Topological phases and phase transitions in two-dimensional fermionic lattices

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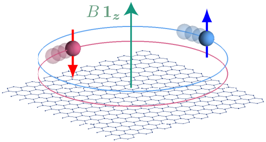
August 21, 2012

Topological states of matter

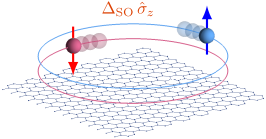
Insulating bulk and conducting edges

- Quantum Hall effect
  Magnetic field ➡ Chiral edge currents
  ➡ Quantised Hall conductivity



➤ [Von Klitzing (1980)]

- Quantum spin Hall effect
  Spin-orbit coupling ➡ Helical edge currents
  ➡ Quantised spin Hall conductivity



➤ [Theory: C. L. Kane and E. J. Mele (2005)]

➤ [Experiment: Molenkamp group, Hasan group]

Main Question

What happens if we have
a magnetic field and spin-orbit coupling?

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What happens if we have
a magnetic field and spin-orbit coupling?

Naive answer (from QSH perspective):
Breaking TR symmetry destroys QSH state

Actual answer (from QH perspective):
Study effect of SO coupling on QH states

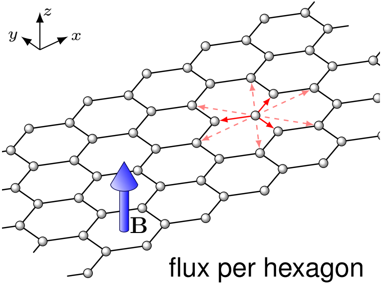
Outline

- Model – Honeycomb lattice
- Topological phases
  - Edge-state analysis
  - Intrinsic SO coupling and Zeeman effect
  - Rashba SO coupling
- Topological phase transitions
  - Honeycomb lattice, driven by intrinsic SO
  - Driven by real NNN hopping
  - In the Lieb and kagome lattices
- Experimental realisations
  - Graphene and 2D topological insulators
  - Artificial honeycomb lattices on a substrate
  - Ultracold atoms in an optical lattice
- Conclusions

Honeycomb lattice – Model

Tight-binding model on a honeycomb lattice:

$$H = H_{\mathrm{nn}}$$



$$H_{\mathrm{nn}} = -t \sum_{\langle i,j \rangle} \left(e^{i\theta_{ij}} c_i^\dagger c_j \right)$$

$$\theta_{ij} = 2\pi \frac{e}{h} \int_{\mathbf{r}_j}^{\mathbf{r}_i} \mathbf{A} \cdot \mathrm{d}\mathbf{l} \propto \phi$$

gauge potential

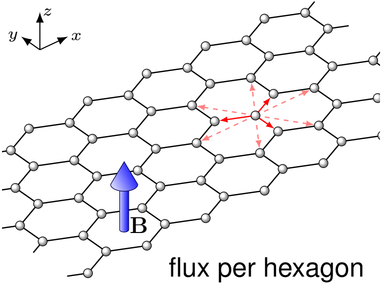
flux per hexagon

$$B \times \mathrm{area} = \Phi \equiv \phi h/e$$

Honeycomb lattice – Model

Tight-binding model on a honeycomb lattice:

$$H = H_{\rm nn} + H_{\rm Z} + H_{\rm I} + H_{\rm R}$$



flux per hexagon

$$B \times \text{area} = \Phi \equiv \phi h/e$$

$$H_{\rm nn} = -t \sum_{\langle i,j \rangle} \left(e^{i\theta_{ij}} c_i^\dagger c_j \right)$$

$$H_{\rm Z} = -2\pi\phi\lambda_{\rm Z} \sum_i c_i^\dagger \sigma_z c_i$$

Zeeman effect

$$H_{\rm I} = -it_{\rm I} \sum_{\langle\langle i,j \rangle\rangle} e^{i\theta_{ij}} \nu_{ij} c_i^\dagger \sigma_z c_j$$

intrinsic SO coupling

$$H_{\rm R} = -it_{\rm R} \sum_{\langle i,j \rangle} e^{i\theta_{ij}} c_i^\dagger (\sigma_x \mathbf{d}_{ij}^y - \sigma_y \mathbf{d}_{ij}^x) c_j$$

Rashba SO coupling

Bulk spectrum

- Let $\phi = p/q \in \mathbb{Q}$
- Harper's equation ➡ eigenvalues of $4q \times 4q$ matrix

$$E \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \vdots \\ \Psi_{q-1} \\ \Psi_q \end{pmatrix} = \begin{pmatrix} \mathcal{D}_1 & \mathcal{R}_1 & 0 & \cdots & 0 & \mathcal{R}_q^\dagger \\ \mathcal{R}_1^\dagger & \mathcal{D}_2 & \mathcal{R}_2 & \cdots & 0 & 0 \\ 0 & \mathcal{R}_2^\dagger & \mathcal{D}_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \mathcal{D}_{q-1} & \mathcal{R}_{q-1} \\ \mathcal{R}_q & 0 & 0 & \dots & \mathcal{R}_{q-1}^\dagger & \mathcal{D}_q \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \vdots \\ \Psi_{q-1} \\ \Psi_q \end{pmatrix},$$

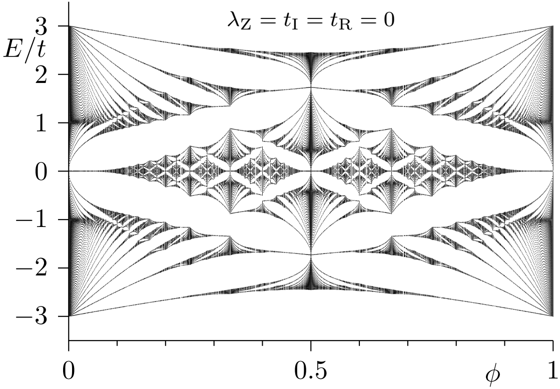
$$\mathcal{D}_n = \begin{pmatrix} 2t_\mathrm{I}\hat{\sigma}_z \sin\big(2\pi\Phi(n+\frac{1}{6})+k\big) + 2\pi\Phi\lambda_\mathrm{Z}\hat{\sigma}_z & t\hat{1} - it_\mathrm{R}\hat{\sigma}_y \\ t\hat{1} + it_\mathrm{R}\hat{\sigma}_y & -2t_\mathrm{I}\hat{\sigma}_z \sin\big(2\pi\Phi(n+\frac{1}{6})+k\big) + 2\pi\Phi\lambda_\mathrm{Z}\hat{\sigma}_z \end{pmatrix},$$

$$\mathcal{R}_n = \begin{pmatrix} it_\mathrm{I}\hat{\sigma}_z\big(e^{i\pi\Phi(n+\frac{2}{3})} - e^{-i\pi\Phi(n+\frac{2}{3})-ik}\big) & 0 \\ e^{i\pi\Phi(n+1)}\big(t\hat{1} - it_\mathrm{R}\hat{\gamma}_-\big) + e^{-i\pi\Phi(n+1)-ik}\big(t\hat{1} - it_\mathrm{R}\hat{\gamma}_+\big) & -it_\mathrm{I}\hat{\sigma}_z\big(e^{i2\pi\Phi(n+\frac{7}{6})} - e^{-i2\pi\Phi(n+\frac{7}{6})-ik}\big) \end{pmatrix},$$

$$\hat{\gamma}_\pm = \pm\frac{\sqrt{3}}{2}\hat{\sigma}_x + \frac{1}{2}\hat{\sigma}_y.$$

Bulk spectrum

- Let $\phi = p/q \in \mathbb{Q}$
- Harper's equation ➡ eigenvalues of $4q \times 4q$ matrix
- $4q$ energy bands (dispersions)



Hofstadter butterfly

➤ [D. R. Hofstadter, Phys. Rev. B **14**, 2239 (1976)]

➤ [R. Rammal, J. Phys. (Paris) **46**, 1345 (1985)]

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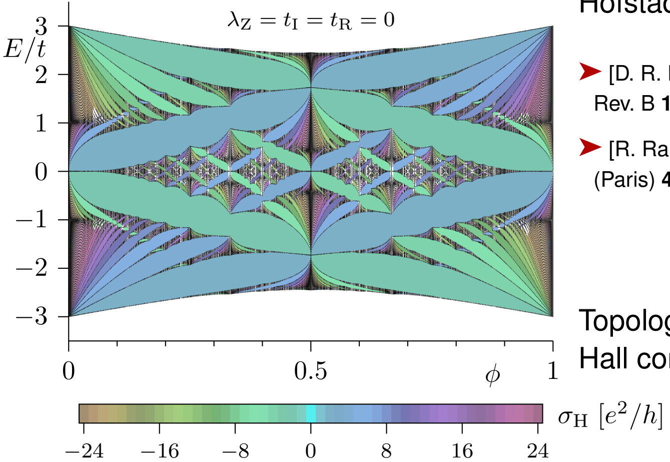

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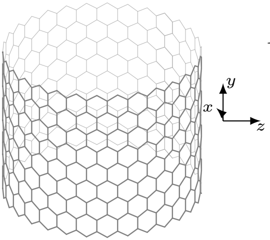
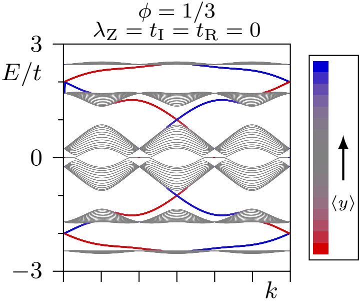
Topological invariant: Hall conductivity σ_H

Edge-state analysis

Compute dispersion in cylindrical geometry





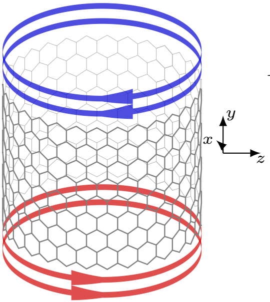
Location $\langle y \rangle$

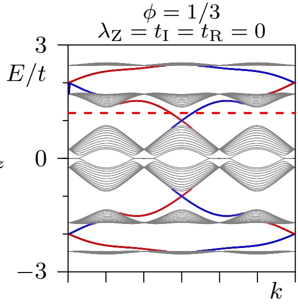
Direction $\frac{\partial E}{\partial k}$

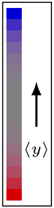
Spin $\langle \sigma_{x,y,z} \rangle$

Edge-state analysis

Compute dispersion in cylindrical geometry







Location $\langle y \rangle$

Direction $\frac{\partial E}{\partial k}$

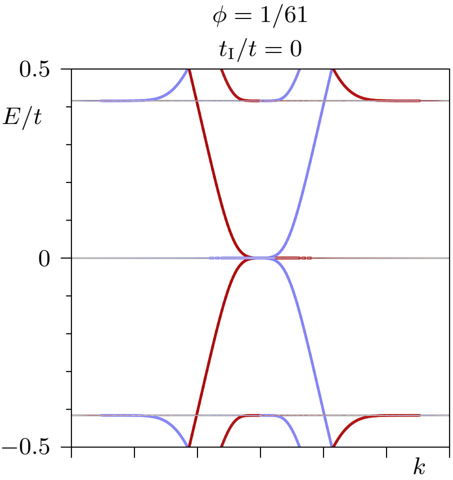
Spin $\langle \sigma_{x,y,z} \rangle$

Hall conductivities

charge $[e^2/h]$:
$\sigma_H = N_\uparrow + N_\downarrow = 2$

spin $[e/4\pi]$:
$\sigma_H^{sp} = N_\uparrow - N_\downarrow = 0$

Topological phases – B + Intrinsic SO coupling



➤ [W. Beugeling, N. Goldman, and C. Morais Smith, Phys. Rev. B **86**, 075118 (2012)]

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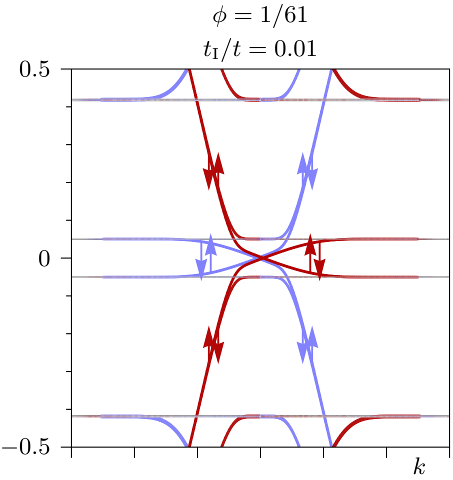
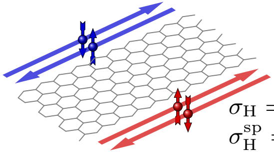


→ Weak QSH phase

$N_{\uparrow} = 1, N_{\downarrow} = -1$

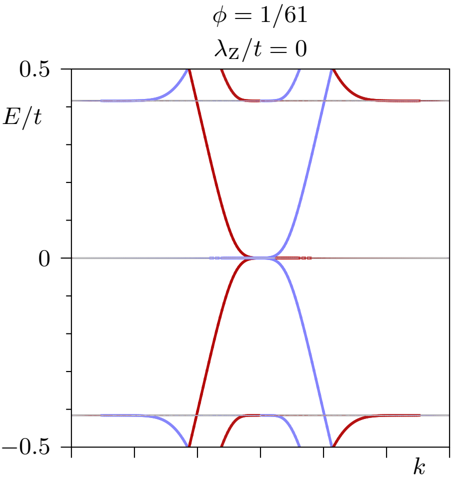


$\sigma_{\mathrm{H}} = 0$
$\sigma_{\mathrm{H}}^{\mathrm{sp}} = 2$

Persists under TRS breaking!

➤ [W. Beugeling, N. Goldman, and C. Morais Smith, Phys. Rev. B **86**, 075118 (2012)]

Topological phases – B + Zeeman



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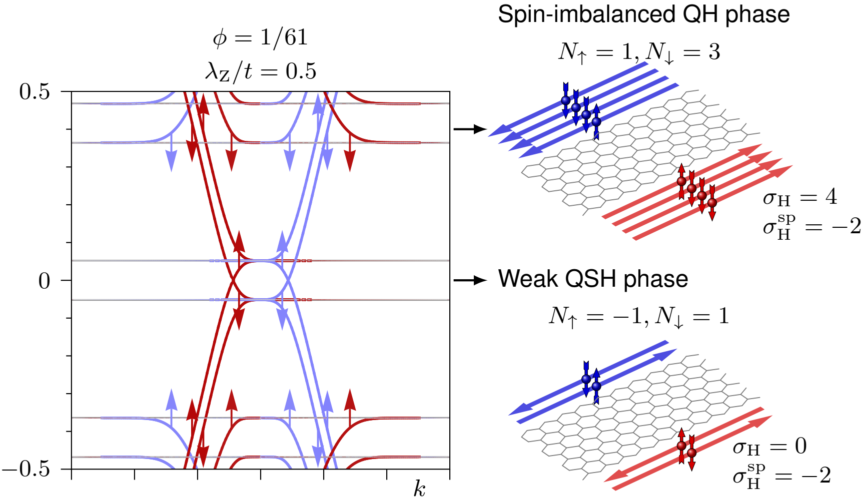
Topological phases – B + Zeeman



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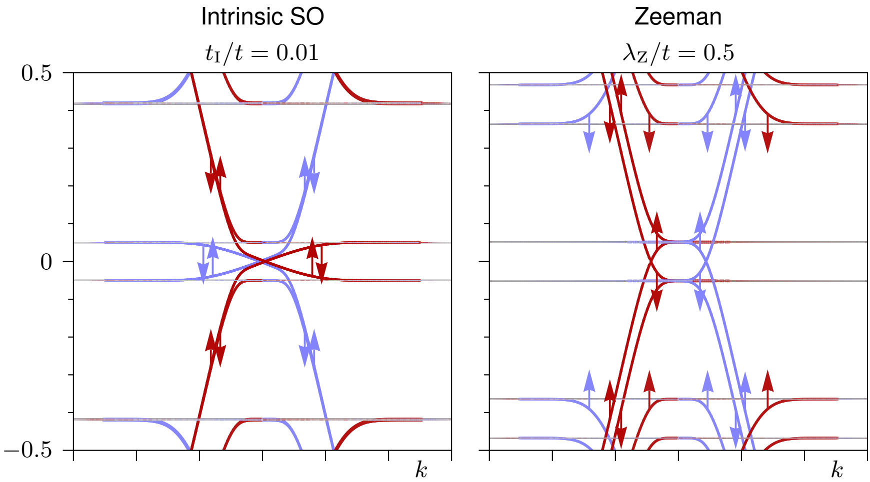
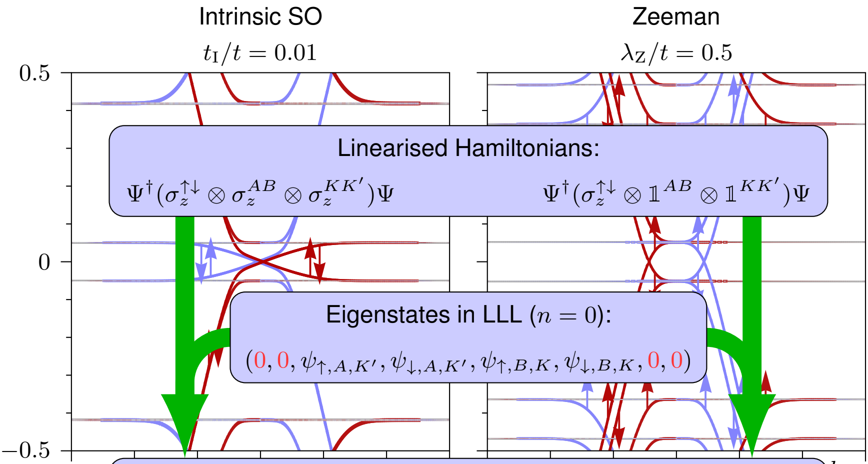
Equivalence of intrinsic SO and Zeeman at LLL



Equivalence of intrinsic SO and Zeeman at LLL



Linearised Hamiltonians:

$\Psi^\dagger(\sigma_z^{\uparrow\downarrow} \otimes \sigma_z^{AB} \otimes \sigma_z^{KK'})\Psi$ $\quad\quad$ $\Psi^\dagger(\sigma_z^{\uparrow\downarrow} \otimes \mathbb{1}^{AB} \otimes \mathbb{1}^{KK'})\Psi$

Eigenstates in LLL ($n = 0$):

$(0, 0, \psi_{\uparrow,A,K'}, \psi_{\downarrow,A,K'}, \psi_{\uparrow,B,K}, \psi_{\downarrow,B,K}, 0, 0)$

In both cases:

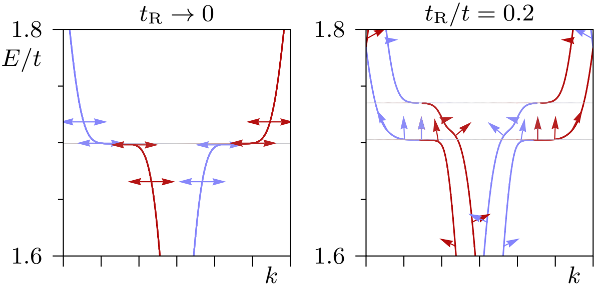
$\psi^\dagger_{\uparrow,A,K'}\psi_{\uparrow,A,K'} - \psi^\dagger_{\downarrow,A,K'}\psi_{\downarrow,A,K'} + \psi^\dagger_{\uparrow,B,K}\psi_{\uparrow,B,K} - \psi^\dagger_{\downarrow,B,K}\psi_{\downarrow,B,K}$

Topological phases – B + Rashba SO coupling

$$H_\mathrm{R} = -it_\mathrm{R} \sum_{\langle i,j\rangle} e^{i\theta_{ij}} c_i^\dagger (\sigma_x \mathbf{d}_{ij}^y - \sigma_y \mathbf{d}_{ij}^x) c_j$$

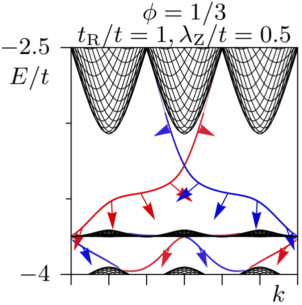
σ_x, σ_y ➡ spin-z not conserved

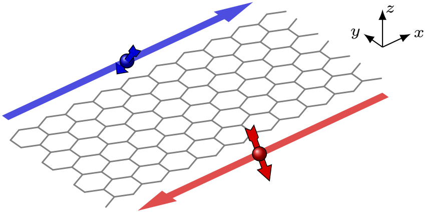
- Low energy, low flux: No gap at zero energy
  Spin degeneracy lifted ➡ Splitting of LL
- High energy, high flux (e.g., $\phi = 7/15 \approx 1/2$, $E/t \approx \sqrt{3}$)



Spin manipulation with Rashba SO coupling

$$H_{\mathrm{R}} = -it_{\mathrm{R}} \sum_{\langle i,j \rangle} e^{i\theta_{ij}} c_i^\dagger (\sigma_x \mathbf{d}_{ij}^y - \sigma_y \mathbf{d}_{ij}^x) c_j$$





- spin eigenstates $\perp \hat{x}$ (edge/momentum)
- spin manipulation by tuning Fermi energy

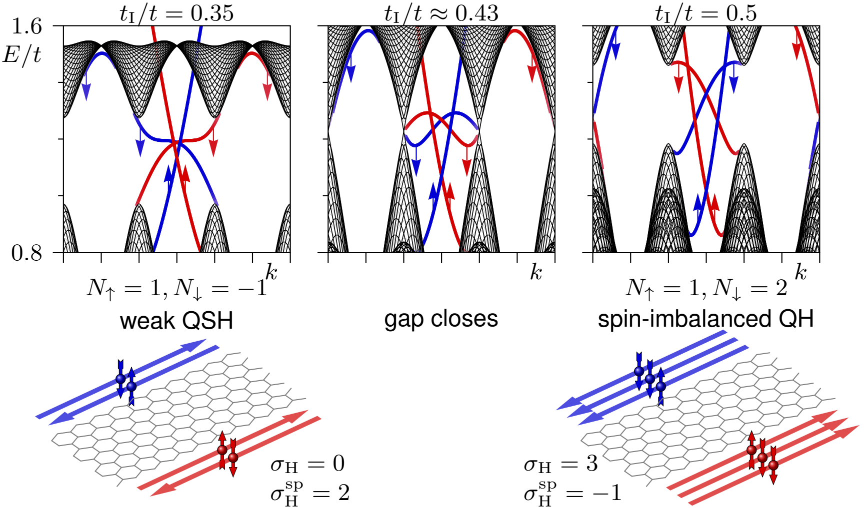
➤ [N. Goldman, W. Beugeling, and C. Morais Smith, EPL **97**, 23003 (2012)]

Topological phase transitions

Topological phases are interesting,
but what about transitions between them?

Topological phase transitions

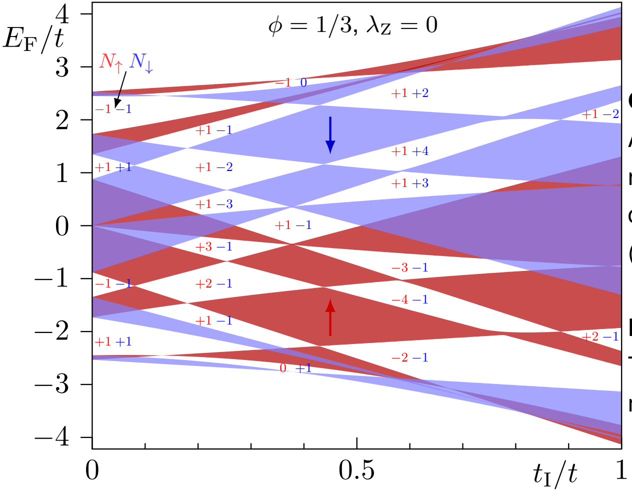
Phase transition driven by ISO ($\phi = 1/3$, $\lambda_Z/t = 0.5$, $t_R = 0$)



➤ [N. Goldman, W. Beugeling, and C. Morais Smith, EPL **97**, 23003 (2012)]

Topological phase transitions

Variation of ISO drives many top. phase transitions



Observation:

At phase transitions, number of edge states $N_\uparrow, N_\downarrow$ changes by ± 3, ± 6 (a multiple of q; $\phi = p/q$)

Reason:

There are q copies of magnetic BZ in the full BZ

➤ [W. Beugeling, N. Goldman, and C. Morais Smith, Phys. Rev. B **86**, 075118 (2012)]

Topological phase transitions

Are there other mechanisms to drive topological phase transitions?

Topological phase transitions

Are there other mechanisms to drive topological phase transitions?

Yes

Real NNN hopping will do the trick!

(assuming $\phi \neq 0$)

real NNN hopping

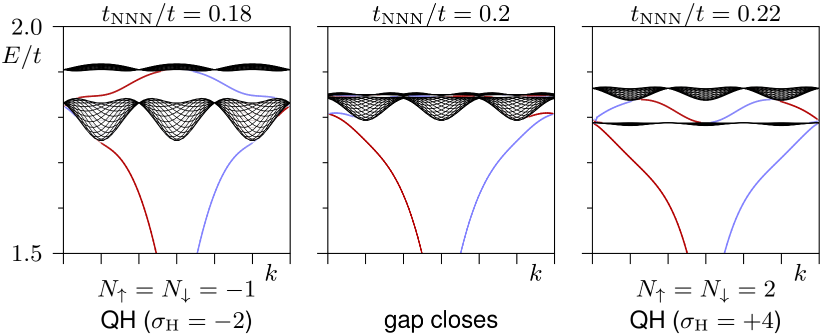
$$H_{\mathrm{NNN}} = -t_{\mathrm{NNN}} \sum_{\langle\langle i,j \rangle\rangle} e^{i\theta_{ij}} c_i^\dagger c_j$$

cf. intrinsic SO coupling

$$H_{\mathrm{I}} = -it_{\mathrm{I}} \sum_{\langle\langle i,j \rangle\rangle} e^{i\theta_{ij}} \nu_{ij} c_i^\dagger \sigma_z c_j$$

Topological phase transitions

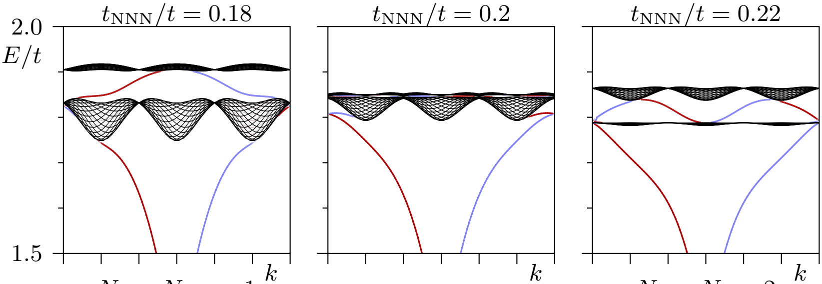
Phase transition driven by NNN ($\phi = 1/3$, $\lambda_{\mathrm{Z}} = t_{\mathrm{R}} = t_{\mathrm{I}} = 0$)



Spin degeneracy ➡ Transitions between QH (chiral) phases

Topological phase transitions

Phase transition driven by NNN ($\phi = 1/3$, $\lambda_Z = t_R = t_I = 0$)



$N_\uparrow = N_\downarrow = -1$
QH ($\sigma_H = -2$)

gap closes

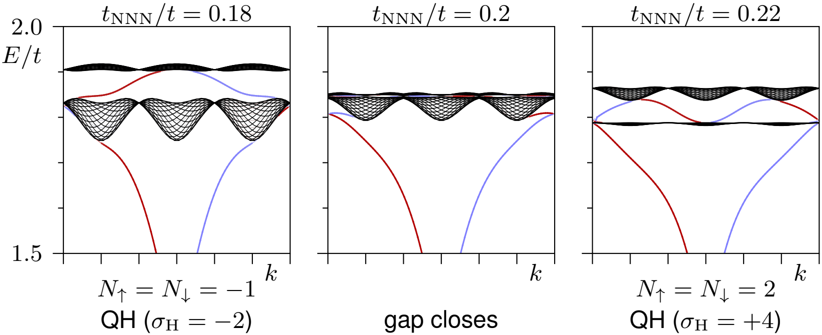
$N_\uparrow = N_\downarrow = 2$
QH ($\sigma_H = +4$)

Spin degeneracy ➡ Transitions between QH (chiral) phases

With $\phi \neq 0$, ISO $t_I \neq 0$: Tuning NNN ➡ Transitions also between nonchiral phases

Topological phase transitions

Phase transition driven by NNN ($\phi = 1/3$, $\lambda_Z = t_R = t_I = 0$)

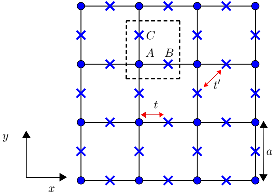


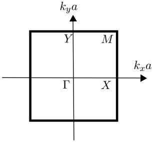
Spin degeneracy ➡ Transitions between QH (chiral) phases

With $\phi \neq 0$, ISO $t_I \neq 0$: Tuning NNN ➡ Transitions also between nonchiral phases

With $\phi = 0$: No phase transitions driven by NNN!

Topological phase transitions in the Lieb lattice

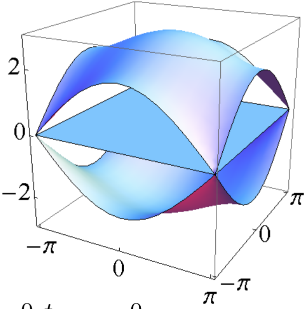




$$\mathcal{H}_{\mathbf{k}} = \mathcal{H}^0_{\mathbf{k}} \otimes \mathbb{1}_{2\times 2} + \mathcal{H}^{\mathrm{ISO}}_{\mathbf{k}} \otimes \sigma_z$$

in the basis $\hat{\Psi}_{\mathbf{k}} \equiv (\hat{\Psi}_{\mathbf{k},\uparrow}, \hat{\Psi}_{\mathbf{k},\downarrow})$

$[\hat{\Psi}_{\mathbf{k},\sigma} \equiv (\hat{c}_{A,\mathbf{k},\sigma}, \hat{c}_{B,\mathbf{k},\sigma}, \hat{c}_{C,\mathbf{k},\sigma})]$



$t_{\mathrm{I}} = 0, t_{\mathrm{NNN}} = 0$

and with

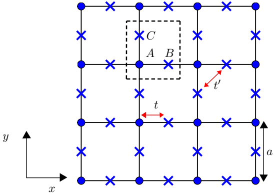
$$\mathcal{H}^0_{\mathbf{k}} = \begin{pmatrix} 0 & -2tc_x & -2tc_y \\ -2tc_x & 0 & -4t_{\mathrm{NNN}}c_xc_y \\ -2tc_y & -4t_{\mathrm{NNN}}c_xc_y & 0 \end{pmatrix}$$

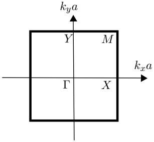
$$\mathcal{H}^{\mathrm{ISO}}_{\mathbf{k}} = 4it_{\mathrm{I}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -s_xs_y \\ 0 & s_xs_y & 0 \end{pmatrix}$$

$(s_\mu \equiv \sin(k_\mu a/2),\ c_\mu \equiv \cos(k_\mu a/2))$

➤ [W. Beugeling, J. C. Everts, and C. Morais Smith, arXiv:1207.6545]

Topological phase transitions in the Lieb lattice





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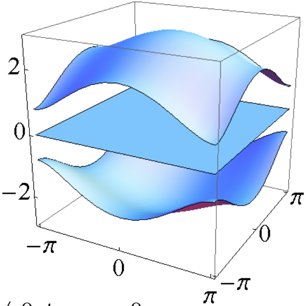

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and with

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$$\mathcal{H}^{\mathrm{ISO}}_{\mathbf{k}} = 4it_{\mathrm{I}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -s_xs_y \\ 0 & s_xs_y & 0 \end{pmatrix}$$

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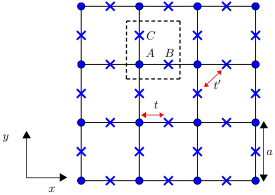

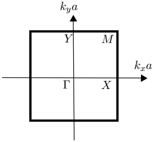

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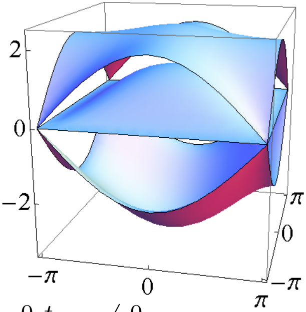


$t_{\mathrm{I}} = 0, t_{\mathrm{NNN}} \neq 0$

and with

$$\mathcal{H}^0_{\mathbf{k}} = \begin{pmatrix} 0 & -2tc_x & -2tc_y \\ -2tc_x & 0 & -4t_{\mathrm{NNN}}c_xc_y \\ -2tc_y & -4t_{\mathrm{NNN}}c_xc_y & 0 \end{pmatrix}$$

$$\mathcal{H}^{\mathrm{ISO}}_{\mathbf{k}} = 4it_{\mathrm{I}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -s_xs_y \\ 0 & s_xs_y & 0 \end{pmatrix}$$

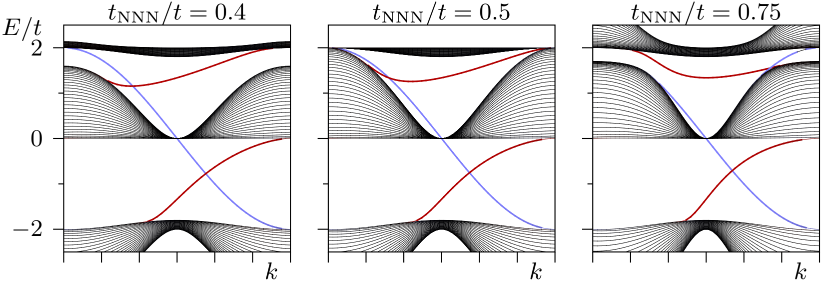
$(s_\mu \equiv \sin(k_\mu a/2),\ c_\mu \equiv \cos(k_\mu a/2))$

- [W. Beugeling, J. C. Everts, and C. Morais Smith, arXiv:1207.6545]

TPTs driven by real NNN hopping in the Lieb lattice

No magnetic field (➡ TRS ➡ helical phases)

ISO coupling $t_\mathrm{I}/t = 0.45$ opens gaps



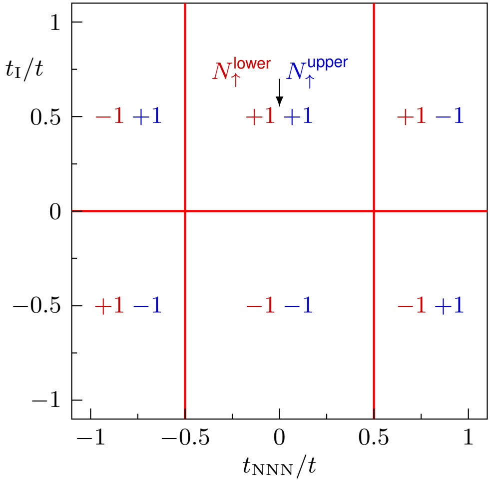
(only ↑ shown; ↓ follows from TRS)

	$t_\mathrm{NNN}/t = 0.4$	$t_\mathrm{NNN}/t = 0.5$	$t_\mathrm{NNN}/t = 0.75$
upper gap:	$N_\uparrow = -N_\downarrow = 1$ QSH ($\sigma_\mathrm{H}^\mathrm{sp} = 2$)	closes	$N_\uparrow = -N_\downarrow = -1$ QSH ($\sigma_\mathrm{H}^\mathrm{sp} = -2$)
lower gap:	$N_\uparrow = -N_\downarrow = 1$ QSH ($\sigma_\mathrm{H}^\mathrm{sp} = 2$)	$N_\uparrow = -N_\downarrow = 1$ QSH ($\sigma_\mathrm{H}^\mathrm{sp} = 2$)	$N_\uparrow = -N_\downarrow = 1$ QSH ($\sigma_\mathrm{H}^\mathrm{sp} = 2$)

Directions of edge states in upper gap are inverted

TPTs driven by real NNN hopping in the Lieb lattice

Phase diagram:



TRS ➡ $N_\uparrow^{\text{gap}} = -N_\uparrow^{\text{gap}}$

$\sigma_{\mathrm{H}}^{\mathrm{sp}}(\text{gap}) = N_\uparrow^{\text{gap}} - N_\downarrow^{\text{gap}} = 2N_\uparrow^{\text{gap}}$

(gap = lower, upper)

QSH gaps with $\sigma_{\mathrm{H}}^{\mathrm{sp}} = \pm 2$

➤ [W. Beugeling, J. C. Everts, and C. Morais Smith, arXiv:1207.6545]

Topological phase transitions – summary

➤ [W. Beugeling, J. C. Everts, and C. Morais Smith, arXiv:1207.6545]

We have topological phase transitions in:

- Honeycomb lattice ($\phi \neq 0$)
  - driven by ISO coupling
  - driven by real NNN hopping
- Lieb lattice ($\phi = 0$)
  - driven by real NNN hopping
- Kagome lattice ($\phi = 0$) (not shown)
  - driven by ISO coupling
  - driven by real NNN hopping

Experimental realisations

How to observe these phases and phase transitions?

Experimental realisations – Condensed Matter

Low-flux limit: $|\phi| \lesssim 10^{-3}$

- Graphene

RSO	$t_\mathrm{R}/t \sim 0.01 – 0.1$
ISO	$t_\mathrm{I}/t \sim 10^{-6} – 10^{-4}$
Zeeman	$\lambda_\mathrm{Z}/t \sim g \sim 1$

- 2D topological insulators (e.g., Hg(Cd)Te quantum wells)

RSO	$t_\mathrm{R}/t \sim 10^{-2}$
ISO	$t_\mathrm{I}/t \sim 10^{-2}$
Zeeman	$\lambda_\mathrm{Z}/t \sim g \sim 10 – 50$

➤ [C. Brüne *et al.*, Phys. Rev. Lett. **106**, 126803 (2011)]

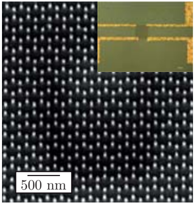
Experimental realisations – Artificial lattices

Patterns on a substrate emulating “real” honeycomb lattices:

- Array of quantum dots on GaAs

  Lattice constant $\sim 100\,\mathrm{nm}$ ➡ high flux
  Possible problem: Small hopping parameter

  ➤ [G. De Simoni *et al.*, Appl. Phys. Lett. **97**, 132113 (2010)]



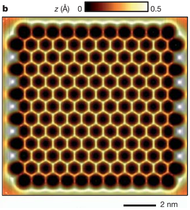
- “Molecular graphene”

  Pattern created by repulsion of CO molecules deposited on Cu(111)

  Lattice constant $\sim 1\,\mathrm{nm}$ ➡ higher flux than graphene
  Choice of substrate ➡ SO coupling?
  High control of lattice parameters (STM)

  ➤ [K. K. Gomes, W. Mar, W. Ko, F. Guinea,

  and H. C. Manoharan, Nature **483**, 306 (2012)]



Experimental realisations – Ultracold atoms

Ultracold atoms (optical lattice with synthetic gauge fields)

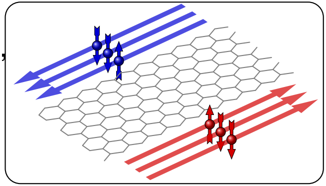
- High flux
- Tunability of the parameters
- Absence of disorder

- [D. Jaksch and P. Zoller, New J. Phys. **5**, 56 (2003)]
- [K. Osterloh *et al.*, Phys. Rev. Lett. **95**, 010403 (2005)]
- [F. Gerbier and J. Dalibard, New J. Phys. **12**, 033007 (2010)]
- [A. Bermudez *et al.*, Phys. Rev. Lett. **105**, 190404 (2010)]
- [N. Goldman *et al.*, Phys. Rev. Lett. **105**, 255302 (2010)]
- [N. Goldman *et al.*, Phys. Rev. Lett. **108**, 255303 (2012)]

Conclusion

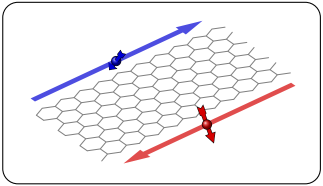
In the honeycomb lattice, the interplay of $\mathbf{B}$, ISO, RSO and Zeeman effect creates

- rich variety of topological phases
- variable spin direction



Topological phase transitions

- driven by ISO, real NNN
- in honeycomb, Lieb, kagome lattices



Various realisations possible

➤ [N. Goldman, W. Beugeling, and C. Morais Smith, EPL **97**, 23003 (2012)]

➤ [W. Beugeling, N. Goldman, and C. Morais Smith, Phys. Rev. B **86**, 075118 (2012)]

➤ [W. Beugeling, J. C. Everts, and C. Morais Smith, arXiv:1207.6545]

Thank you
for your attention

$* * *$

Topological invariants

Dispersion in ribbon geometry

$\big\downarrow$ Count

$N_\uparrow, N_\downarrow$

\# of edge states in gap

$$\mathbf{A}_{n,\mathbf{k}} = i \langle \psi_{n,\mathbf{k}} | \nabla | \psi_{n,\mathbf{k}} \rangle$$ (Berry conn.)

$$F_{n,\mathbf{k}} = \partial_x A_y - \partial_y A_x$$ (Berry curv.)

$\big\downarrow \int_{\mathrm{BZ}} \mathrm{d}\mathbf{k}$

$C_{\uparrow,n}, C_{\downarrow,n}$

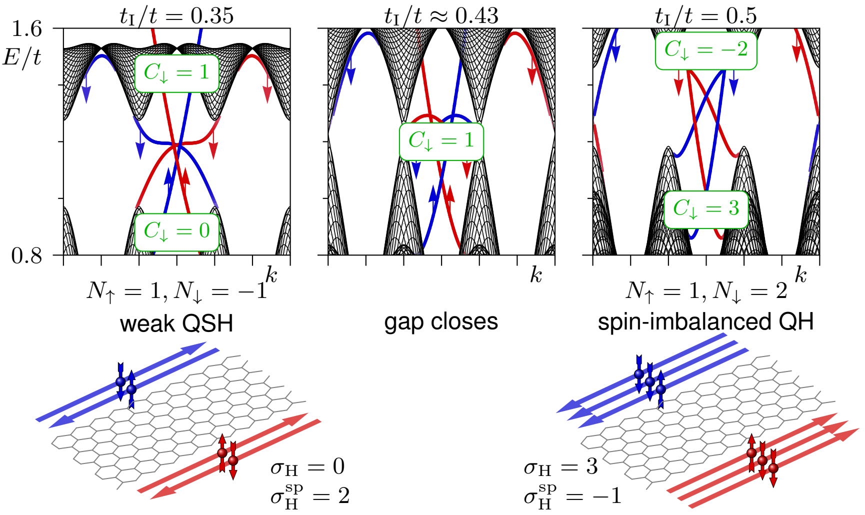
Chern numbers of bulk bands

$$N_\sigma = \sum_{\text{occupied bands } n} C_{\sigma,n}$$

bulk-boundary correspondence

Topological phase transitions – Chern numbers

Phase transition driven by ISO ($\phi = 1/3$, $\lambda_Z/t = 0.5$, $t_R = 0$)



➤ [N. Goldman, W. Beugeling and C. Morais Smith, EPL **97**, 23003 (2012)]

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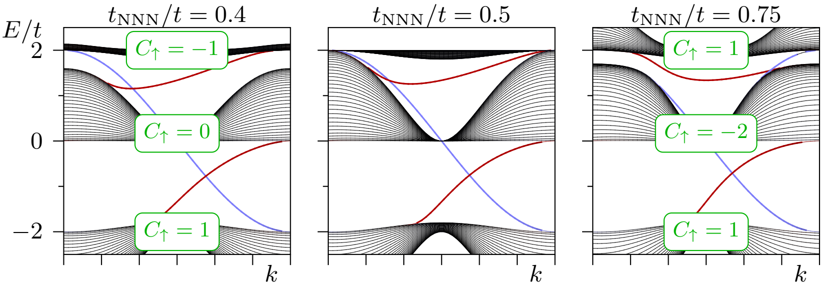

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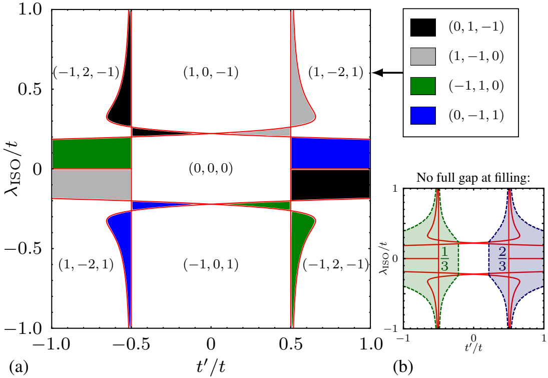
Directions of edge states in upper gap are inverted

Lieb lattice with dimerisation term

Dimerisation:
Change NN hopping t to $t + \alpha$ and $t - \alpha$ alternatingly.

➡ Phase diagram ($\alpha/t = 0.3$):



➤ [W. Beugeling, J. C. Everts, and C. Morais Smith, arXiv:1207.6545]