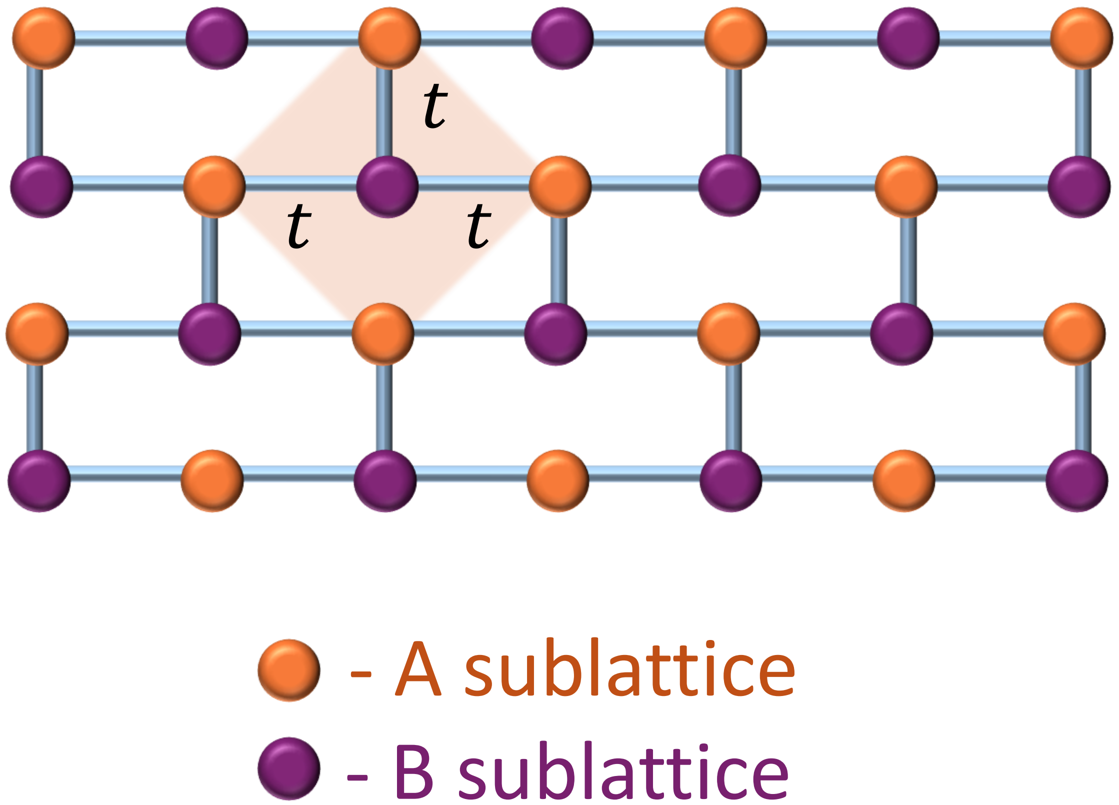
Brickwall lattice



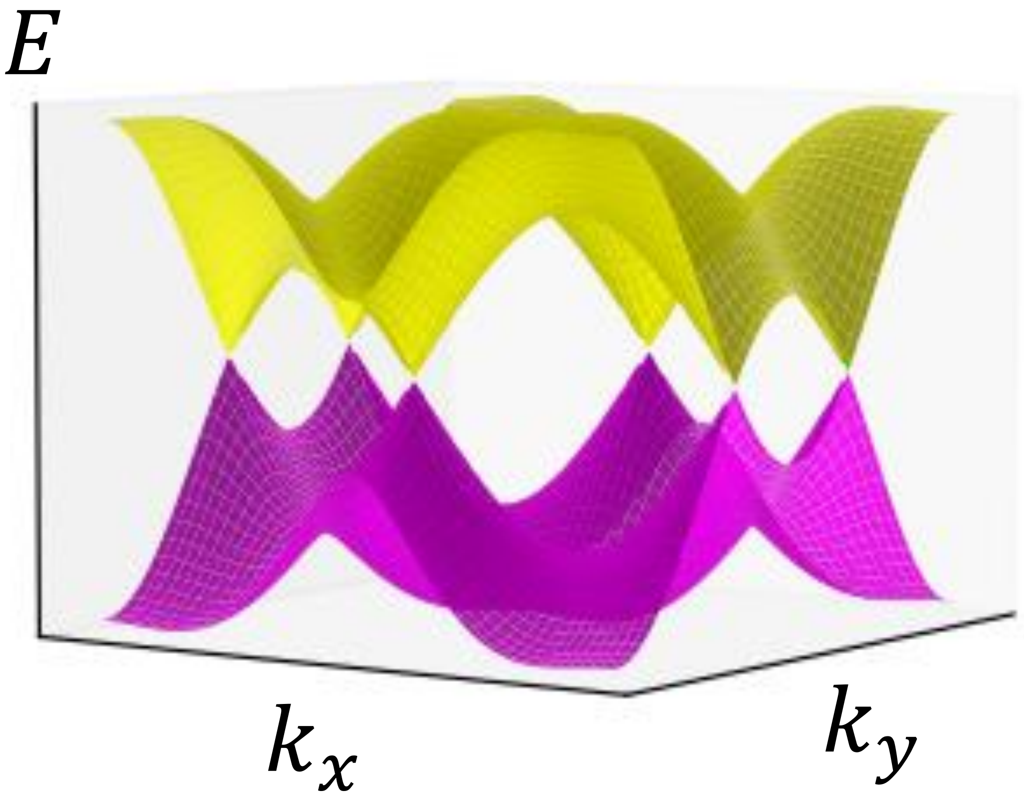
- A sublattice

- B sublattice

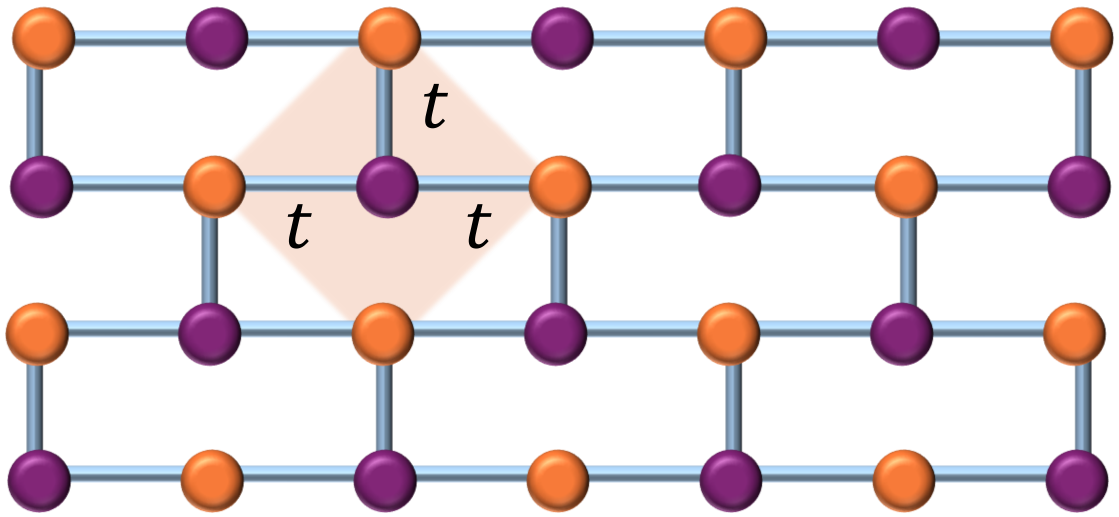
Brickwall lattice



Energy spectrum



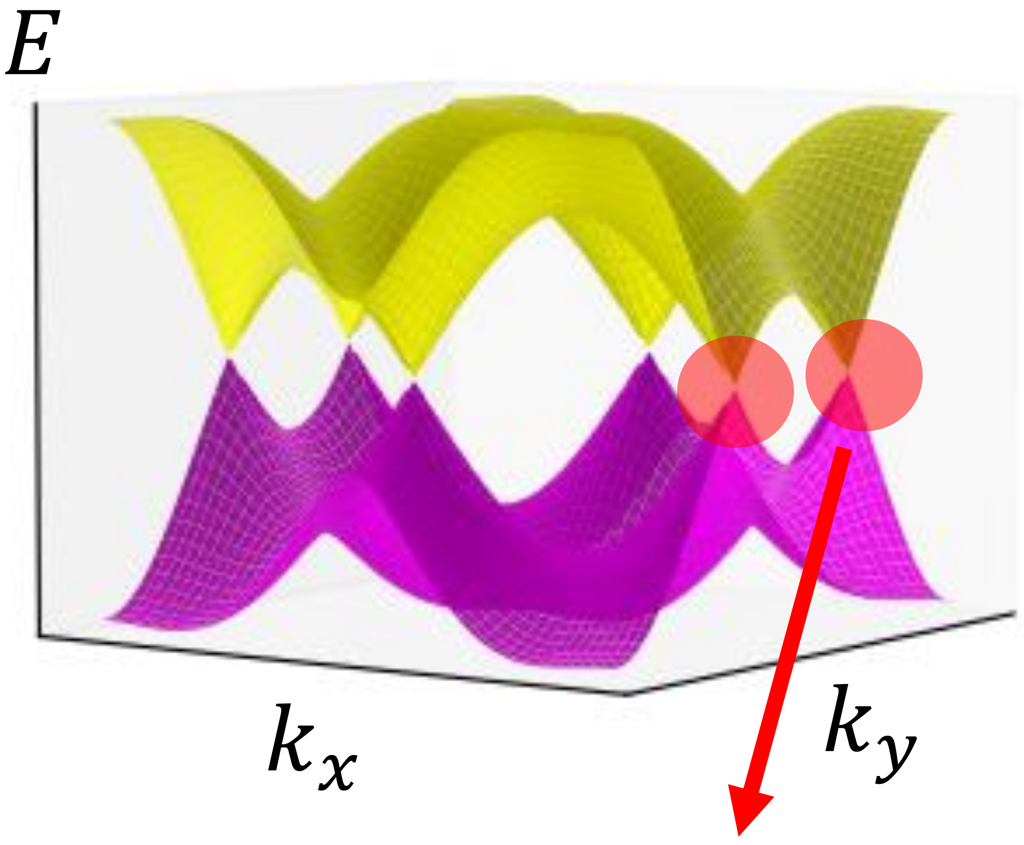
Brickwall lattice



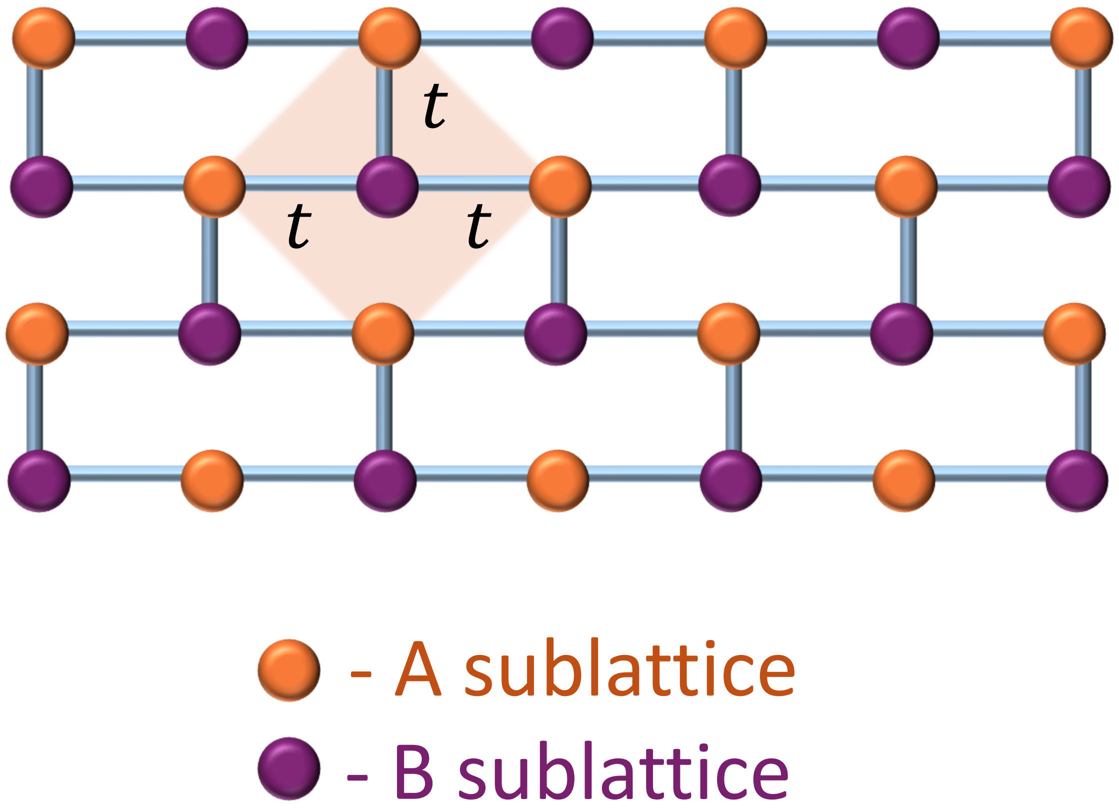
- A sublattice

- B sublattice

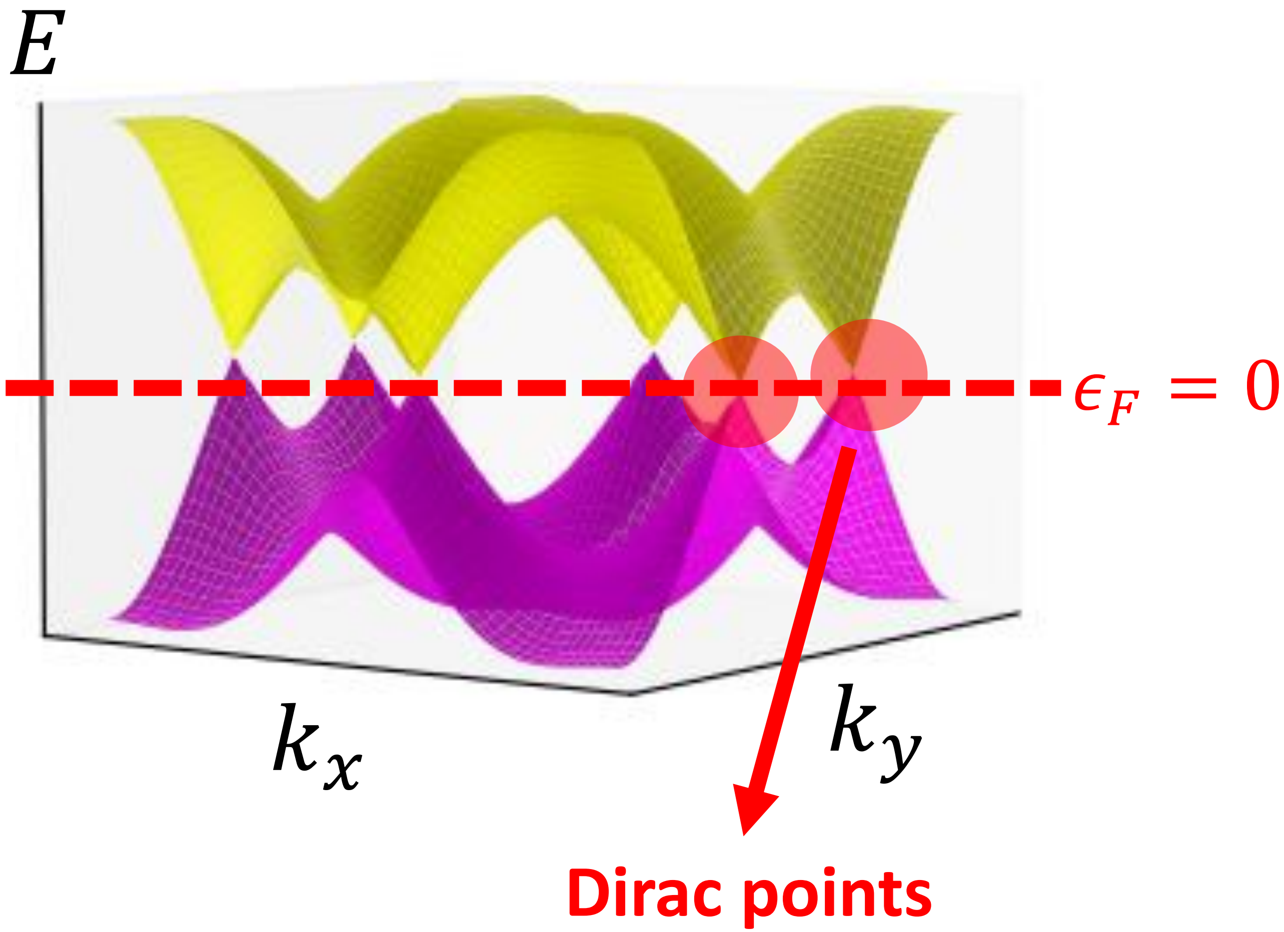
Energy spectrum



Brickwall lattice



Energy spectrum



Brickwall lattice with a defect

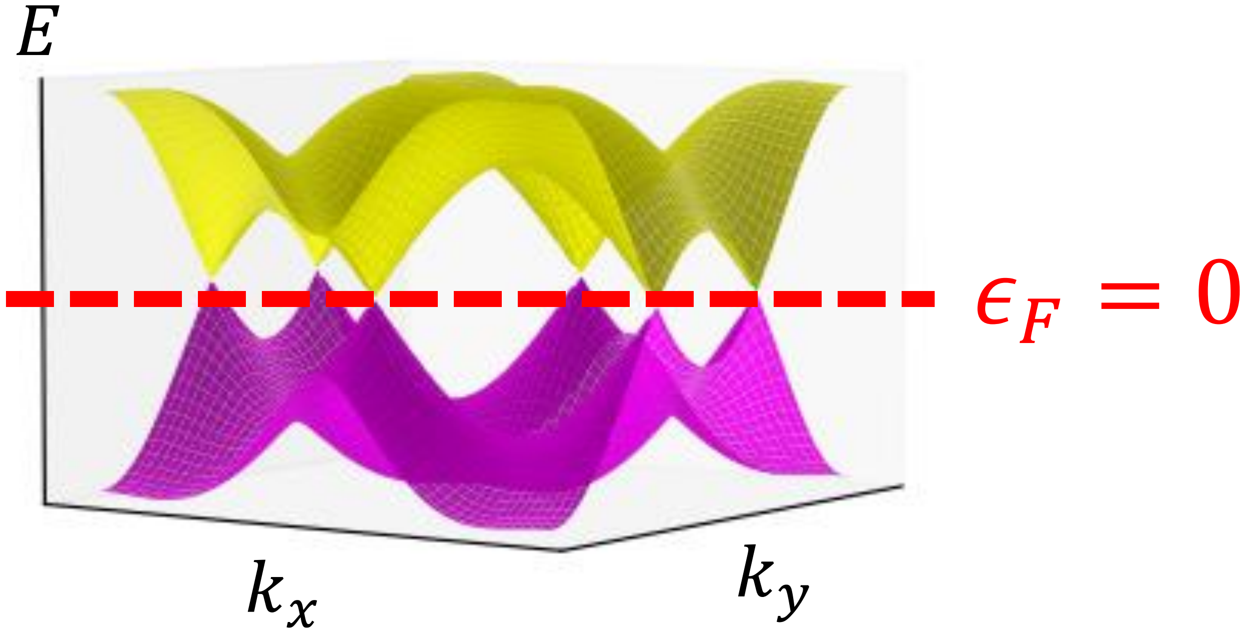
How does the energy spectrum change?

Brickwall lattice with a defect

How does the energy spectrum change? → New mode

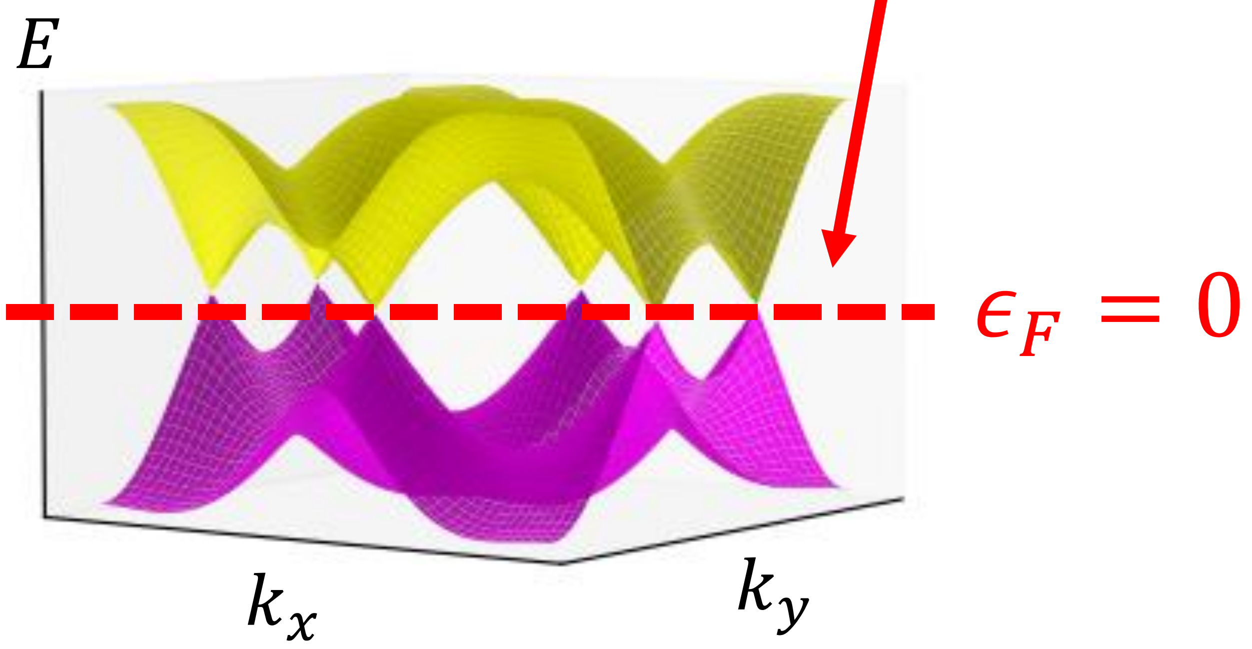
Brickwall lattice with a defect

How does the energy spectrum change? ⇨ New mode



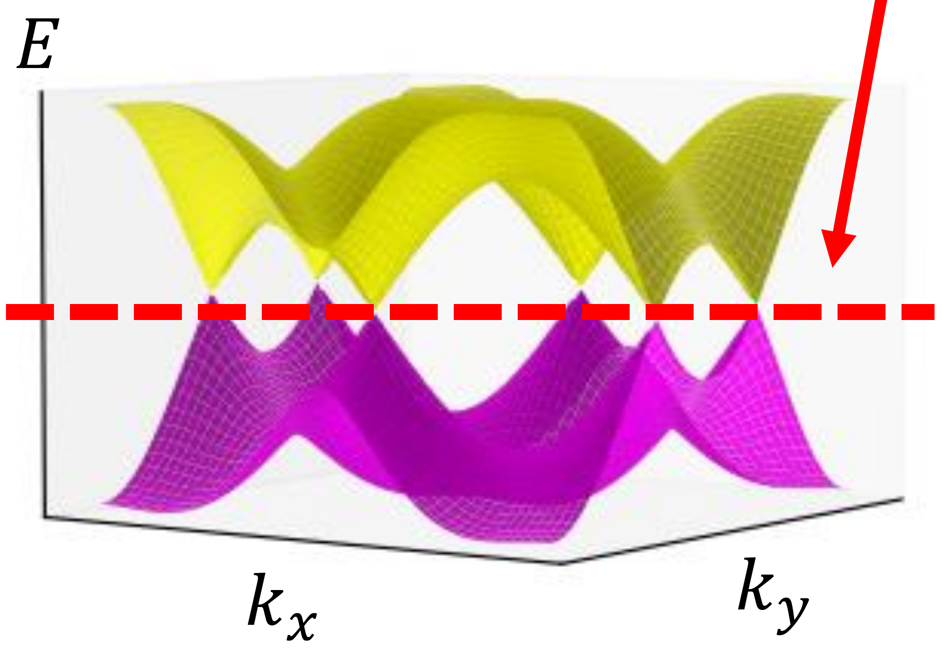
Brickwall lattice with a defect

How does the energy spectrum change? ⇨ New mode



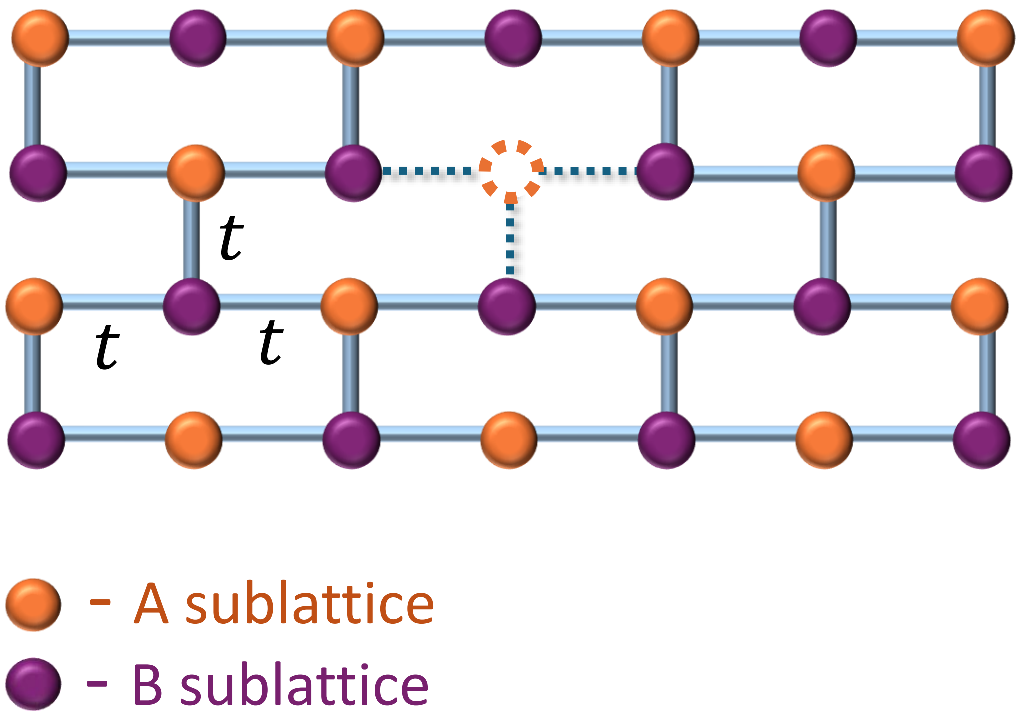
Brickwall lattice with a defect

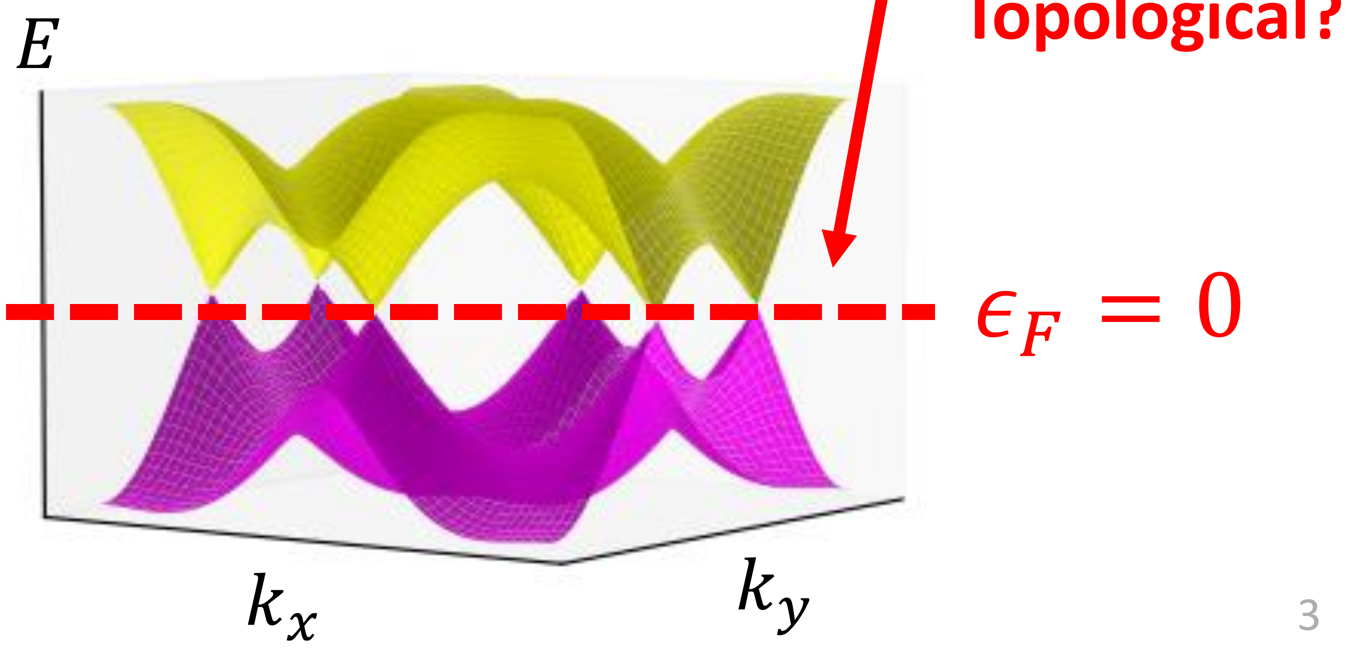
How does the energy spectrum change? ⇨ New mode



Brickwall lattice with a defect (vacancy)

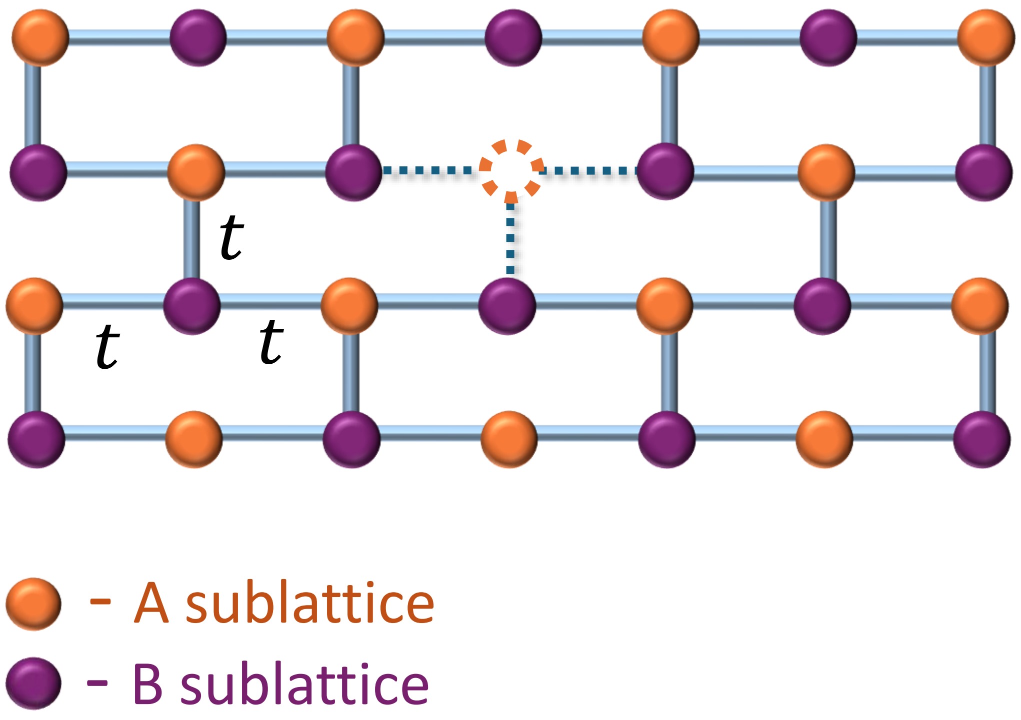
How does the energy spectrum change? → New mode

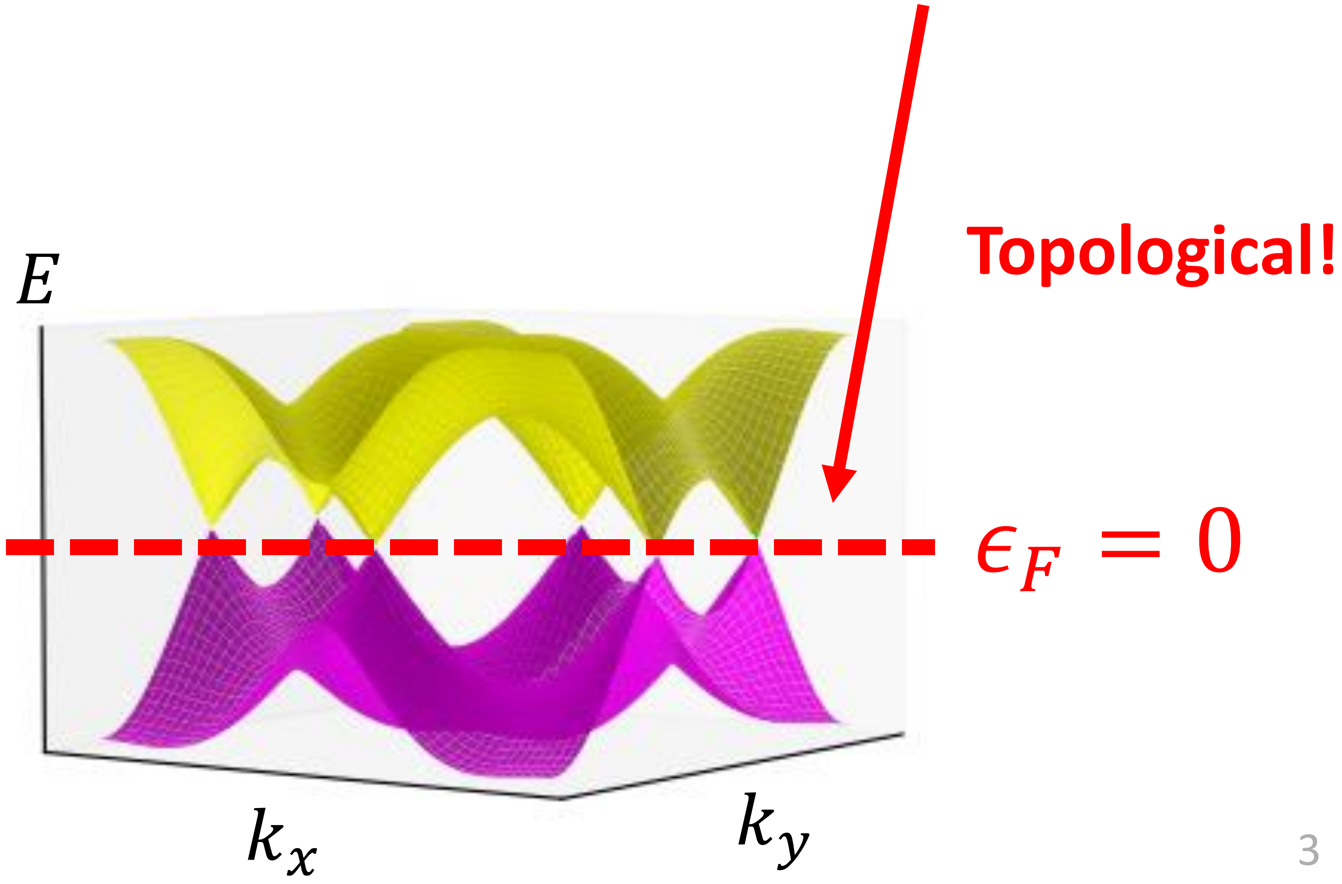




Brickwall lattice with a defect (vacancy)

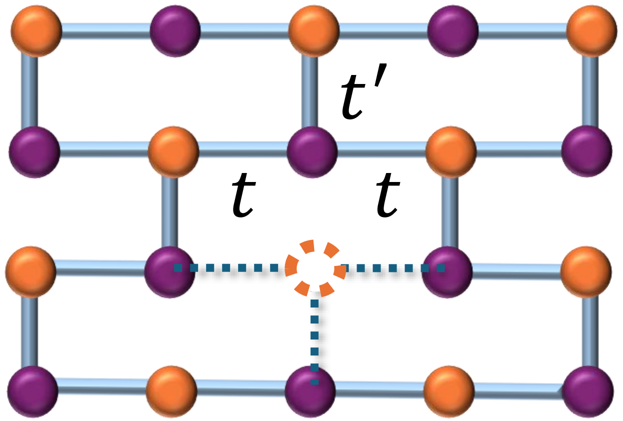
How does the energy spectrum change? → New mode





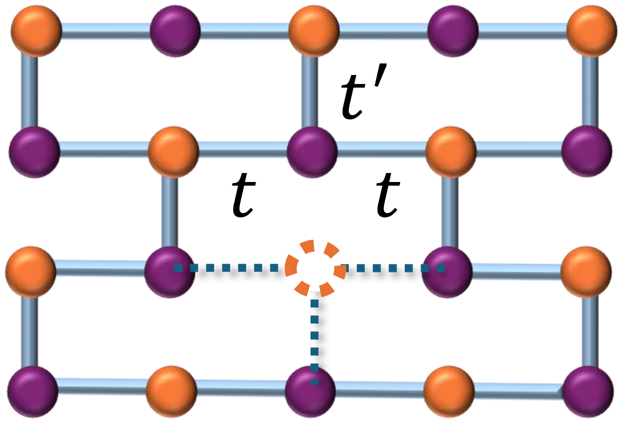
Goft et al (2023) **Abulafia** et al (2023)

Topological mode under a continuous change of parameter



Topological mode under a continuous change of parameter

t'/t



Topological mode under a continuous change of parameter

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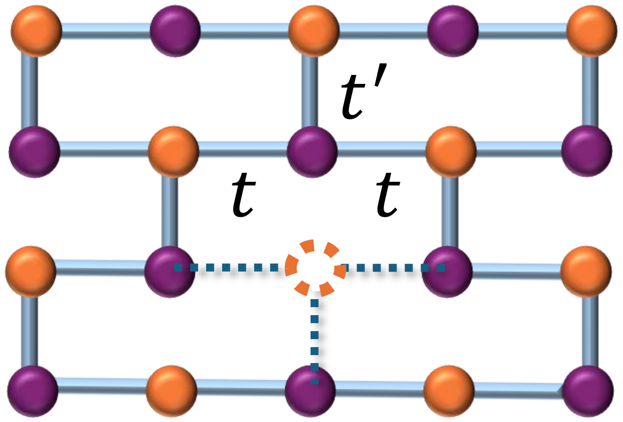
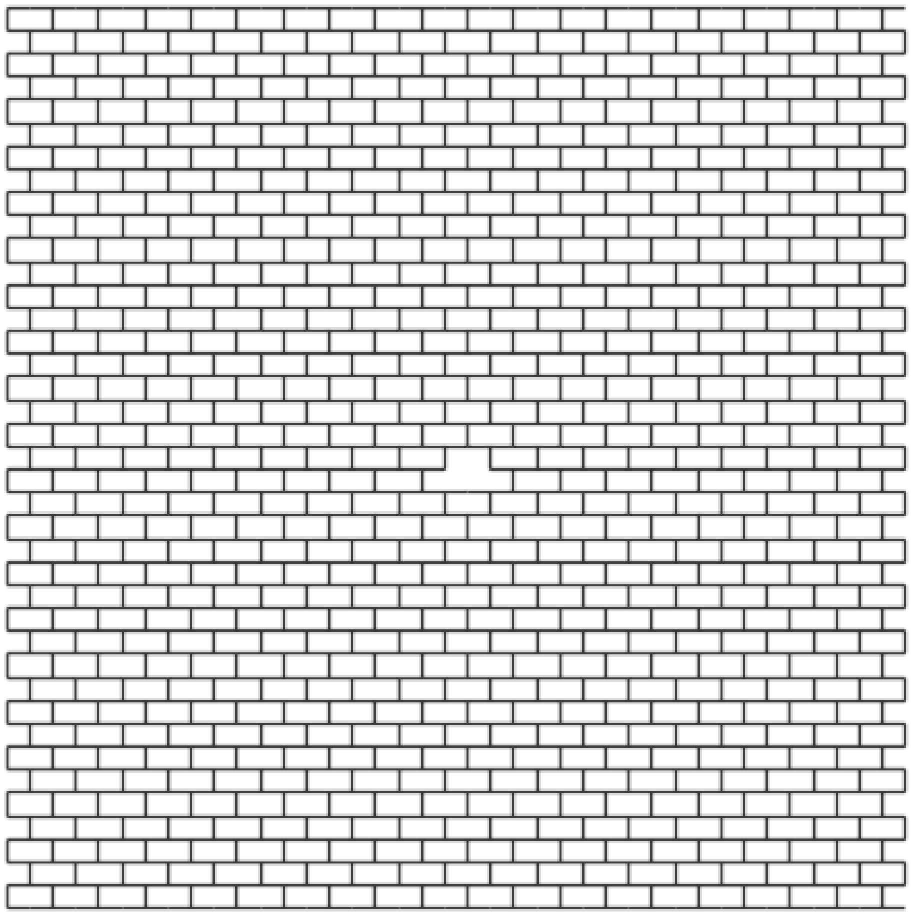
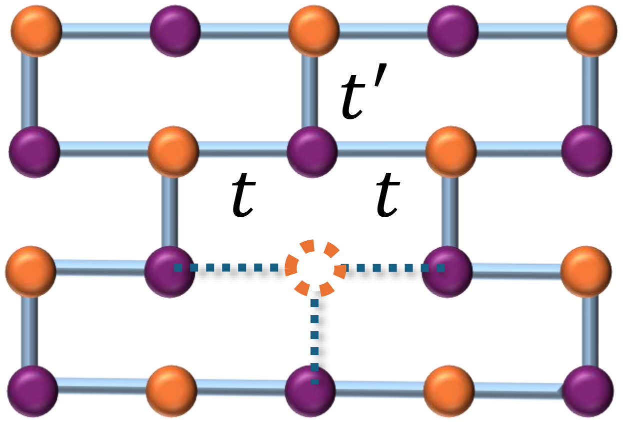


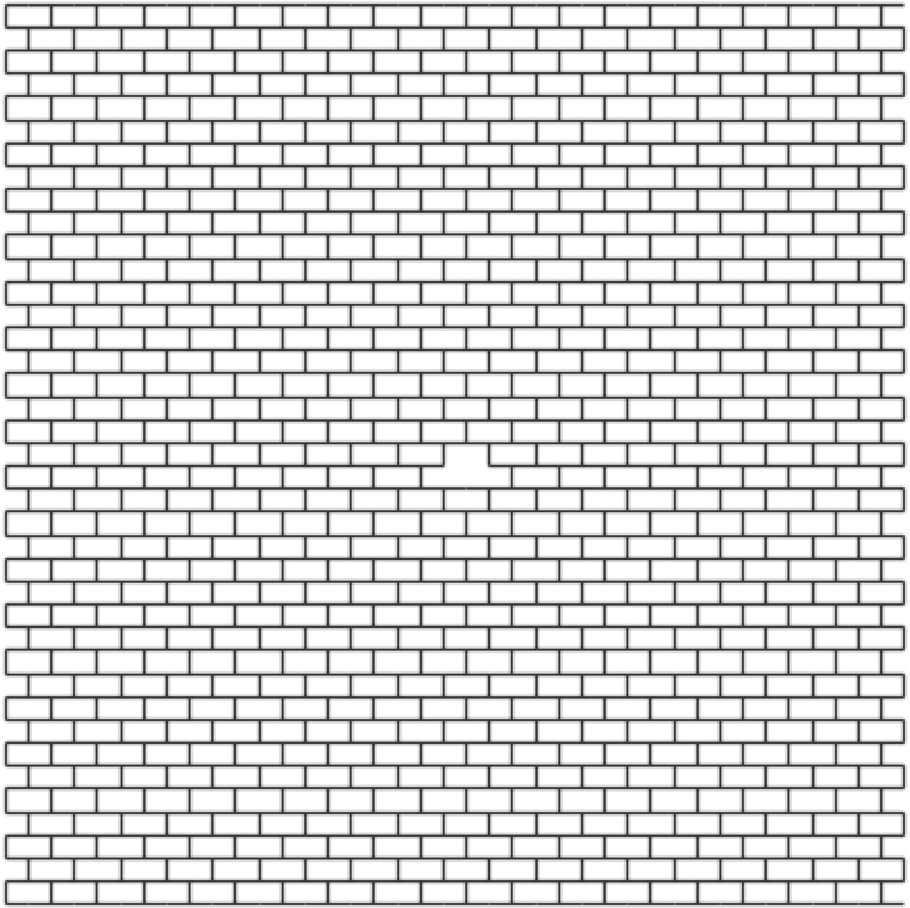


Periodic boundary conditions

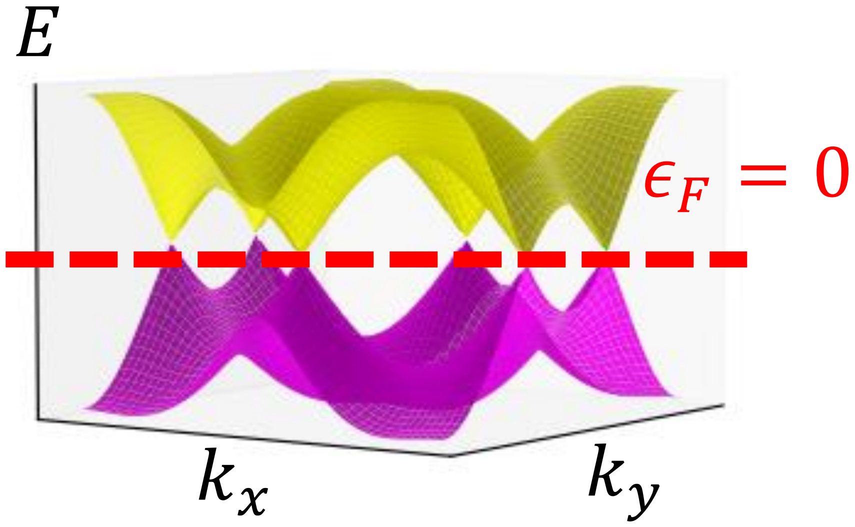
Topological mode under a continuous change of parameter

t'/t

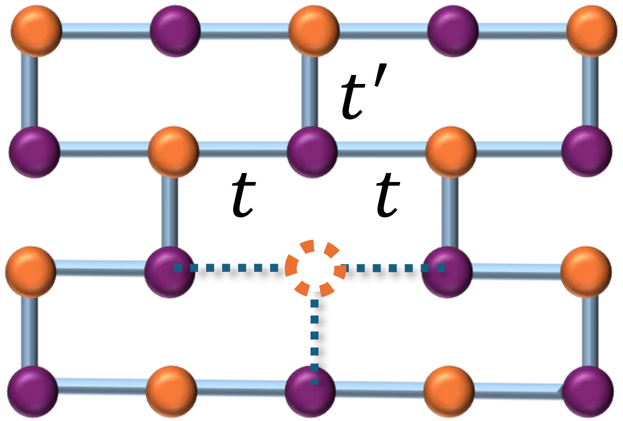




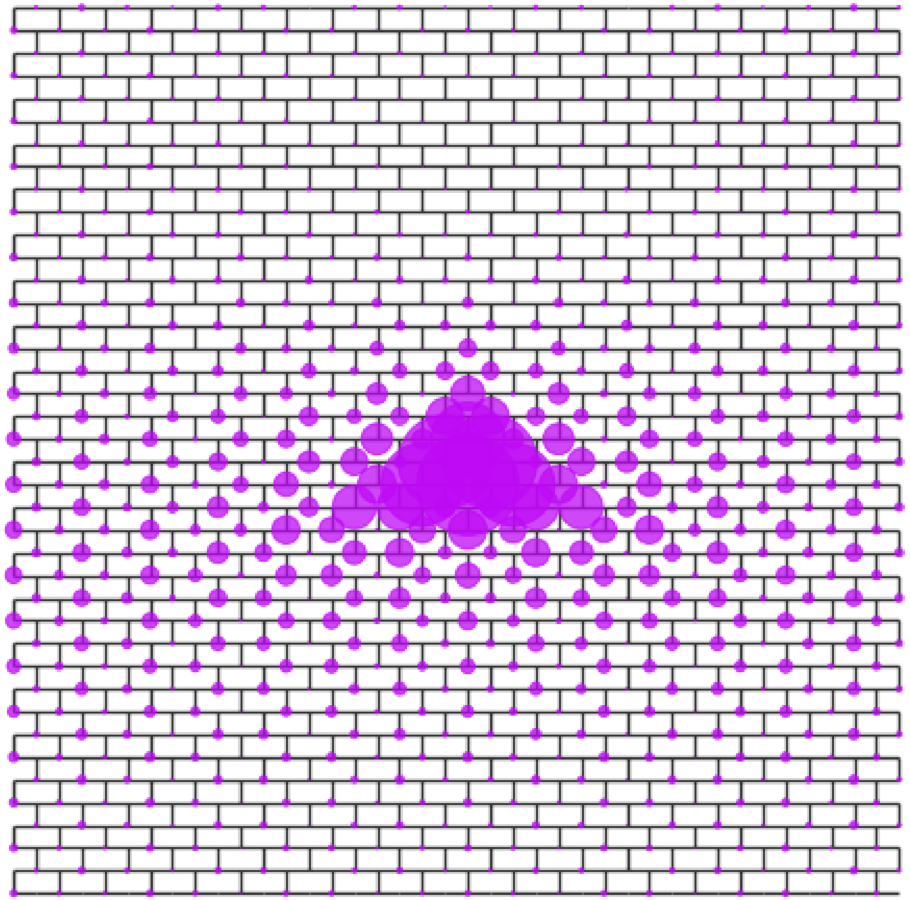
Periodic boundary conditions



Topological mode under a continuous change of parameter

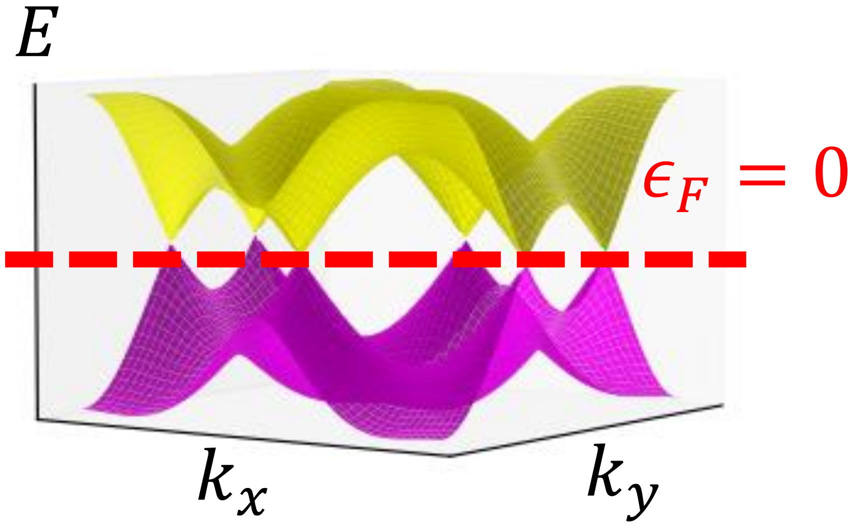


t'/t

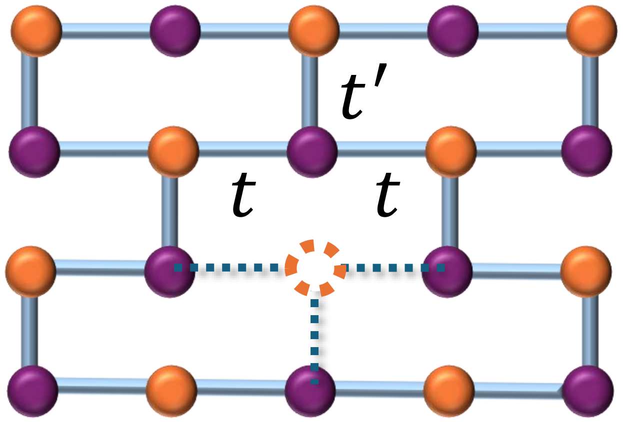


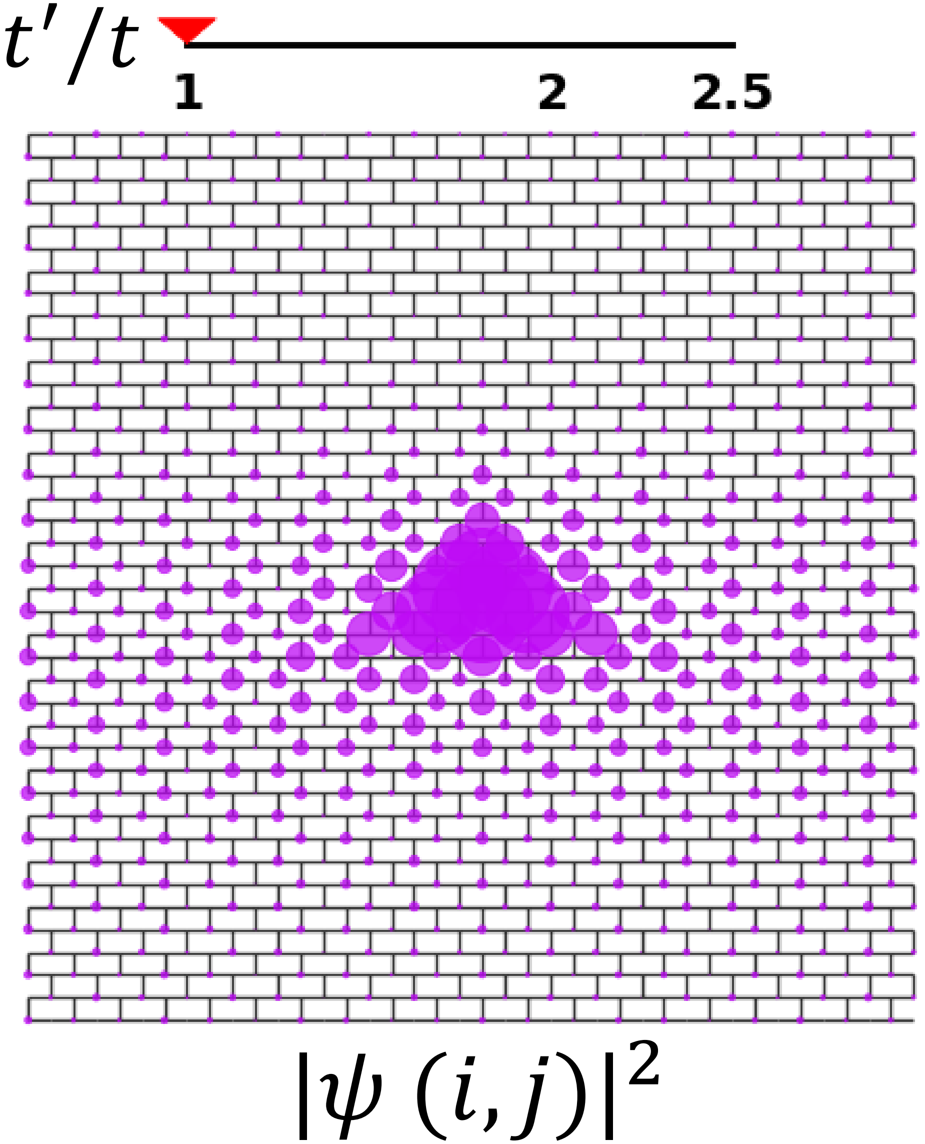
$|\psi\ (i,j)|^2$

Periodic boundary conditions



Topological mode under a continuous change of parameter





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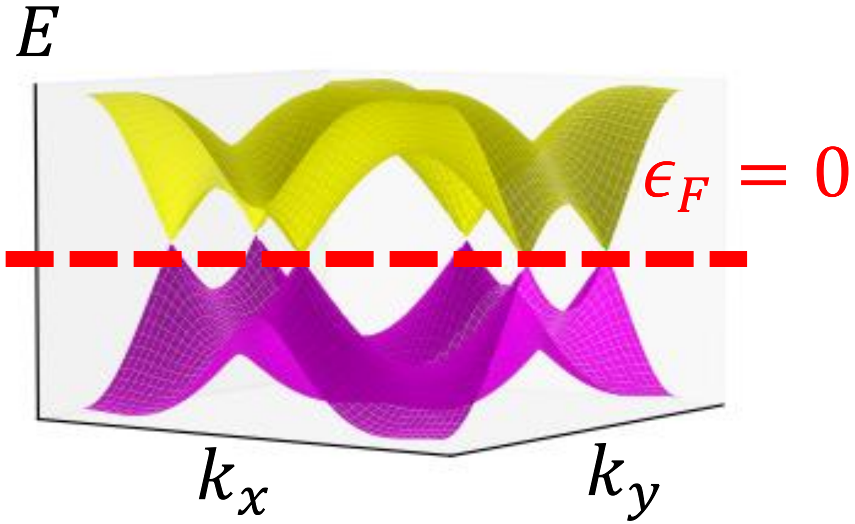
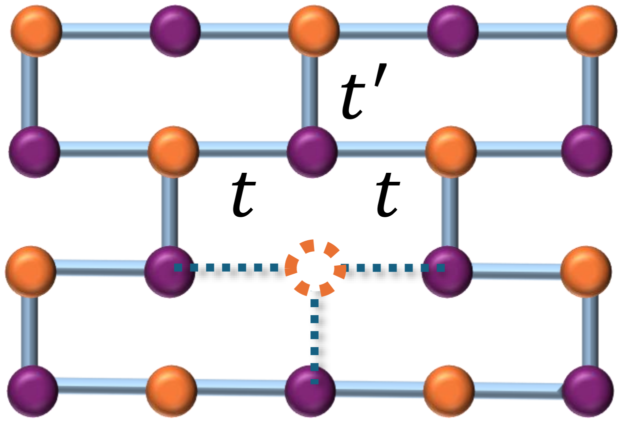
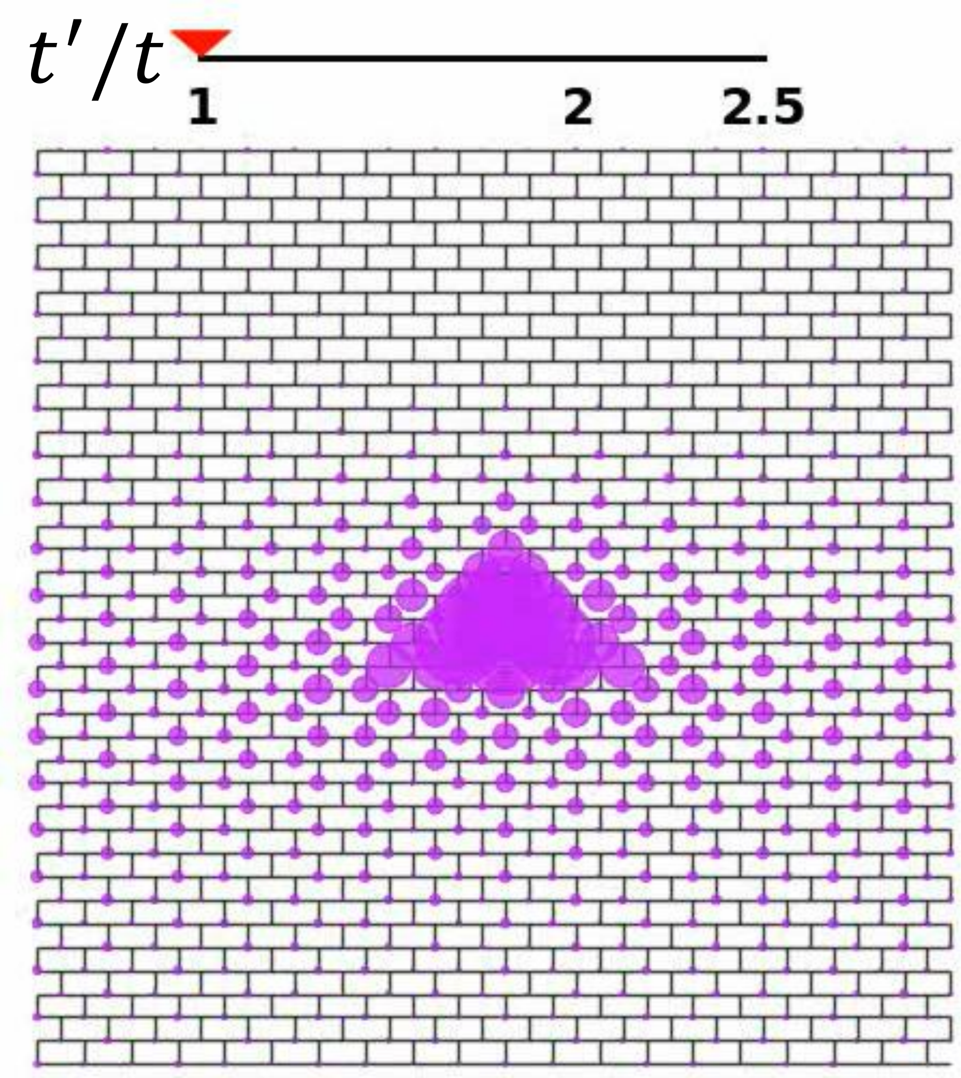


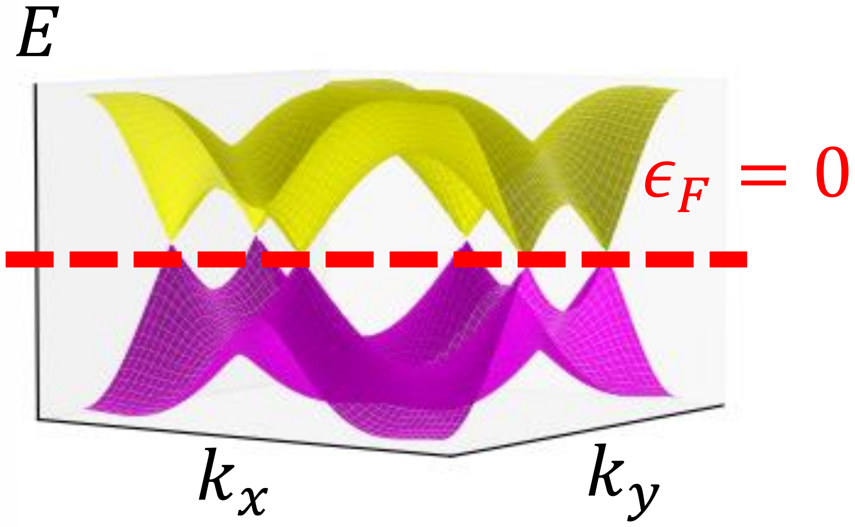
Topological mode under a continuous change of parameter



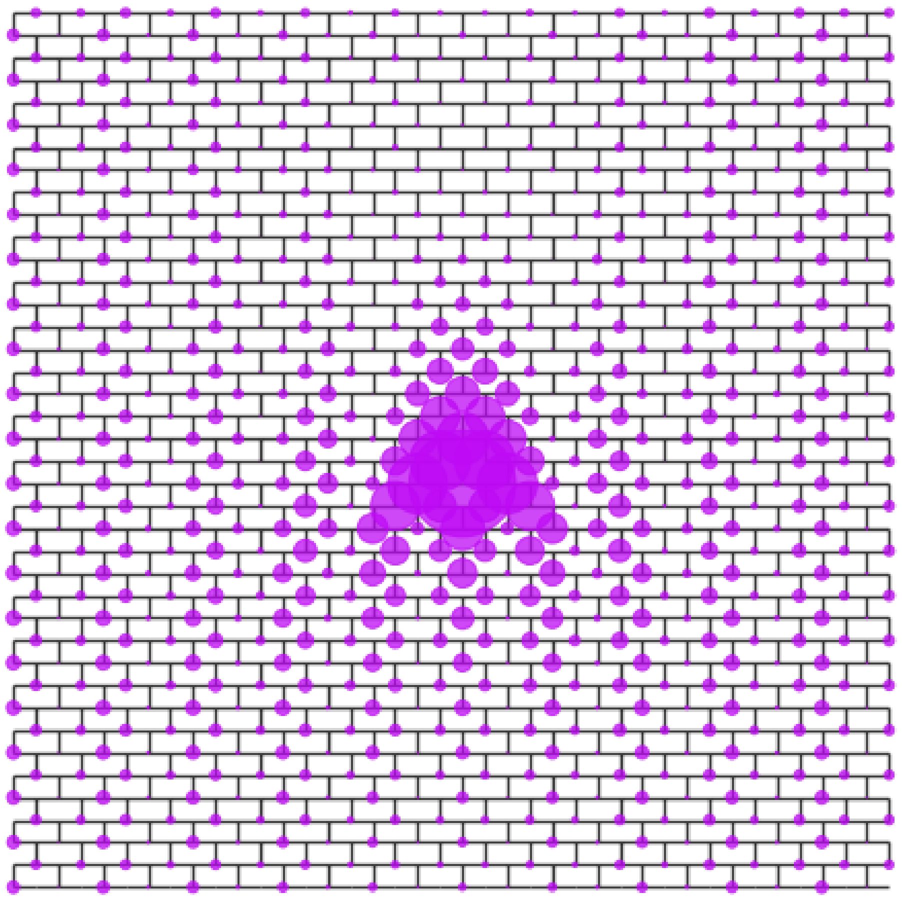


$|\psi\ (i,j)|^2$

Periodic boundary conditions

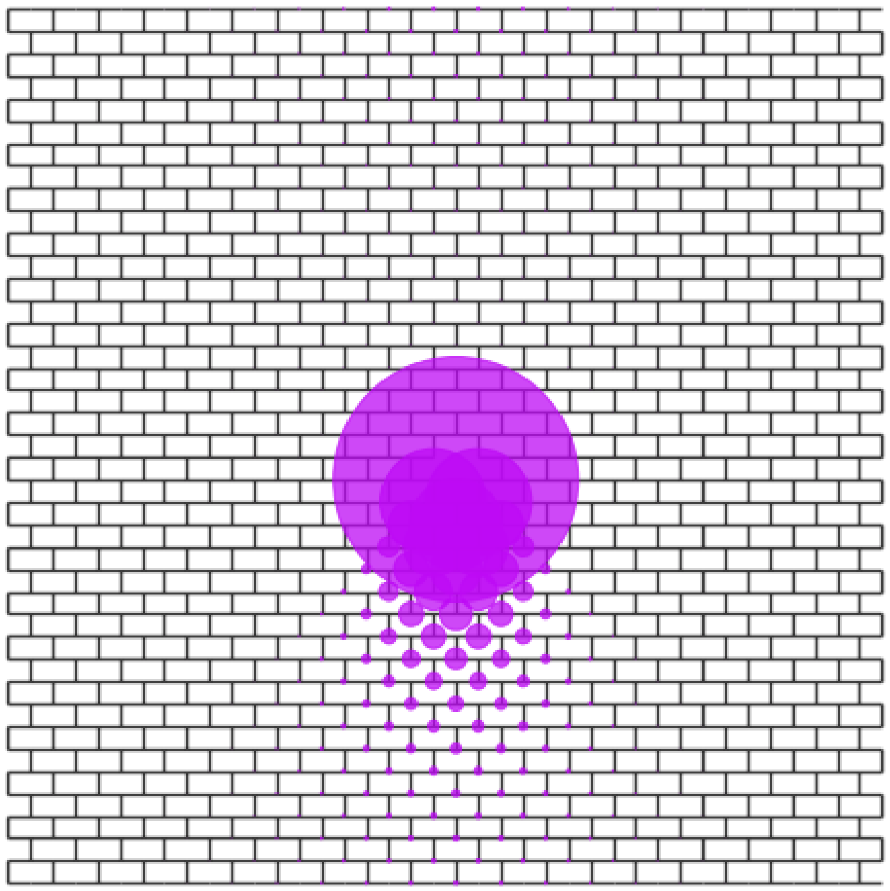


Is there a topological phase transition at the critical point?



Critical

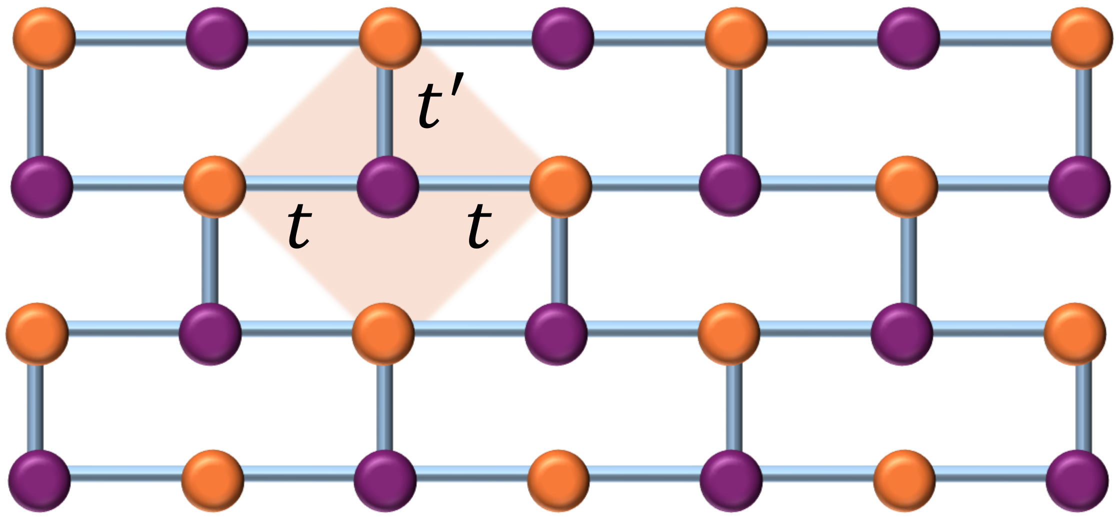
$t'/t = 2$



$|\psi\ (i,j)|^2$ $\quad t'/t < 2$

$t'/t > 2$ $\quad |\psi\ (i,j)|^2$

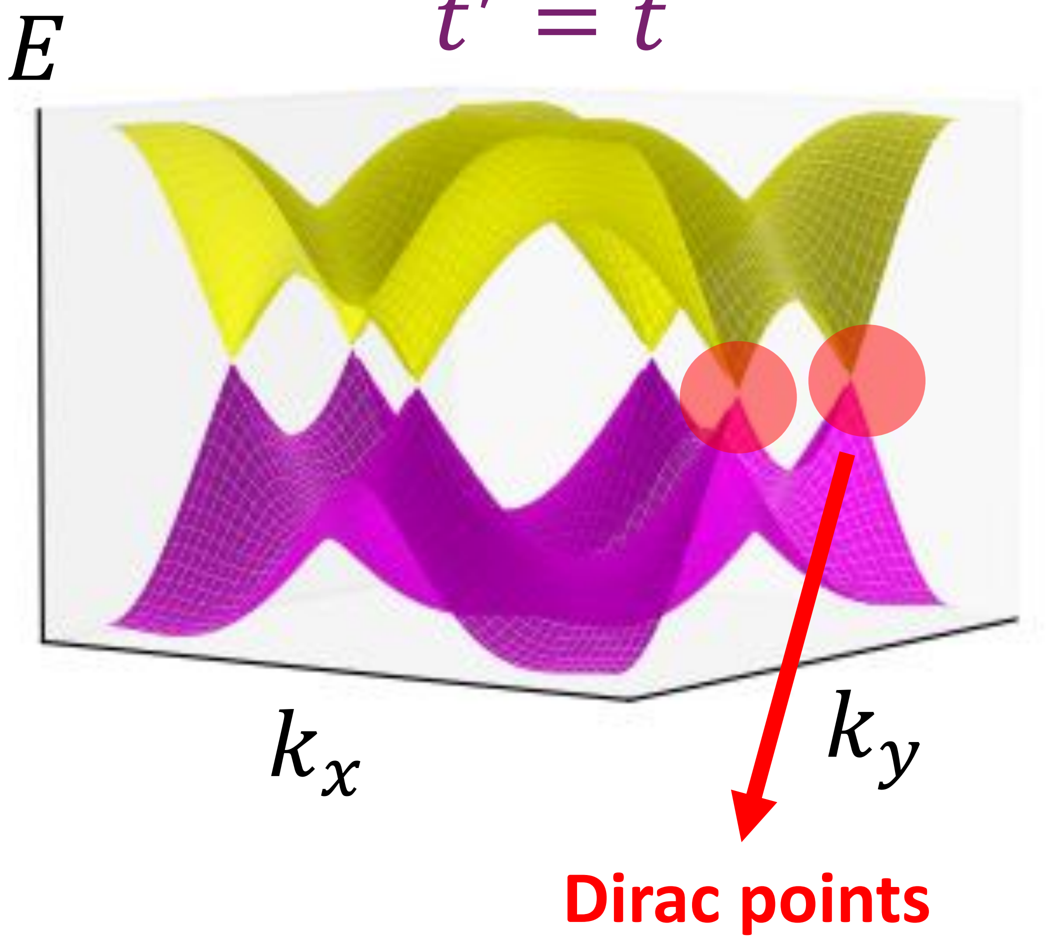
Brickwall lattice



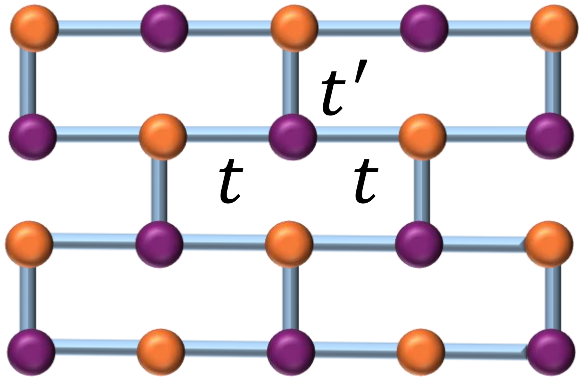
- A sublattice
- B sublattice

Energy spectrum

$t' = t$

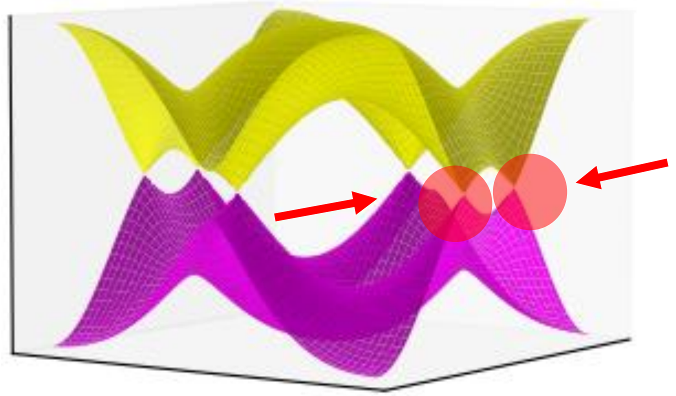


Energy spectrum and critical point

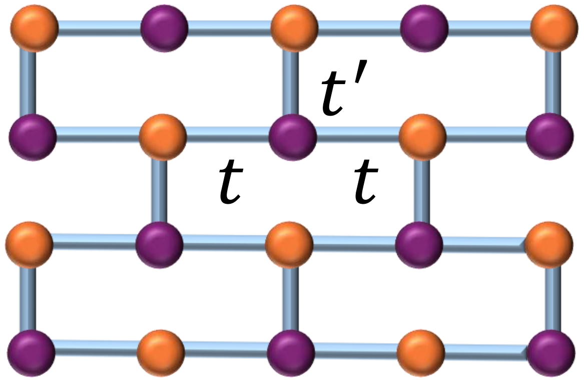


Before

$t' = 1.5t$



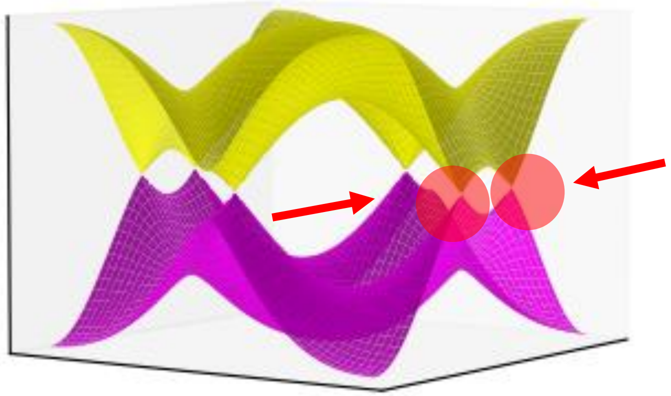
Energy spectrum and critical point

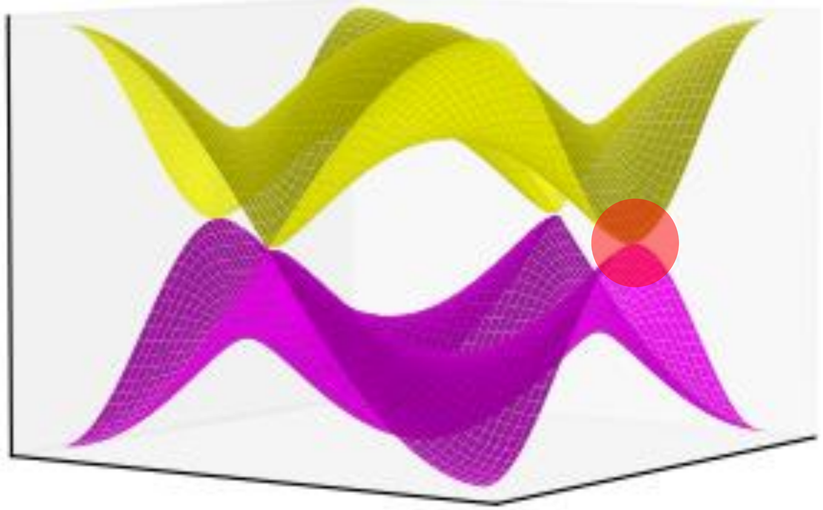


Before

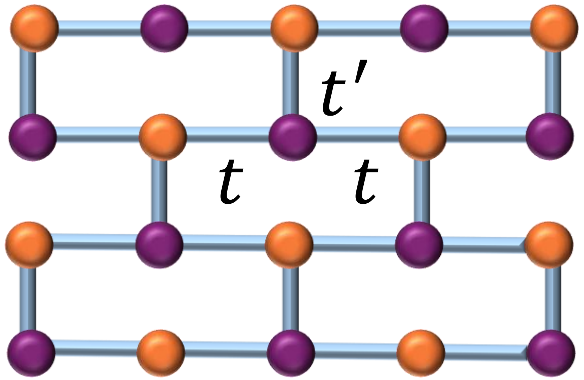
Merging
$t' = 2t$

$t' = 1.5t$



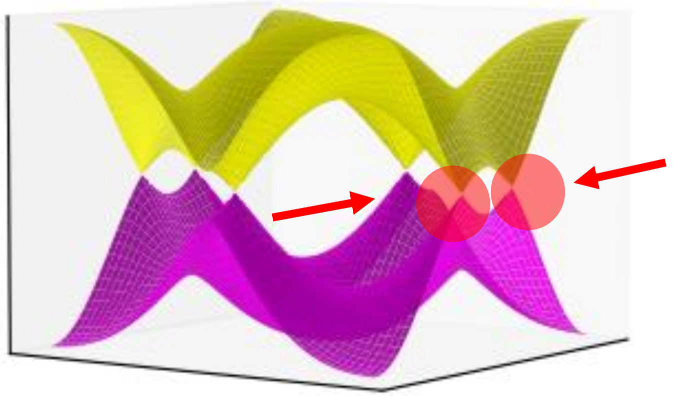


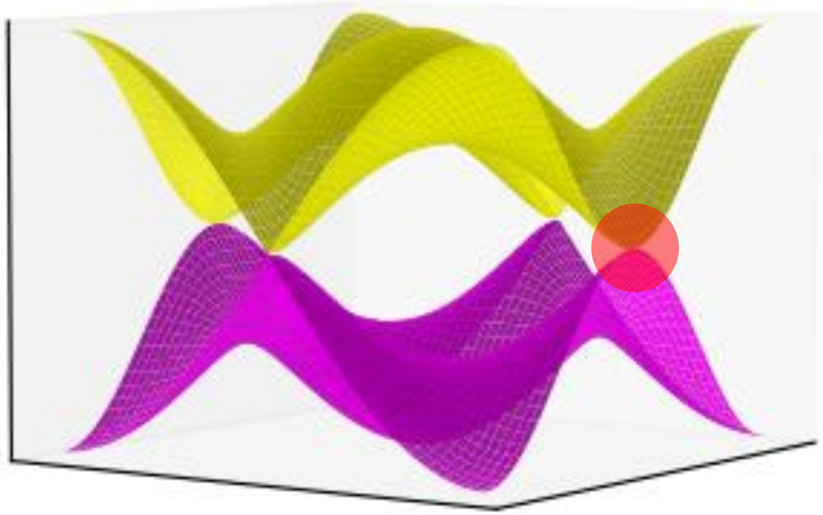
Energy spectrum and critical point



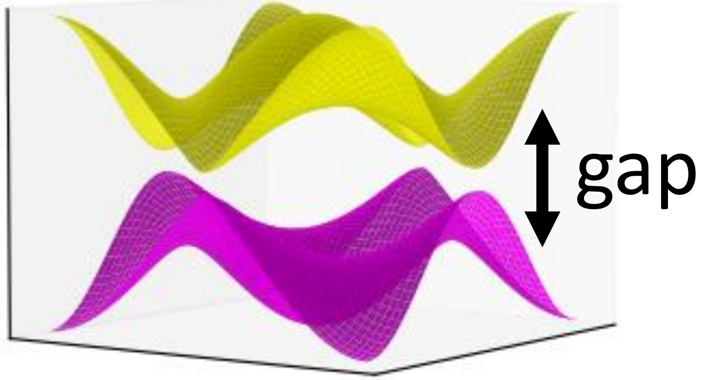
Before → **Merging** $t' = 2t$ → After

$t' = 1.5t$





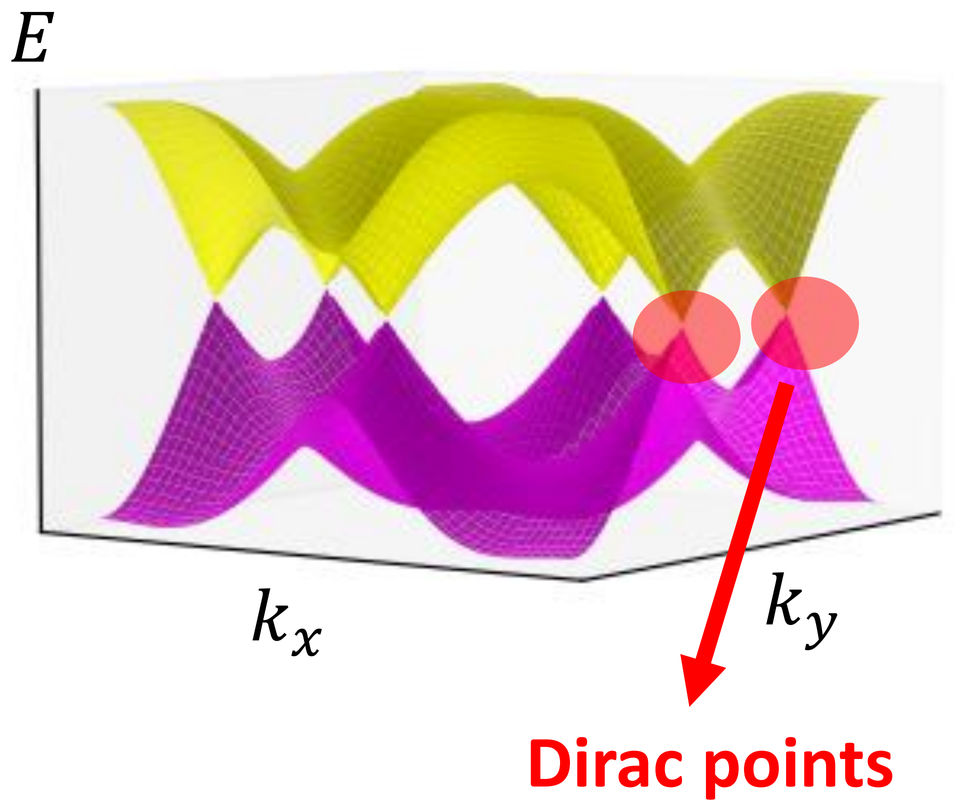
$t' = 2.3t$



Background - Topological materials

1. Topological classification
2. w - Integer invariant

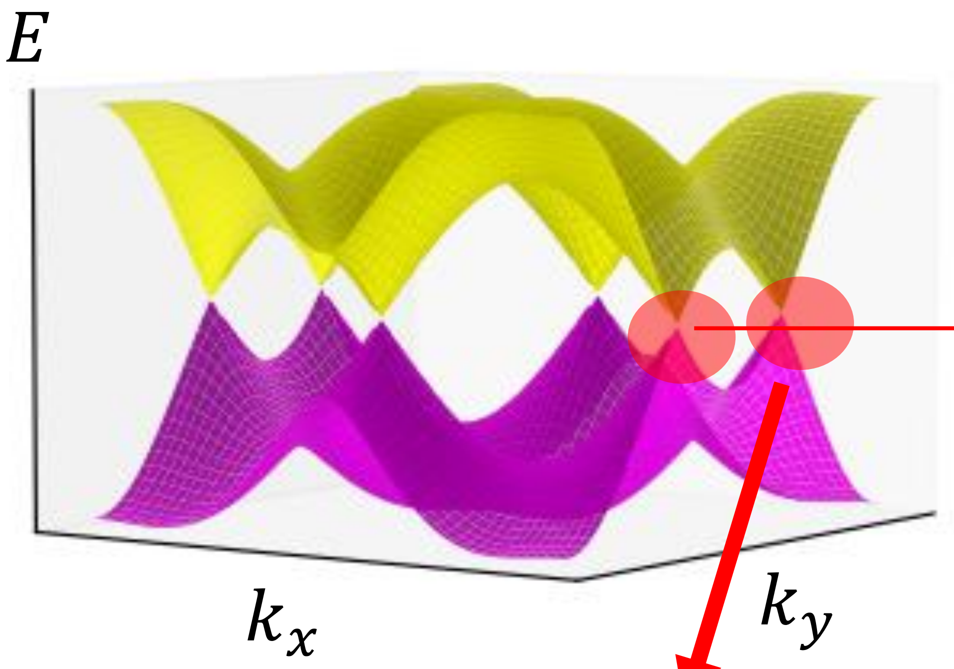
1 Topological classification of materials



1 Topological classification of materials

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}$$

Anti- commuting
Dirac matrices



Dirac points

1 Topological classification of materials

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}$$

Anti- commuting Dirac matrices

Anti-unitary symmetries
- Θ - Time reversal
- C - Particle hole

1 Topological classification of materials

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}$$

Anti- commuting Dirac matrices

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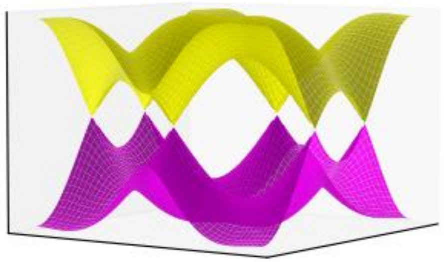

1 Topological classification of materials

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}$$

Anti- commuting Dirac matrices

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$$\Theta^2, C^2 \in \{+,-,0\}$$

1 Topological classification of materials

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}$$

Anti- commuting Dirac matrices

Anti-unitary symmetries
- Θ - Time reversal
- C - Particle hole

$$\Theta^2, C^2 \in \{+,-,0\}$$

S - Chirality $\in \{0,1\}$

1 Topological classification of materials

Class	Θ	C	S
A	0	0	0
AIII	0	0	1
AI	+	0	0
BDI	+	+	1
D	0	+	0
DIII	−	+	1
AII	−	0	0
CII	−	−	1
C	0	−	0
CI	+	−	1

Teo and **Kane** (2010)

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}$$

$\boldsymbol{\gamma}$ → Anti- commuting Dirac matrices

↓

Anti-unitary symmetries:
- Θ - Time reversal
- C - Particle hole

$$\Theta^2, C^2 \in \{+,-,0\}$$

S - Chirality $\in \{0,1\}$

↓

class

1 Topological classification of materials

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

Teo and **Kane** (2010)

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}$$

Anti- commuting Dirac matrices

Anti-unitary symmetries
- Θ - Time reversal
- C - Particle hole

$$\Theta^2, C^2 \in \{+,-,0\}$$

S - Chirality $\in \{0,1\}$

class

1 Topological classification of materials

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

Codimension

$$\delta = d - D$$

Spatial dimension

Defect dimension

Teo and **Kane** (2010)

1 Topological classification of materials

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

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$$\delta = d - D$$

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BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

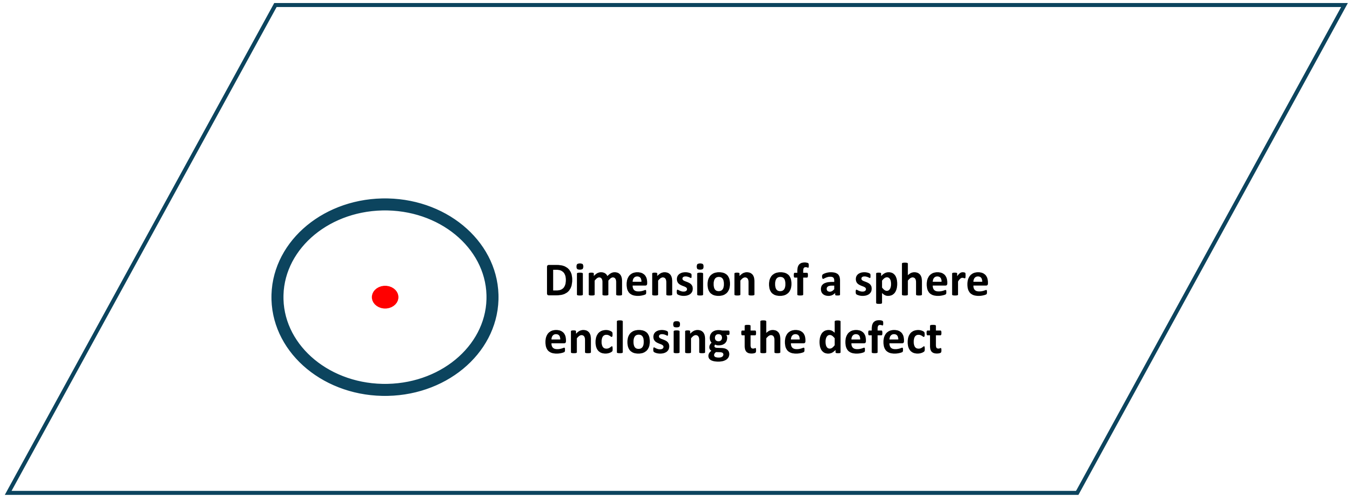
Teo and **Kane** (2010)

Codimension

$$\boldsymbol{\delta} = d - D$$

Spatial dimension

Defect dimension



1 Topological classification of materials

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

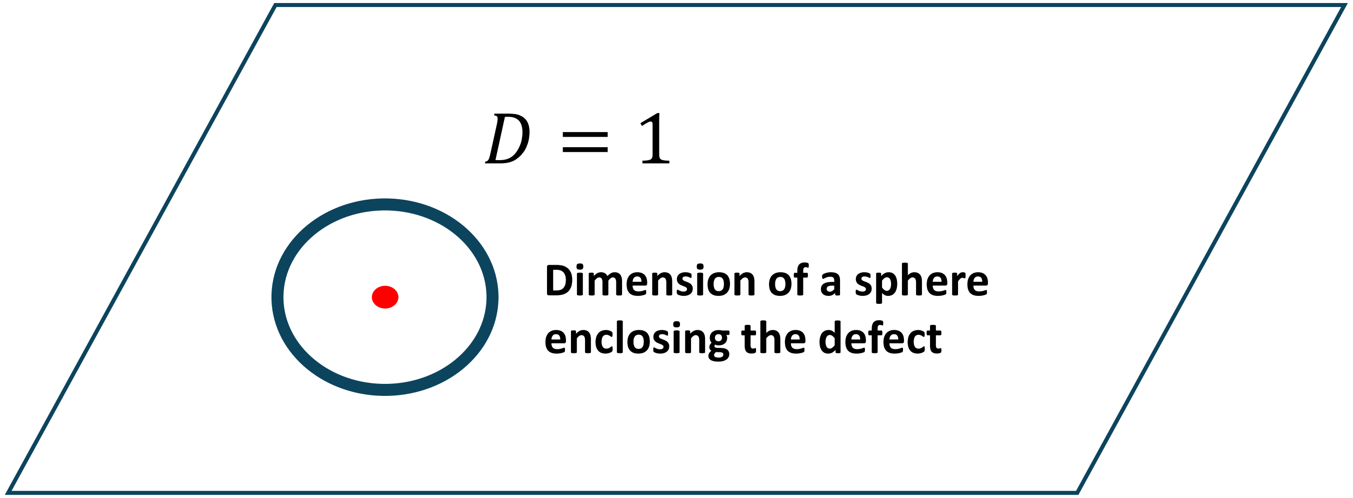
Teo and **Kane** (2010)

Codimension

$$\boldsymbol{\delta} = d - D$$

Spatial dimension

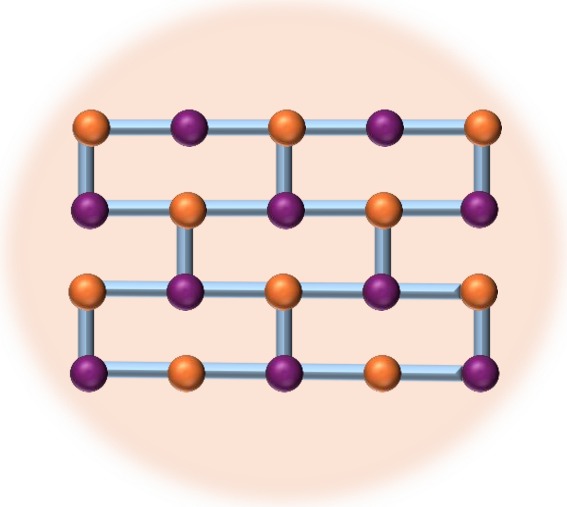
Defect dimension



Example

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

Teo and **Kane** (2010)



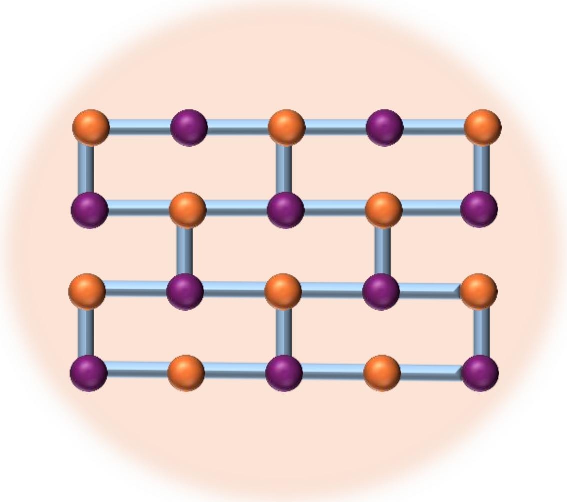
Brickwall lattice

$$\boldsymbol{\delta} = 2 - 0$$

Example

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

Teo and **Kane** (2010)



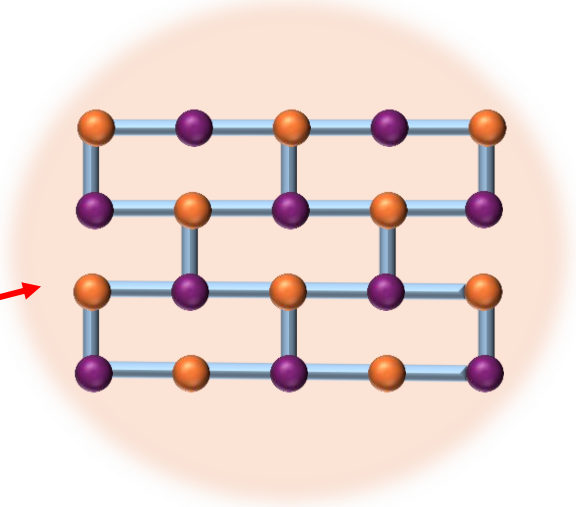
Brickwall lattice

$$\boldsymbol{\delta} = 2 - 0$$

Example

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

Teo and **Kane** (2010)



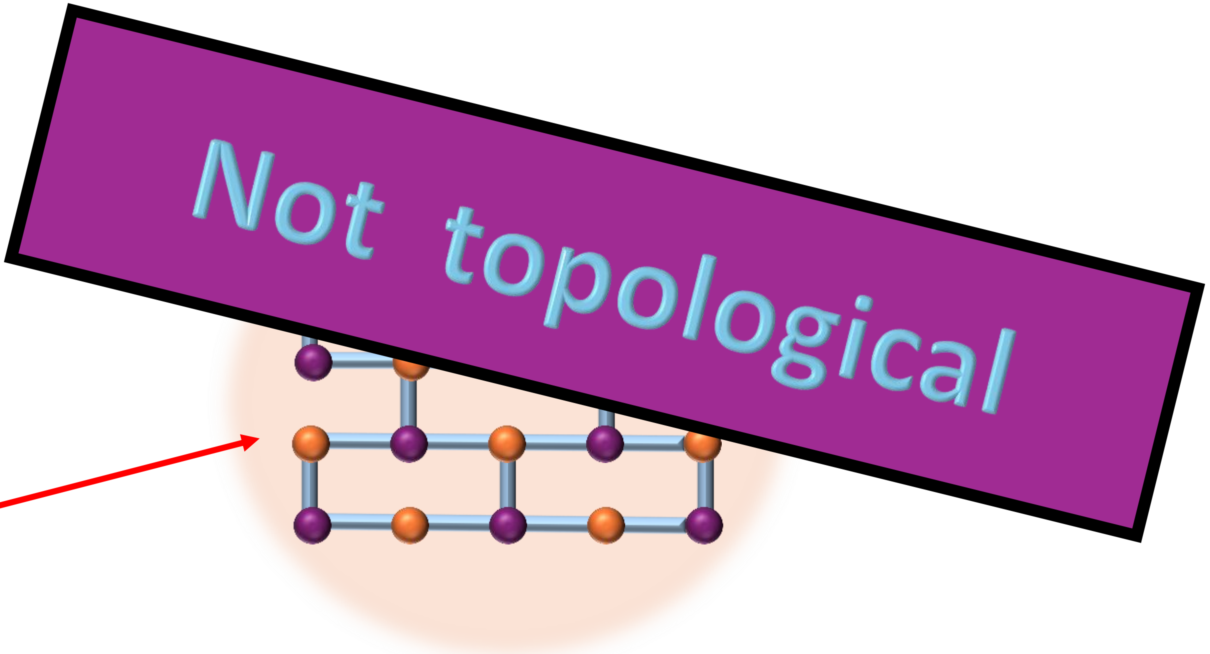
Brickwall lattice

$$\boldsymbol{\delta} = 2 - 0$$

Example

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

Teo and **Kane** (2010)



Brickwall lattice

$$\boldsymbol{\delta} = 2 - 0$$

Example

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

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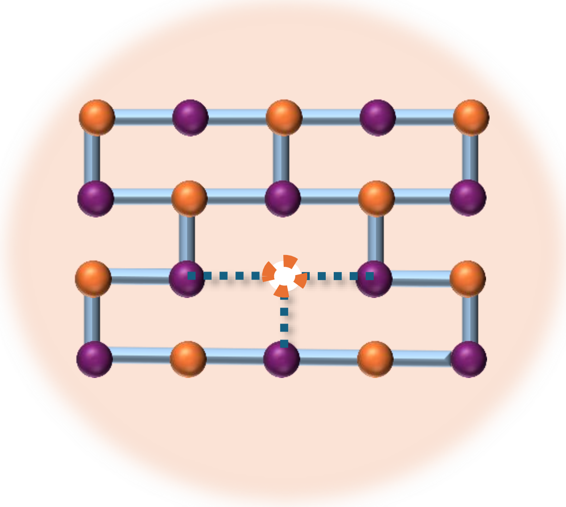
$$\boldsymbol{\delta} = 2 - 1$$



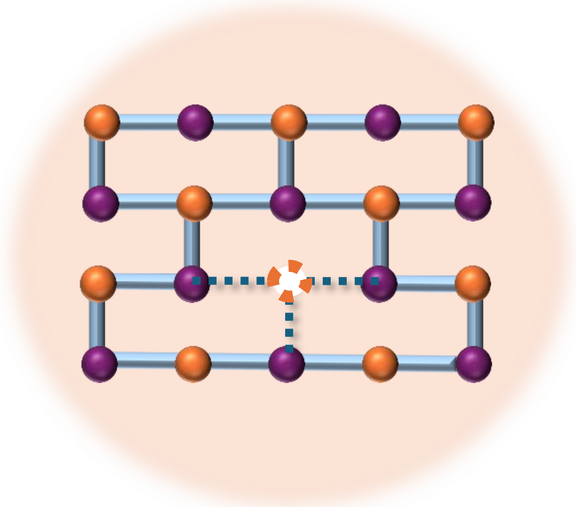
Brickwall lattice + vacancy

Example

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

Teo and **Kane** (2010) **Goft** et al (2023)

$$\boldsymbol{\delta} = 2 - 1$$



Brickwall lattice + vacancy

Example

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

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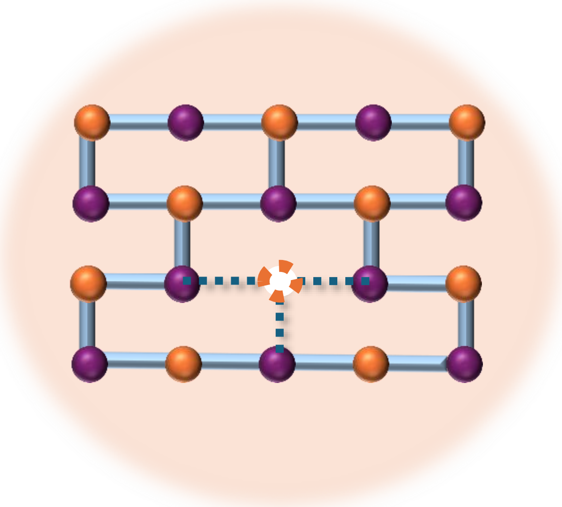
$$\boldsymbol{\delta} = 2 - 1$$



Brickwall lattice + vacancy

Example

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

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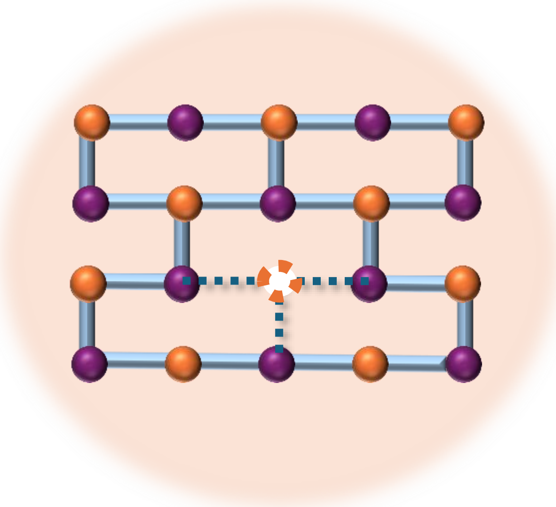
Topological

Integer invariant

$$\delta = 2 - 1$$



Brickwall lattice + vacancy

Background - Topological materials

1. Topological classification
2. w - Integer invariant

2 w - Integer invariant

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
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C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

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Anti- commuting matrices

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}_{2m\times 2m}$$

degrees of freedom

2 w - Integer invariant

Anti- commuting matrices

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}_{2m\times 2m}$$

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DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

m

degrees of freedom

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2 w - Integer invariant

Anti- commuting matrices

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}_{2m\times 2m}$$

Class	Θ	C	S	$\delta = 0$	1	2	3
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AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

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Spatial dimension

Defect dimension

$$2m = d + D + 1$$

degrees of freedom

2 w - Integer invariant

Anti- commuting matrices

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}_{2m\times 2m}$$

Class	Θ	C	S	$\delta = 0$	1	2	3
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

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Spatial dimension

Defect dimension

$$2m = d + D + 1 \Rightarrow w \in \mathbb{Z}$$

degrees of freedom

2 w - Integer invariant

Anti- commuting matrices

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}(\boldsymbol{k},\boldsymbol{r}) \cdot \boldsymbol{\gamma}_{2m\times 2m}$$

Class	Θ	C	S	$\delta = 0$	1	2	3
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BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	0	−	0	0	0	$2\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$

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Spatial dimension

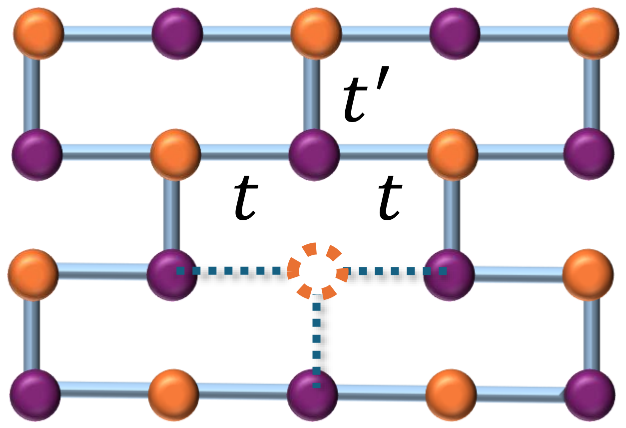
Defect dimension

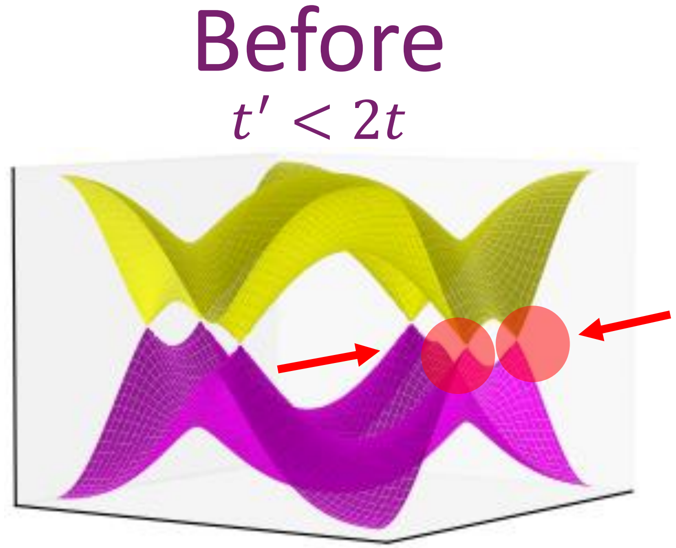
$$2m = d + D + 1 \Rightarrow w \in \mathbb{Z}$$

$$2m \neq d + D + 1 \Rightarrow w \notin \mathbb{Z}$$

Brickwall + vacancy before merging

- Degrees of freedom
  - Sublattice
  - Inequivalent Dirac points

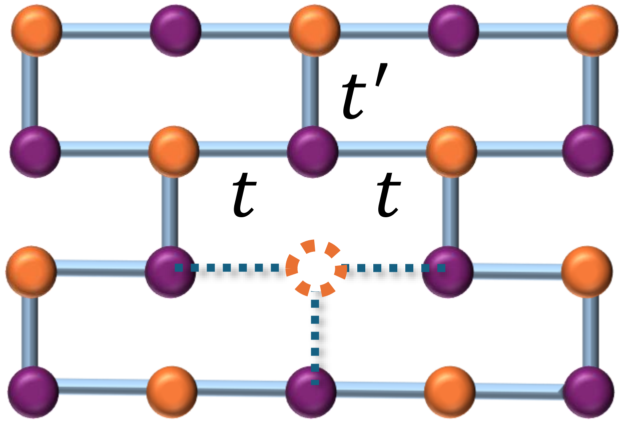


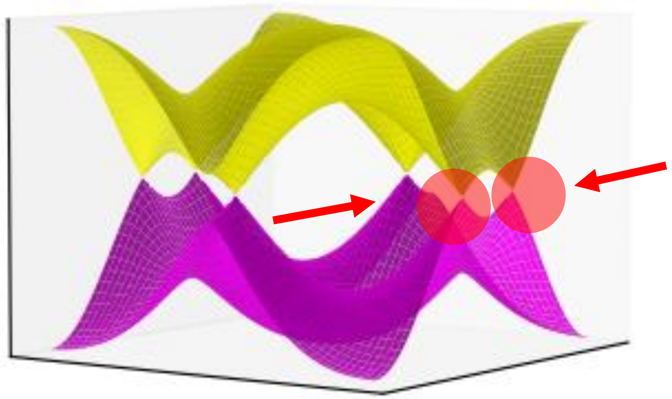


Brickwall + vacancy before merging

- Degrees of freedom
  - Sublattice
  - Inequivalent Dirac points

$$m = 2$$

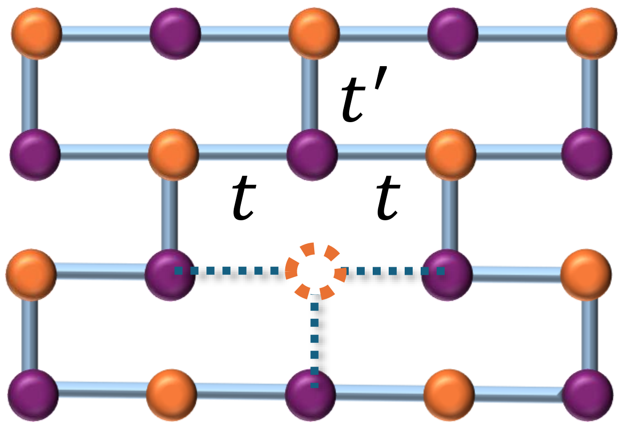


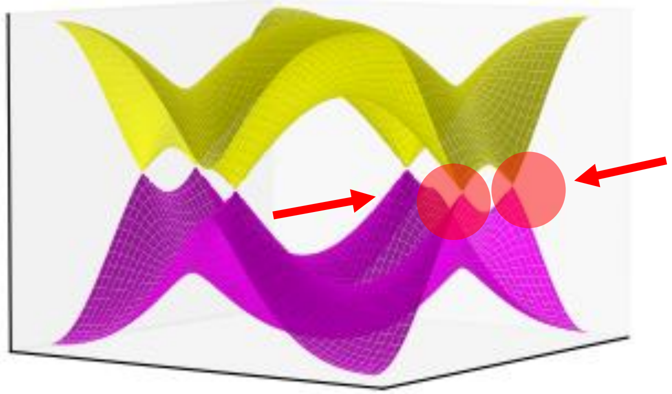


Brickwall + vacancy before merging

- Degrees of freedom
  - Sublattice
  - Inequivalent Dirac points

$m = 2$





- Dirac Hamiltonian:

$$\mathcal{H}_{<} = \sqrt{1-\left(\frac{t'}{2t}\right)^2}\, k_x \sigma_x \otimes \tau_z + \frac{t'}{2t} k_y \sigma_y \otimes \mathrm{I} + \text{defect terms}$$

Brickwall + vacancy before merging

- Degrees of freedom
  - Sublattice
  - Inequivalent Dirac points

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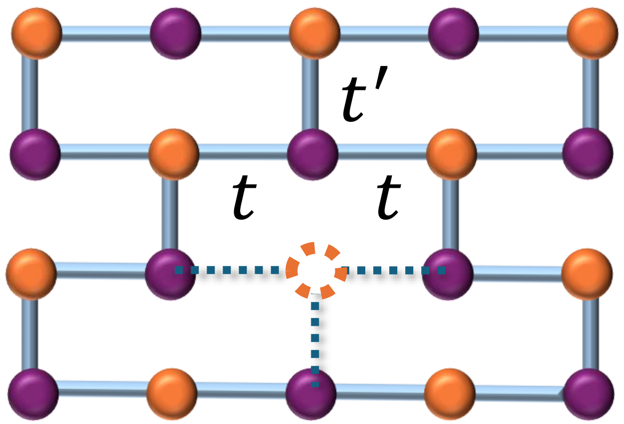

Before

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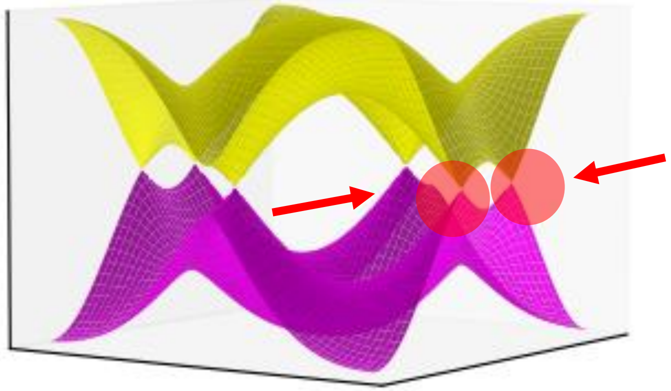

- Dirac Hamiltonian:

$\boldsymbol{\gamma}_{4\times4}$

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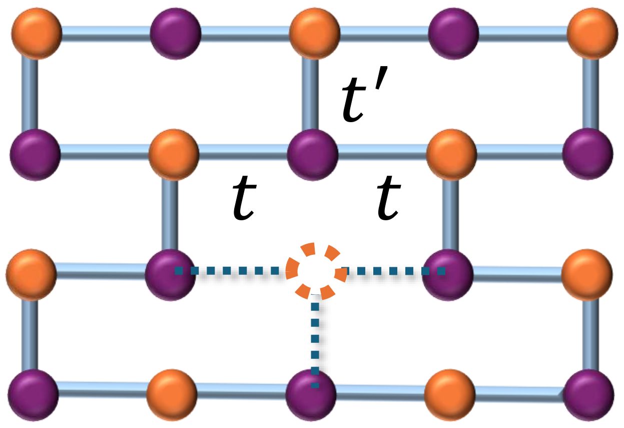

Before

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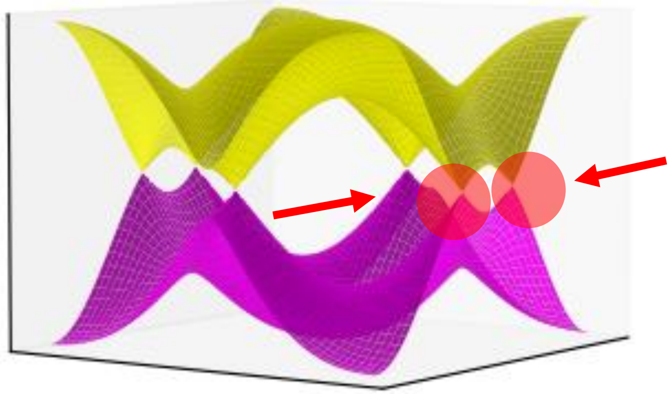

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w - Integer invariant

Spatial dimension

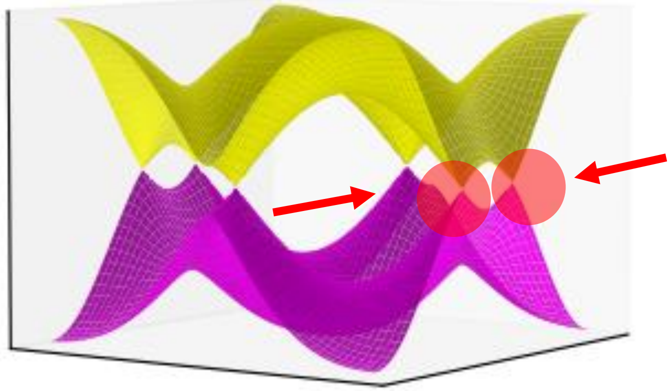
Defect dimension

$$2m = d + D + 1$$

degrees of freedom

Before

$t' < 2t$



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Spatial dimension

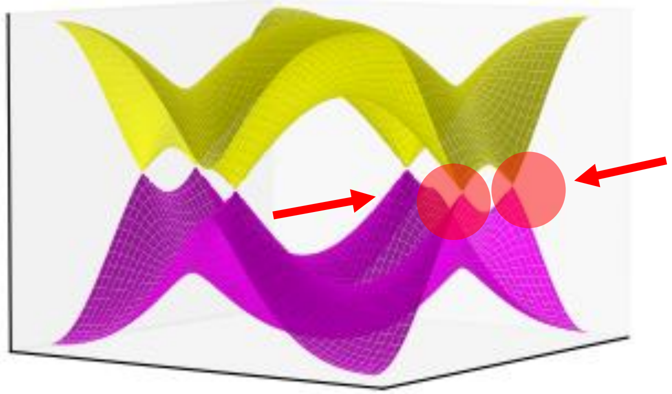
Defect dimension

$$2 \cdot 2 = 2 + 1 + 1$$

degrees of freedom

Before

$t' < 2t$



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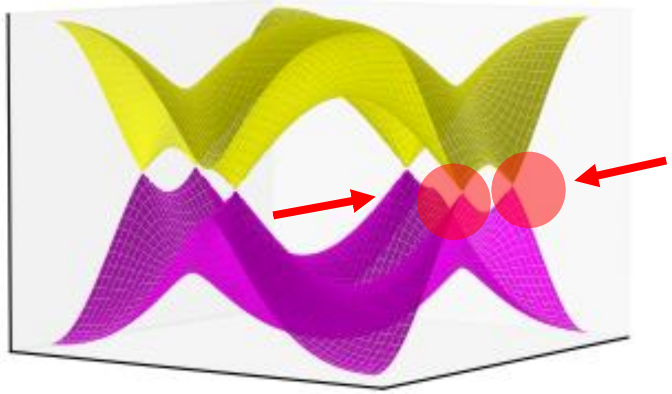
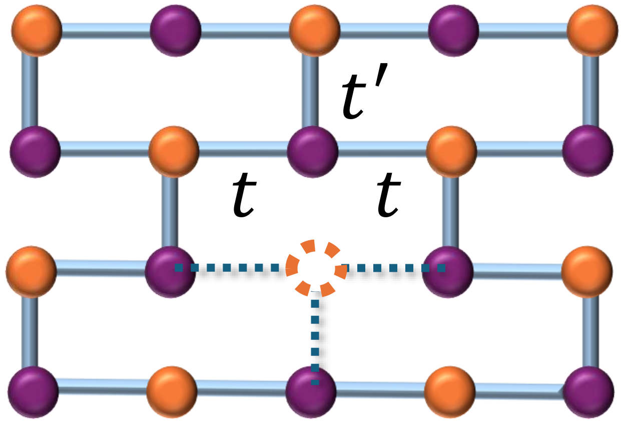


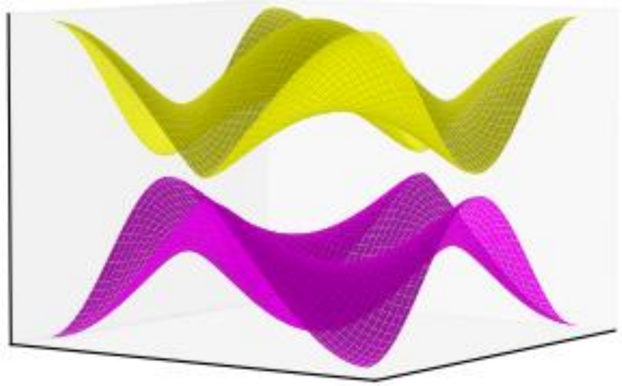
Brickwall + vacancy after merging

- Degrees of freedom
  - Sublattice
  - Inequivalent Dirac points



After

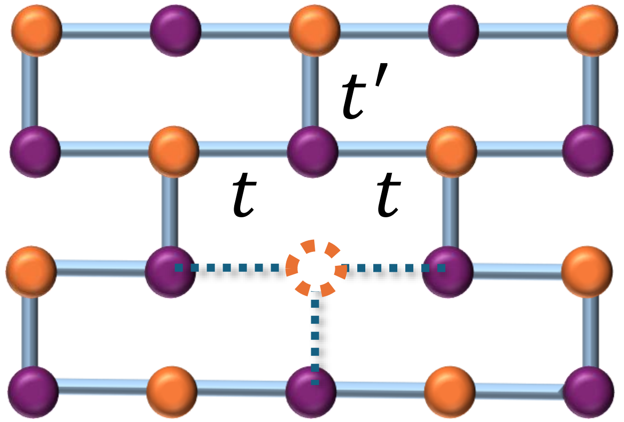
$t' > 2t$



Brickwall + vacancy after merging

- Degrees of freedom
  - Sublattice
  - ~~Inequivalent Dirac points~~

$m = 1$



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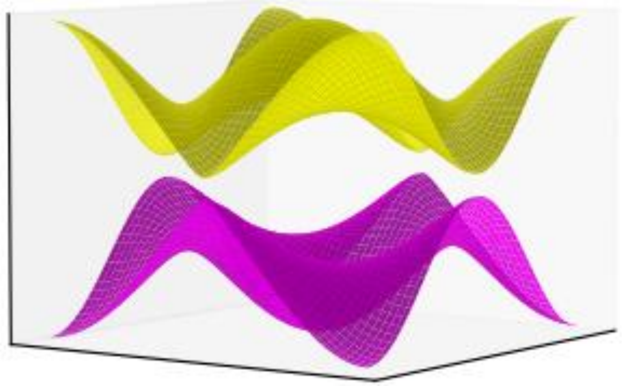

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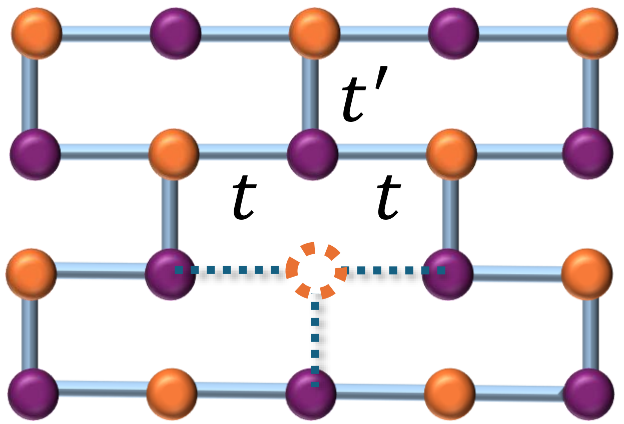
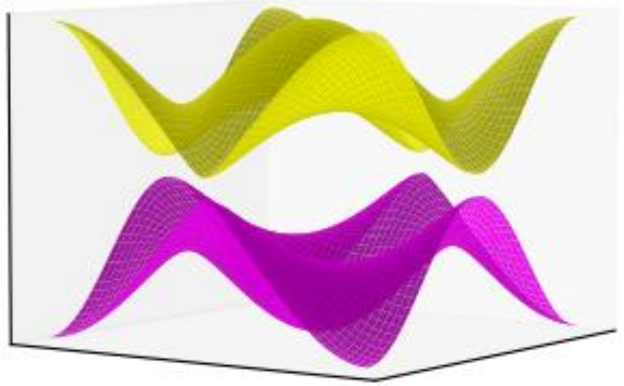


After
$t' > 2t$



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$$\mathcal{H}_{>} = \phi(\boldsymbol{r})\left[\left(1 - \frac{t'}{2t} + \frac{1}{2}k_x^2\right)\sigma_x + \frac{t'}{2t}k_y\sigma_y\right]$$

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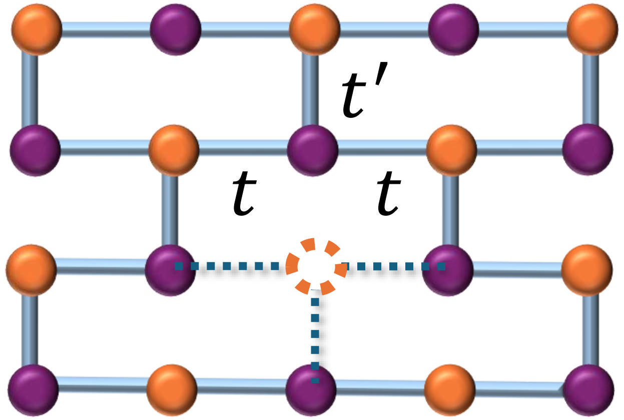

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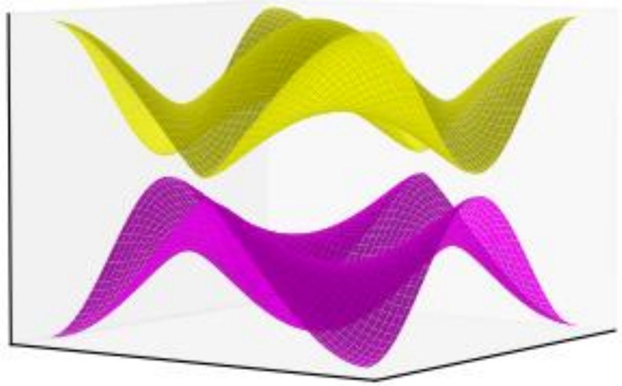
$t' > 2t$



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Spatial dimension

Defect dimension

$$2m = d + D + 1$$

degrees of freedom

After

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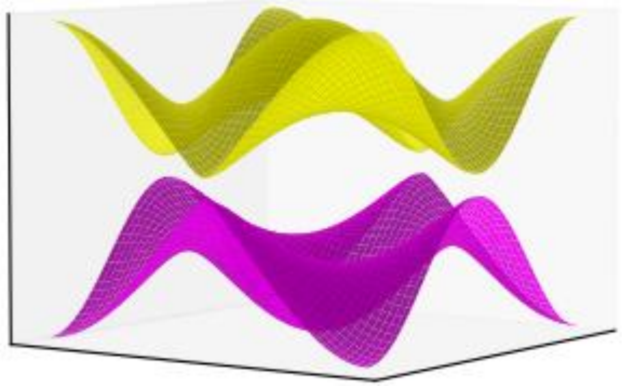

w - Integer invariant

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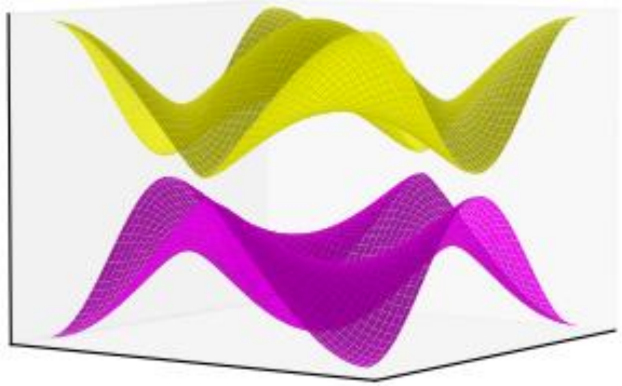
$$2 \cdot 1 \neq 2 + 1 + 1$$

degrees of freedom

After

$t' > 2t$



w - Integer invariant

Spatial dimension

Defect dimension

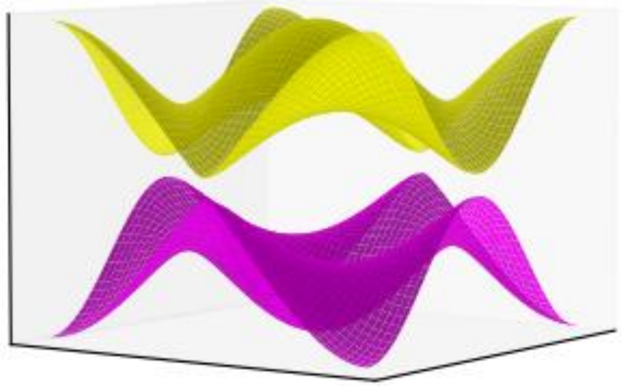
$$2 \cdot 1 \neq 2 + 1 + 1$$

degrees of freedom

⇨ **Not topological**

After

$t' > 2t$



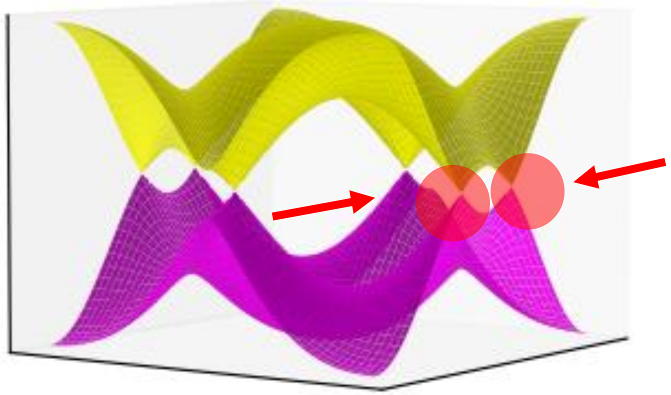
Topological phase transition

Topological

$$\boxed{w = \pm 1}$$

Before

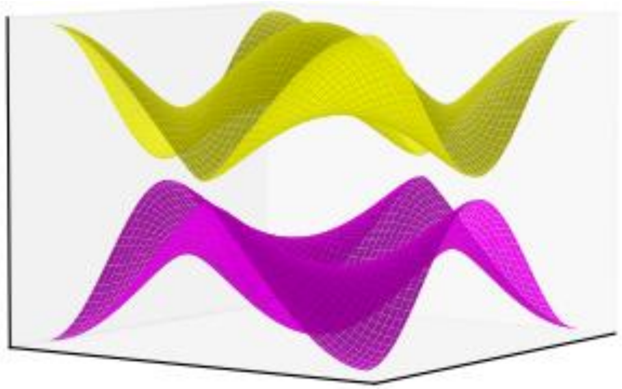
$t' < 2t$



Not topological

After

$t' > 2t$



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Before

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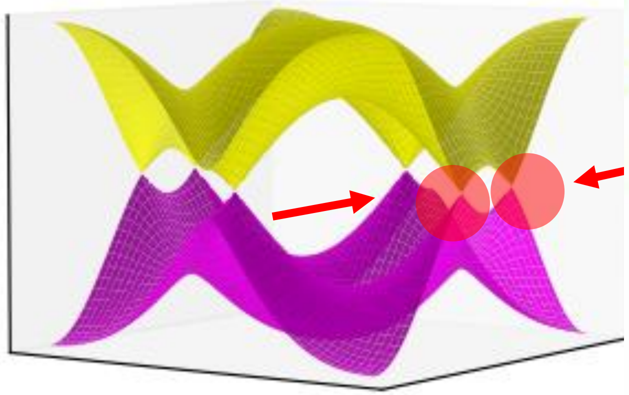
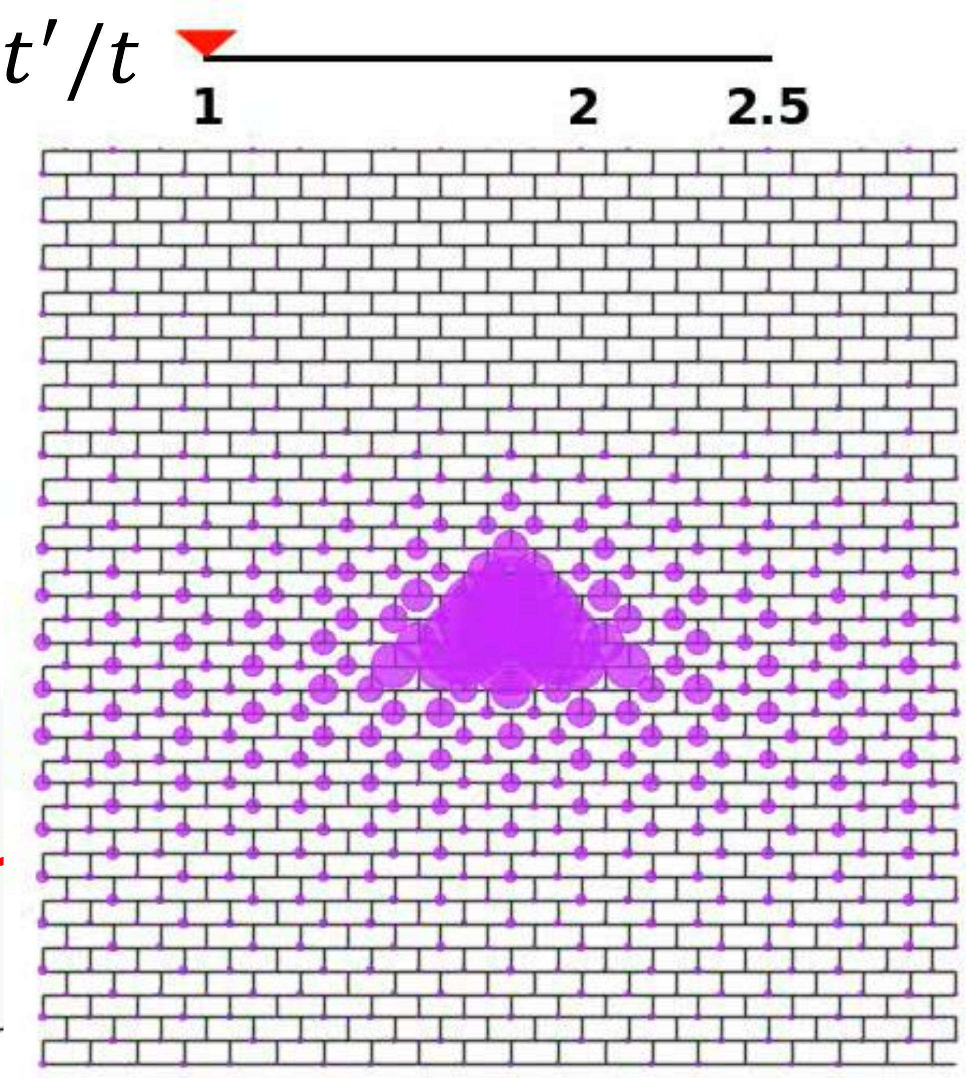


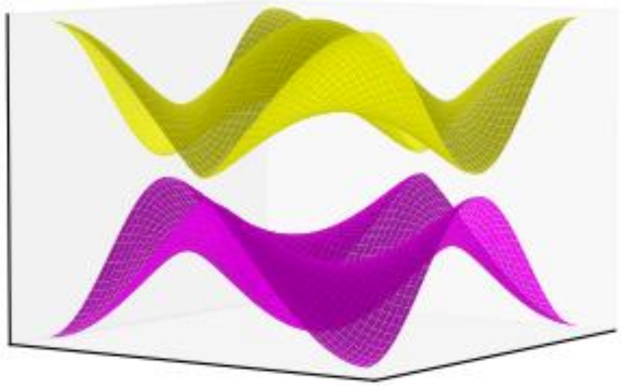


$|\psi\,(i,j)|^2$

Not topological

After

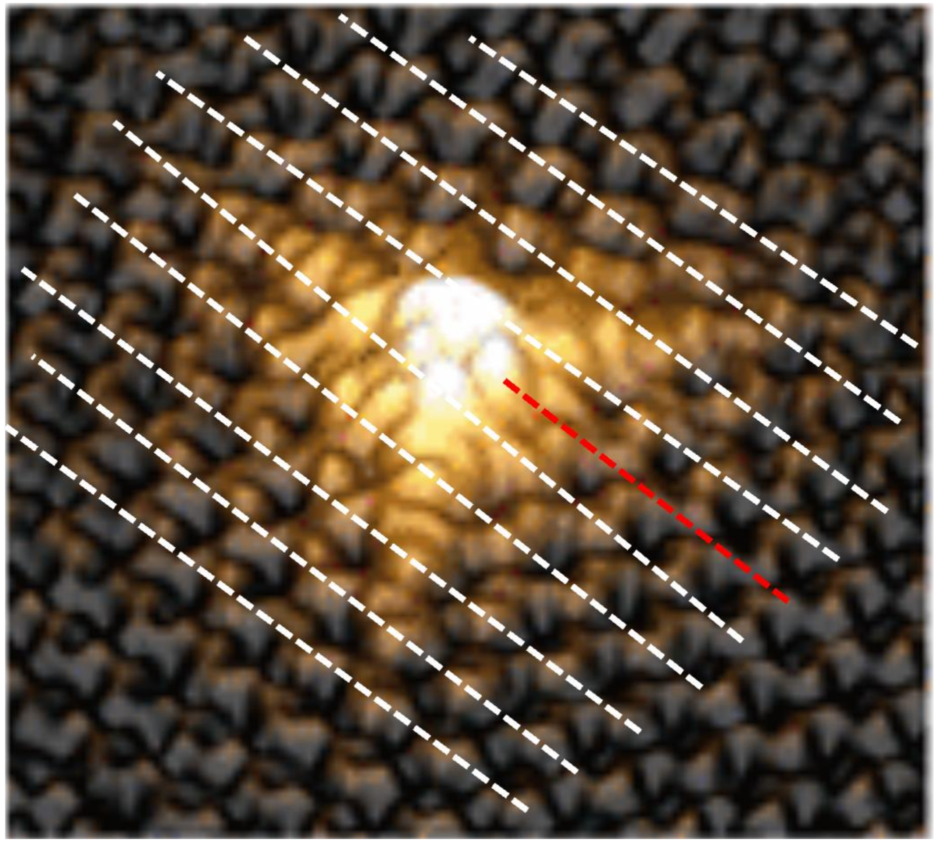
$t' > 2t$



Can we observe the transition and measure w ?

Measuring topology

Vacancy in graphene

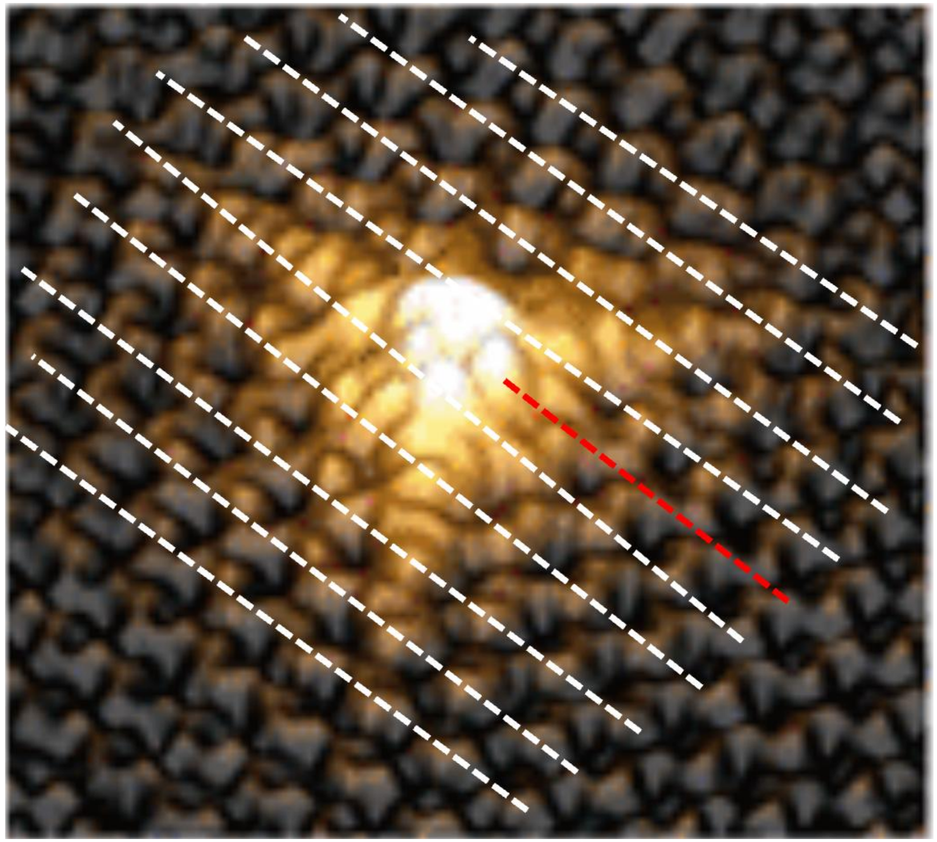


- STM measurement of charge density

Abulafia et al (2023) **Ugeda** et al (2010)

Measuring topology

Vacancy in graphene

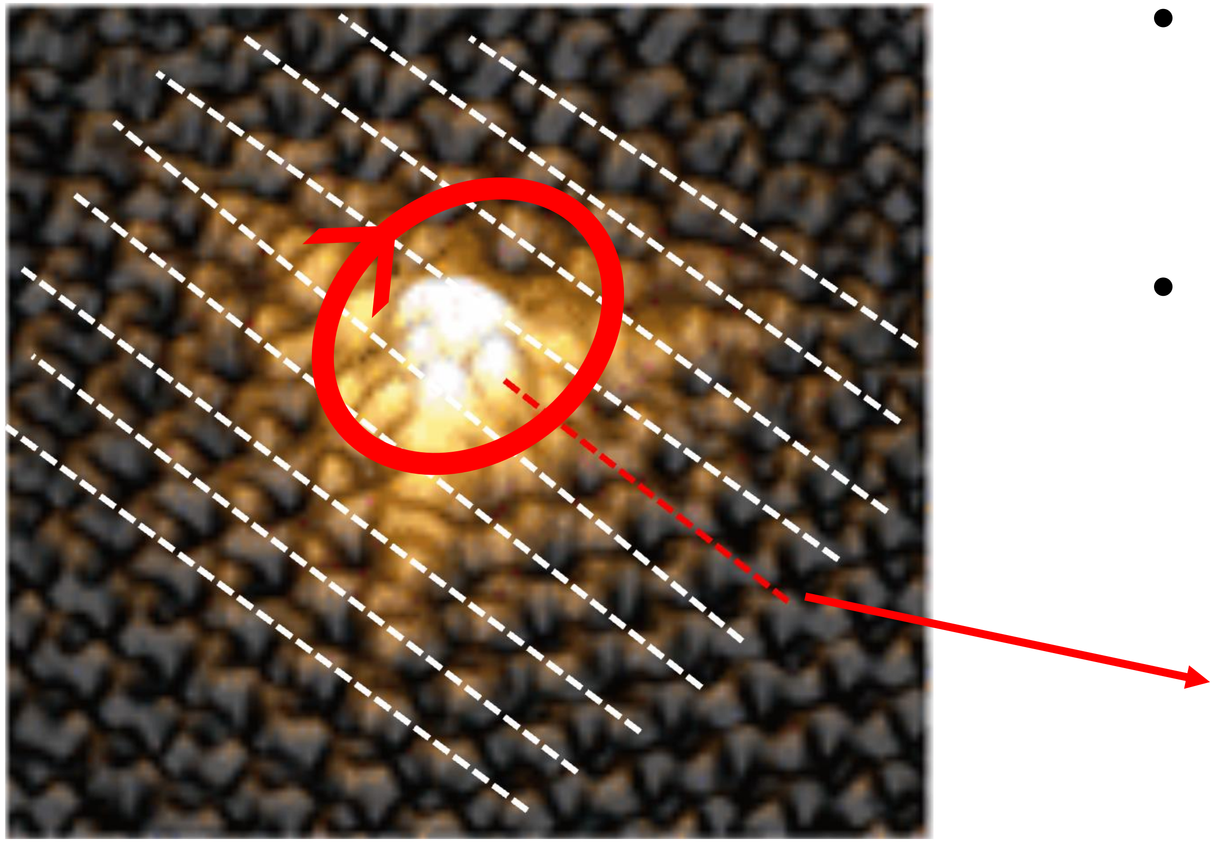


- STM measurement of charge density
- Lines of maximum amplitude

Abulafia et al (2023) **Ugeda** et al (2010)

Measuring topology

Vacancy in graphene



- STM measurement of charge density
- Lines of maximum amplitude

1 dislocation

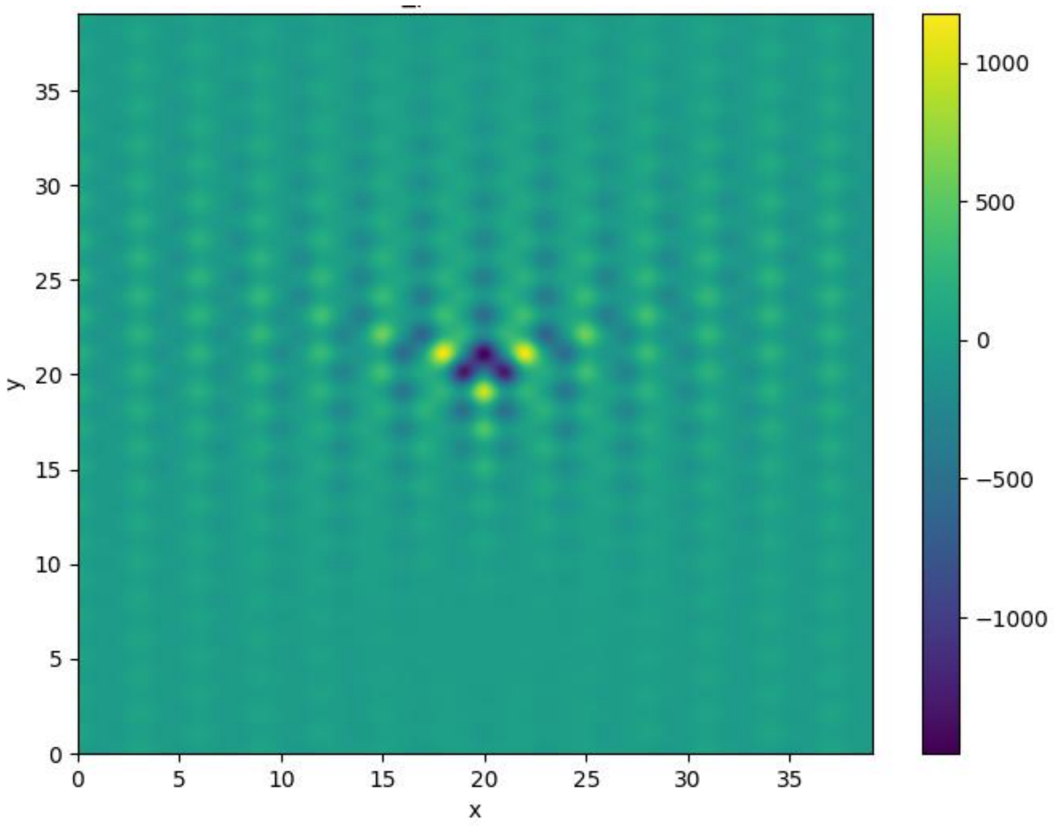
$w = 1$

Abulafia et al (2023) Ugeda et al (2010)

Dislocations in brickwall lattice – numerical

Before
$t' < 2t$

$\psi\ (x, y)$



Dislocations in brickwall lattice – numerical

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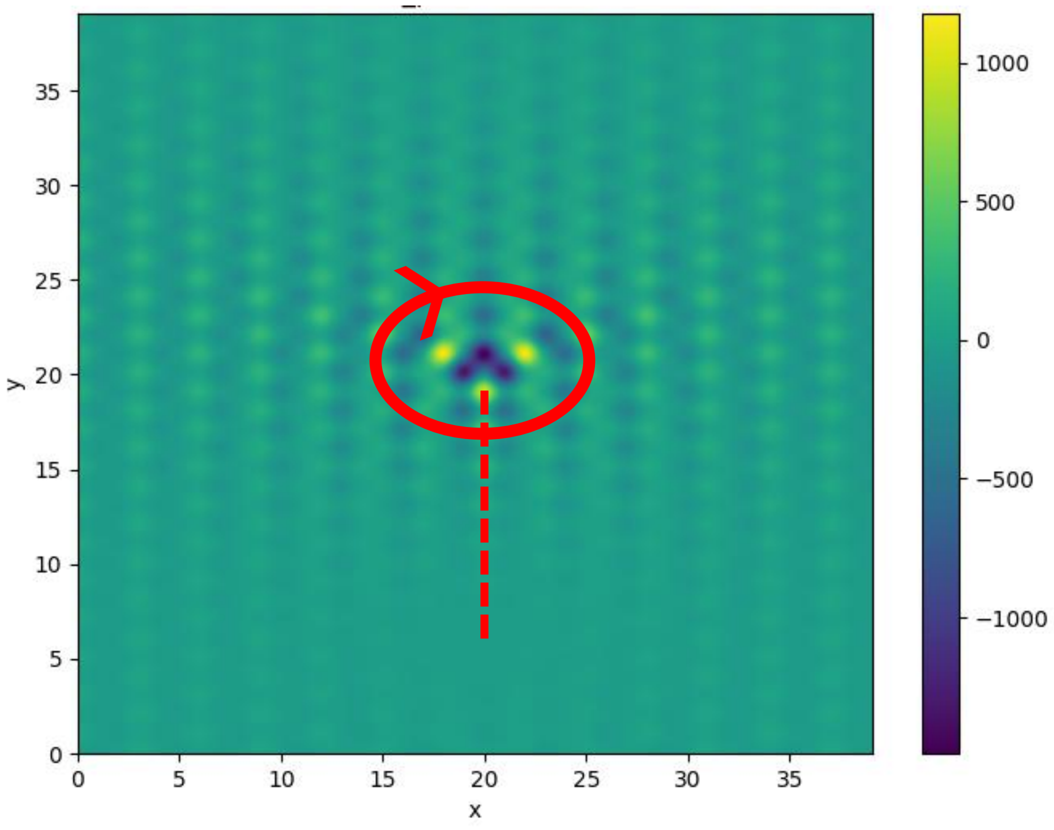


Dislocations in brickwall lattice – numerical

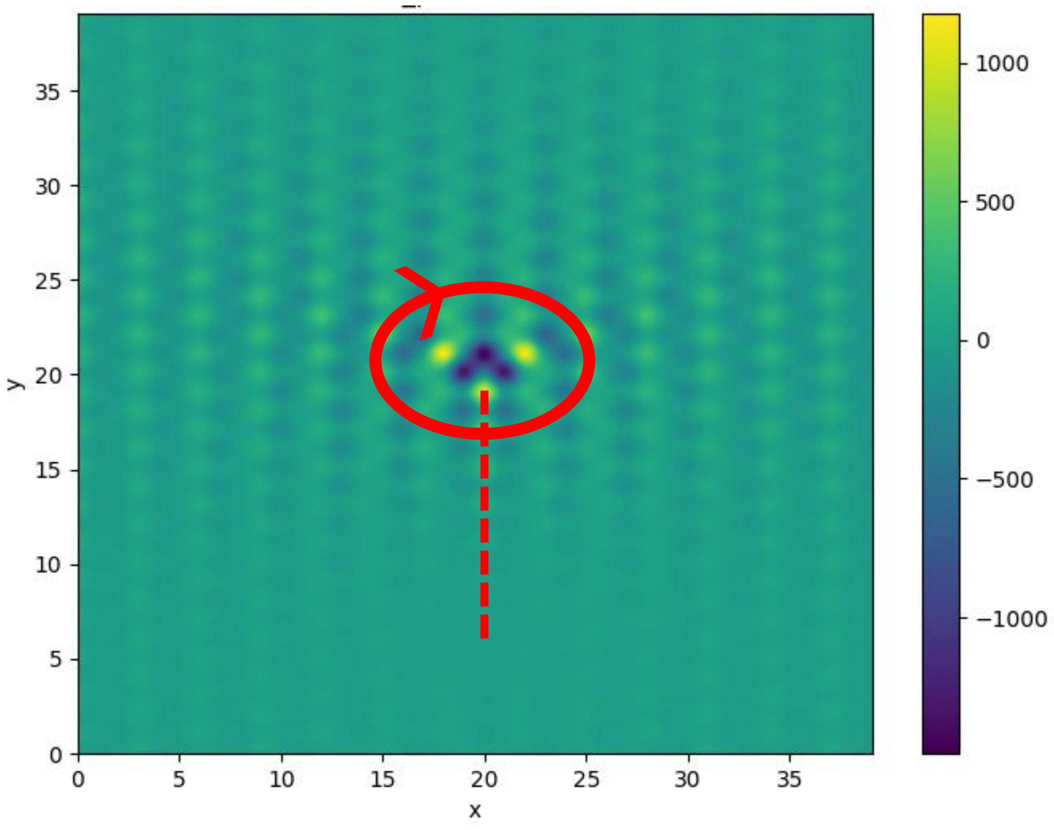
Before

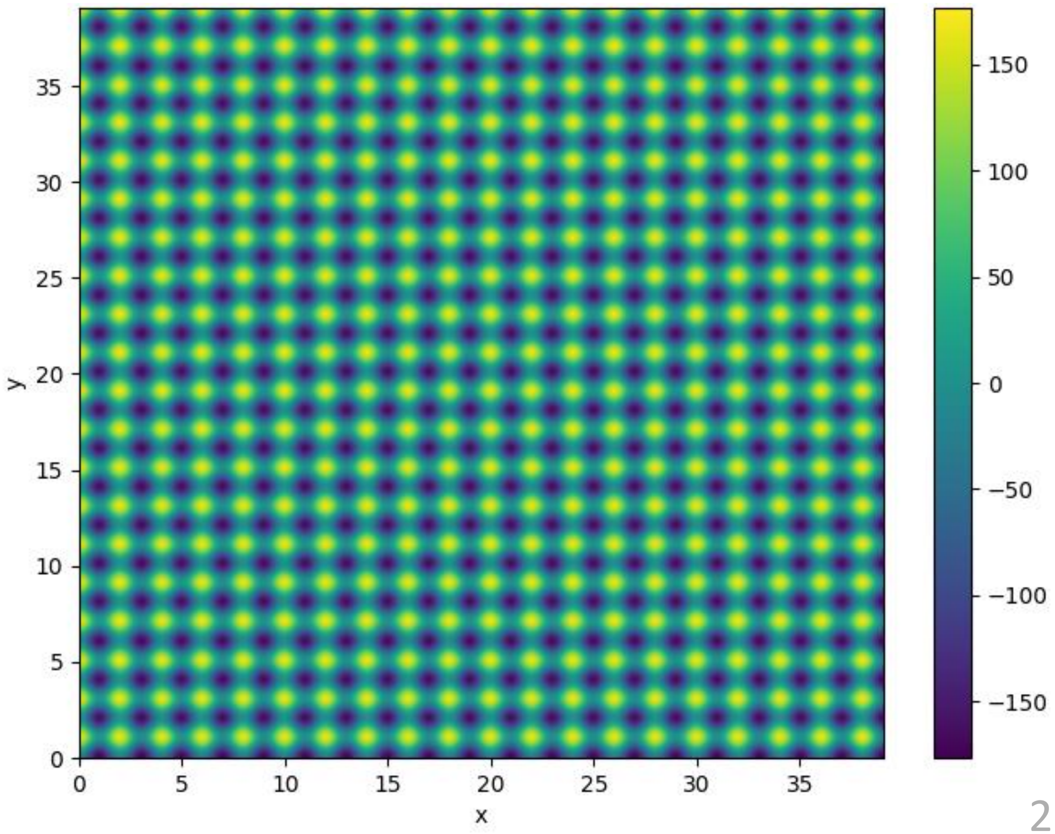
$t' < 2t$

$\psi\,(x, y)$

Merging

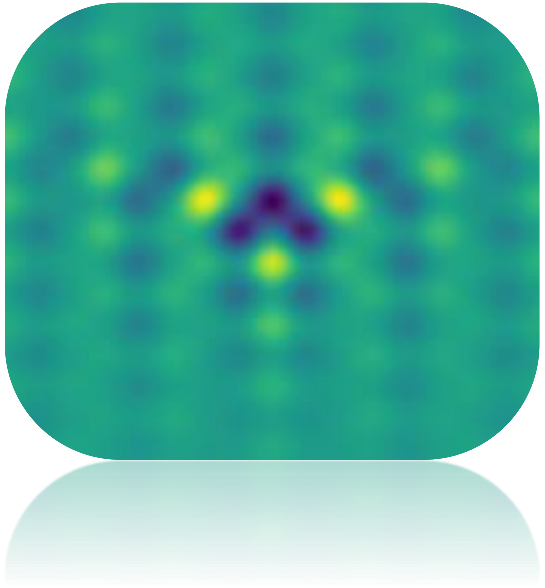
$t' = 2t$



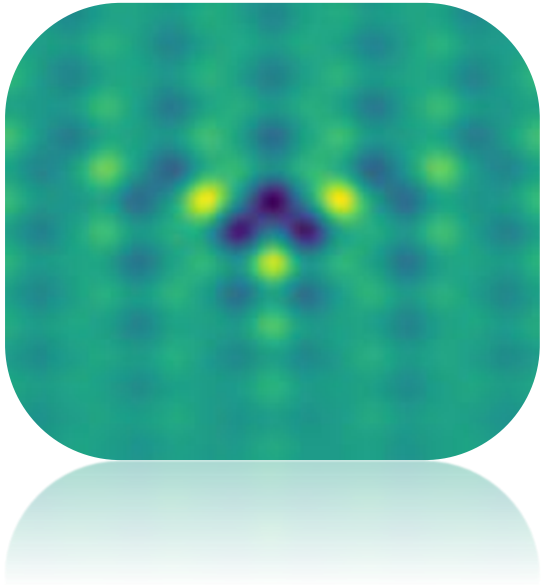


Summary

- Topological transition by merging Dirac points
- Simulation results supporting it



Summary



- Topological transition by merging Dirac points
- Simulation results supporting it

Future work

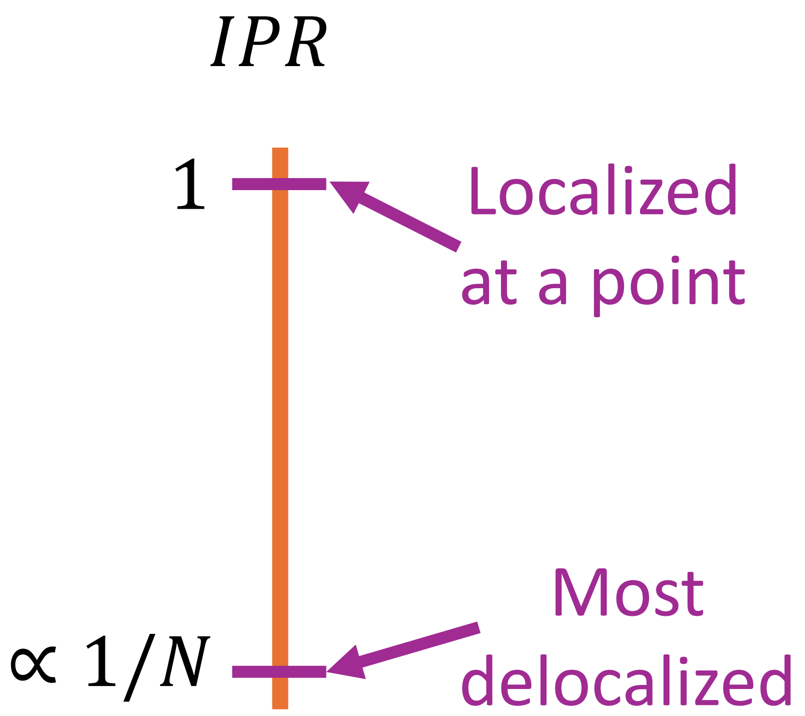
- Inverse participation ratio – spatial localization
- Effects on transport along t' direction

Thank you ☺

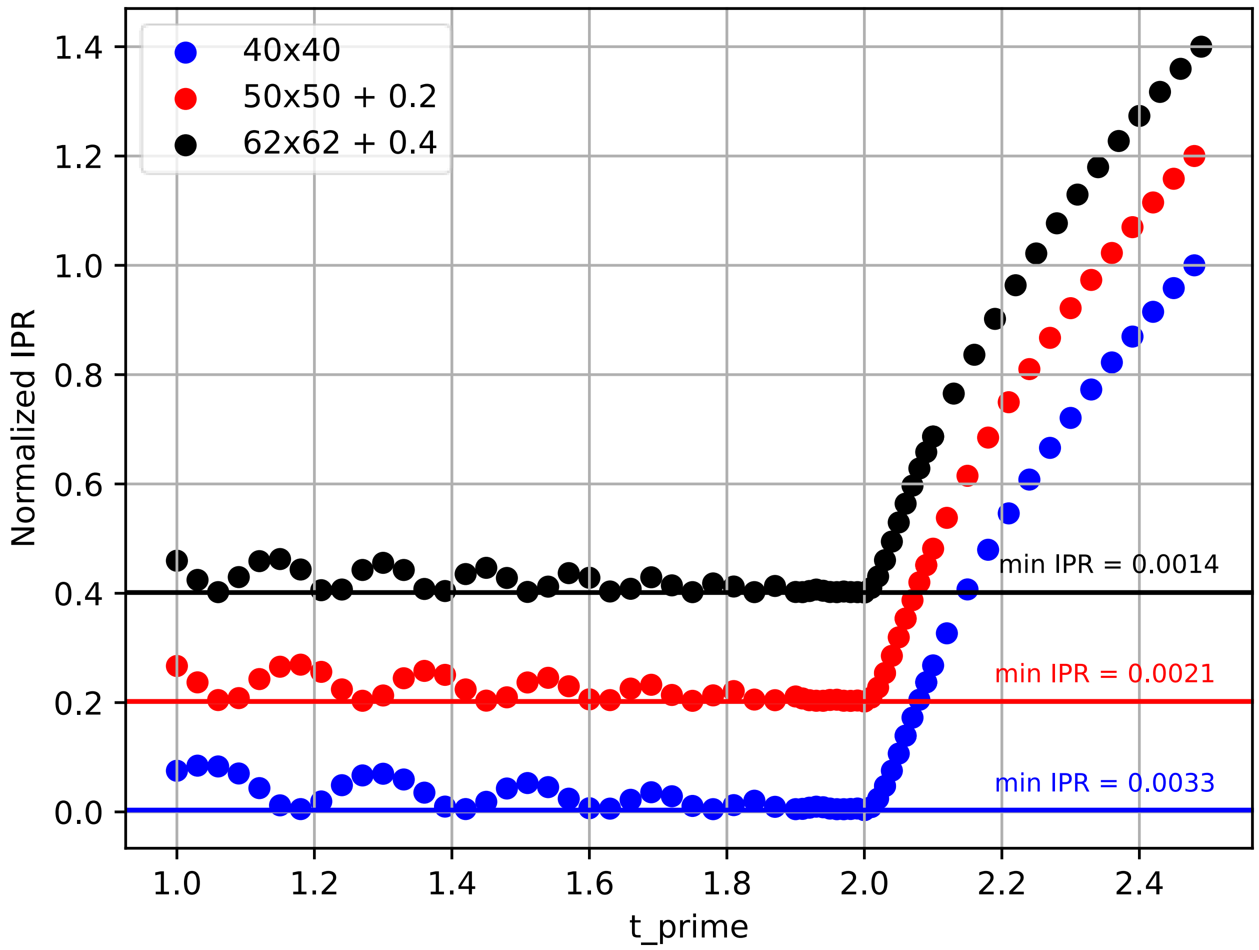
Inverse participation ratio (IPR)

Measure of localization:

$$IPR \propto \int |\psi(\boldsymbol{r})|^4 d\boldsymbol{r}$$



Merging
$t' = 2t$



Dislocations in brickwall lattice – numerical

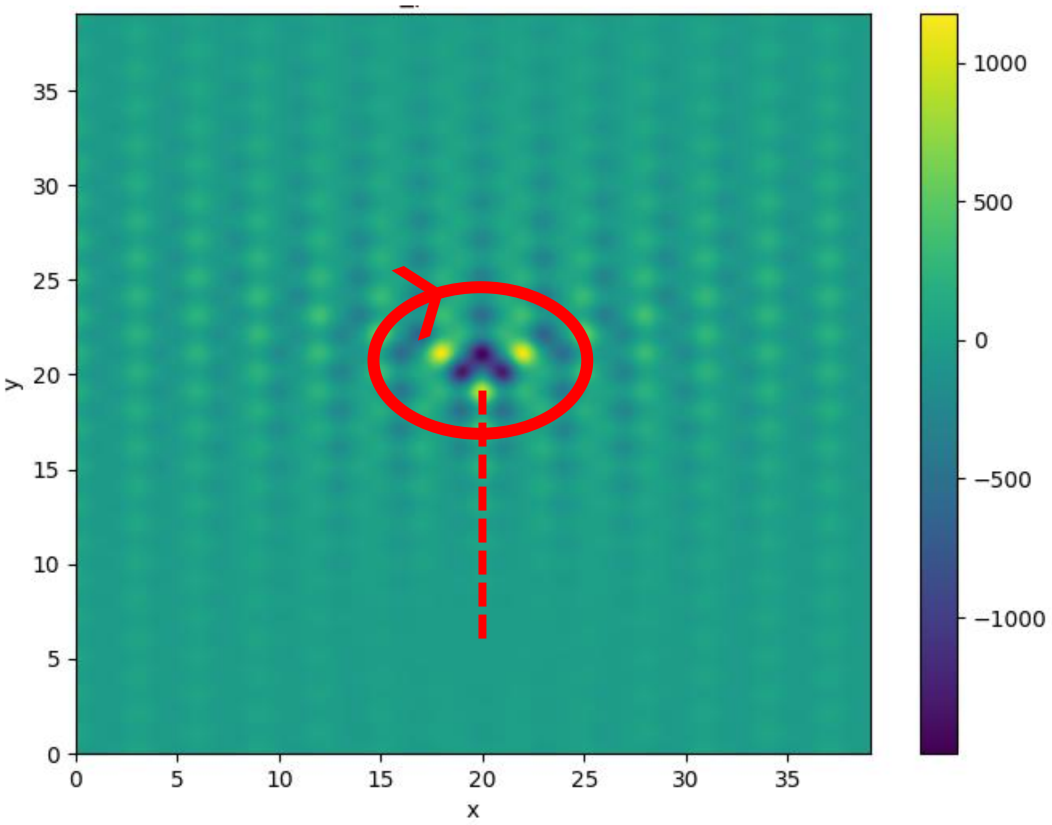
Before

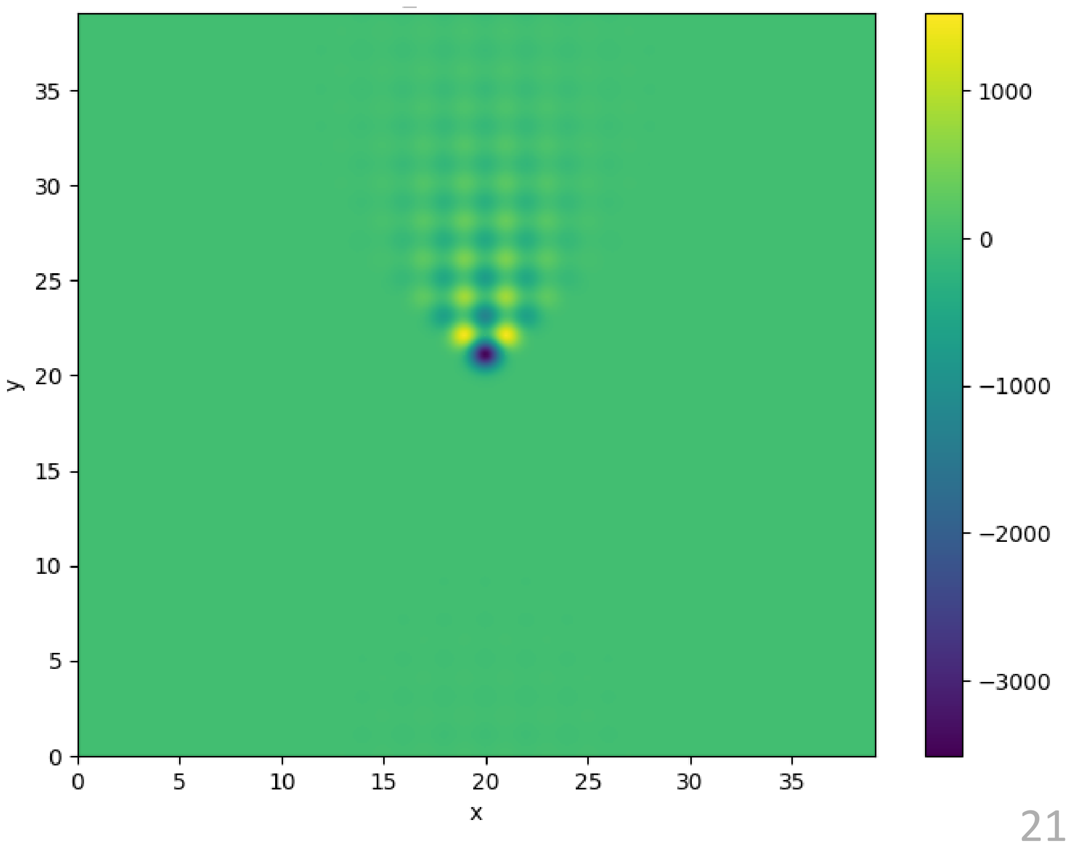
$t' < 2t$

$\psi\,(x, y)$

After

$t' > 2t$

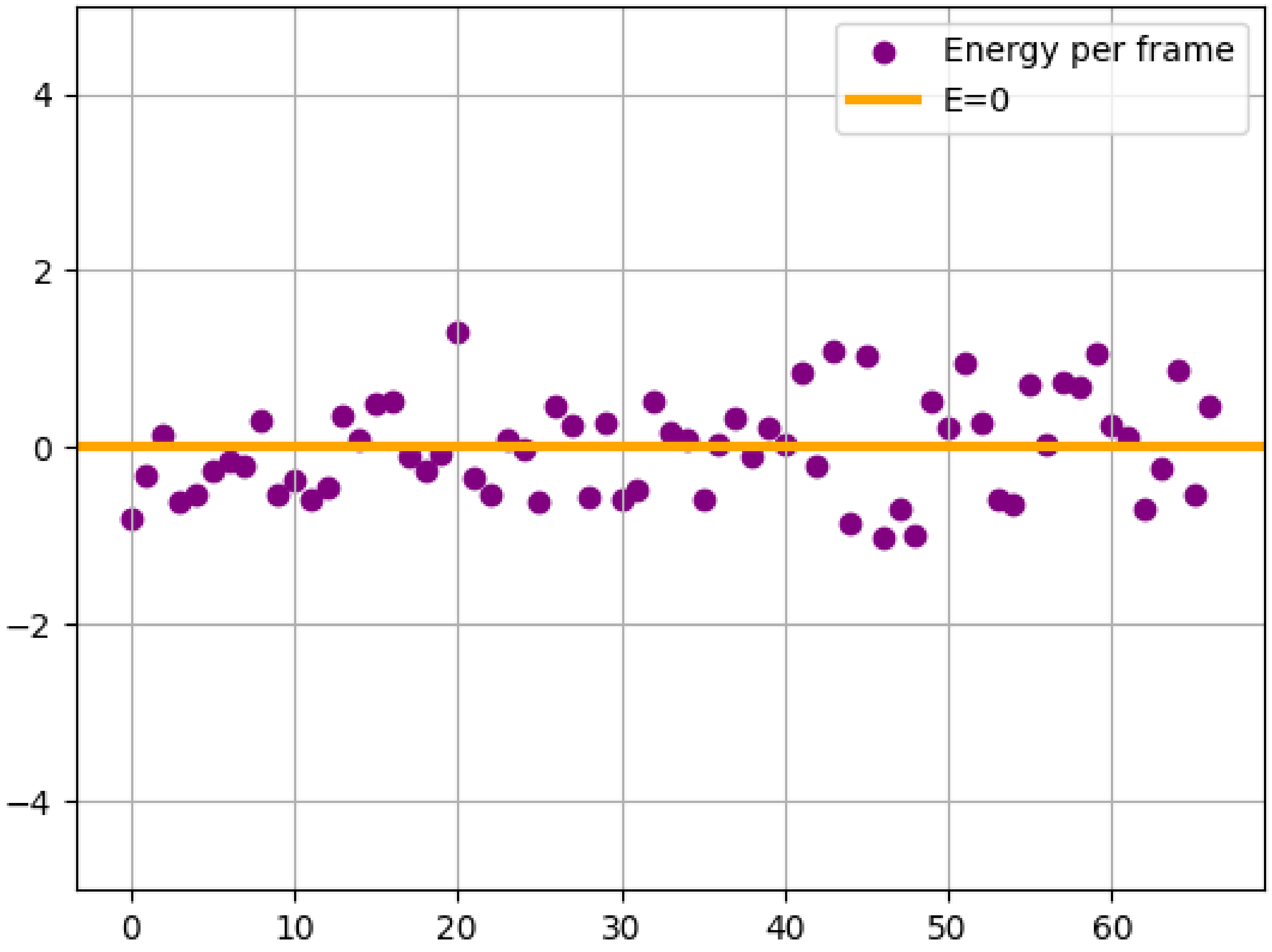




Energy of $|\psi(i,j)|^2$

adjacent energies $\propto \pm 10^{-2} t$

$\times 10^{-15} t$



Frame number