Topological invariants and topological insulators

Ryan Requist
Max Planck Institute of Microstructure Physics, Halle, Germany

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MAX-PLANCK-GESELLSCHAFT

Outline

I. Introduction
   A. Topological invariants in condensed matter physics
   B. Dirac monopole
   C. From geometry to topology

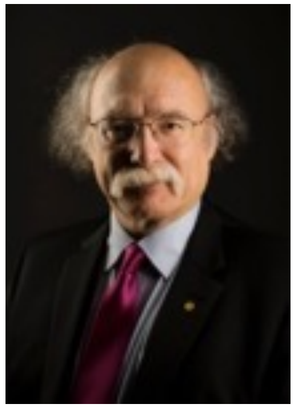
II. Topological invariants in one-dimensional systems
   A. Edge states in the Su-Schrieffer-Heeger model
   B. Polarization in the Su-Schrieffer-Heeger model
   C. Thouless charge pumping in Rice-Mele model
   D. Effect of interactions: Rice-Mele-Hubbard model

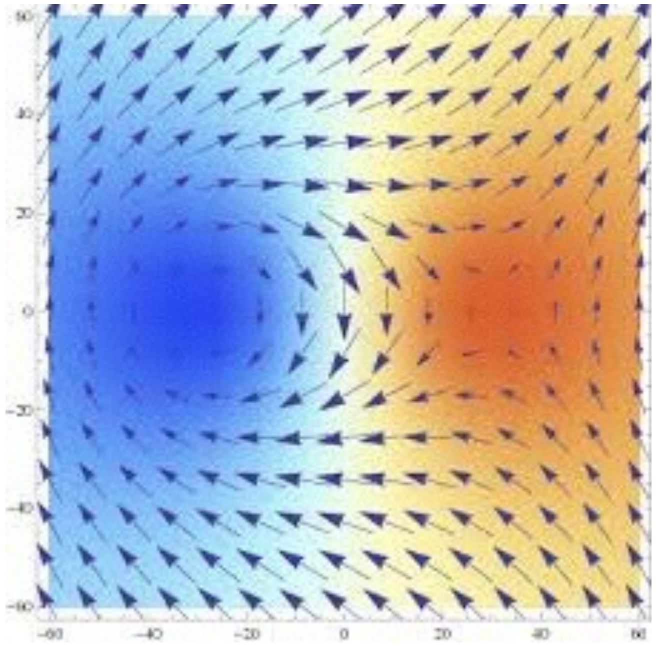
III. Topological invariants in two-dimensional systems
   A. Integer quantum Hall effect
   B. Quantum spin Hall effect

Topology in condensed matter physics

Nobel Prize in Physics 2016

for discoveries of
topological phase transitions &
topological phases of matter



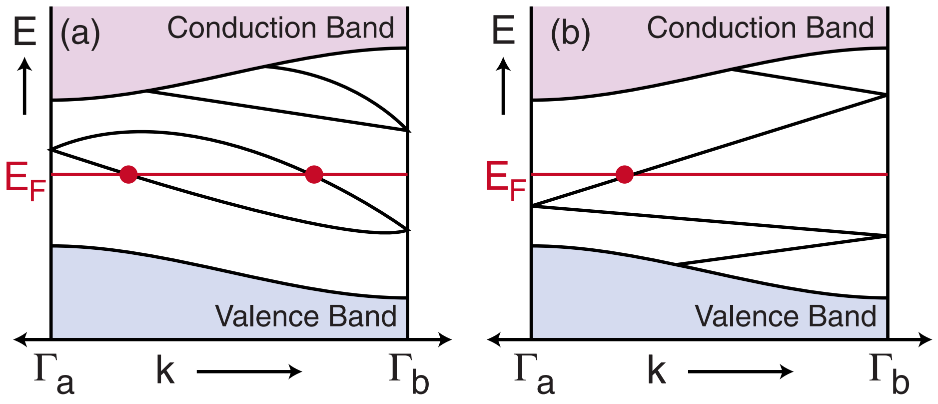


Topological phases of matter

Integer quantum Hall effect Thouless *et al.* 1982

Quantum spin Hall effect Kane Mele 2005

Topological insulators Fu Kane Mele 2007

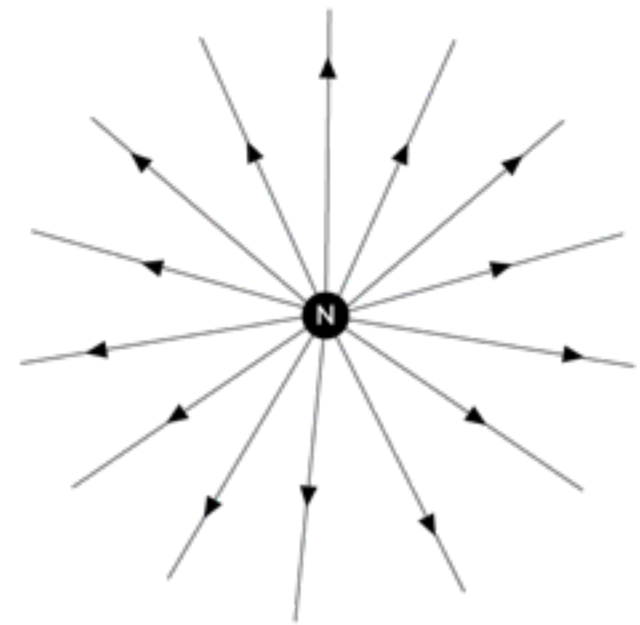


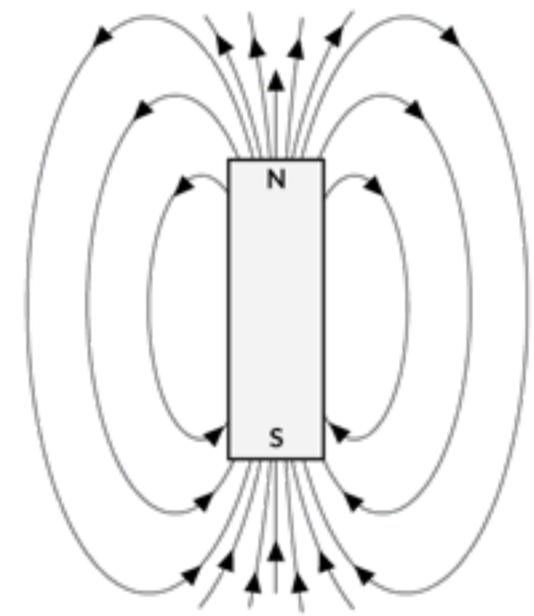
Magnetic monopoles and Dirac's quantization condition

$$\nabla \cdot \mathbf{B} = \sum_i g_i \delta^{(3)}(\mathbf{r} - \mathbf{r}_i)$$

$$\mathbf{B} = B_r \mathbf{r}$$

$$B_r = \frac{1}{r \sin\theta} \frac{\partial}{\partial\theta}(A_\phi \sin\theta)$$





$$A_\phi^+ = g \frac{1 - \cos\theta}{r \sin\theta} \qquad \text{for} \quad \theta < \frac{\pi}{2} + \delta$$

$$A_\phi^- = g \frac{-1 - \cos\theta}{r \sin\theta} \qquad \text{for} \quad \theta > \frac{\pi}{2} - \delta$$

Dirac 1931

Magnetic monopoles and Dirac's quantization condition

$$\nabla \cdot \mathbf{B} = \sum_i g_i \delta^{(3)}(\mathbf{r} - \mathbf{r}_i)$$

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$$A_\phi^- = g\frac{-1 - \cos\theta}{r\sin\theta} \qquad \text{for} \quad \theta > \frac{\pi}{2} - \delta$$

A^+ and A^- are related by a gauge transformation

$$\psi(\mathbf{r}) \to e^{if_{+-}(\theta,\phi)}\psi(\mathbf{r})$$

$$A_\phi^+ = A_\phi^- + \frac{\partial}{\partial\phi} f_{+-}(\theta,\phi)$$

$$A_\phi^+ = A_\phi^- + \frac{\partial}{\partial\phi} \frac{2g\phi}{r\sin\theta}$$

$$g_{-+} : (\theta, \phi, e^{i\alpha_-}) \to (\theta, \phi, e^{if_{+-}(\theta,\phi)} e^{i\alpha_+})$$

Dirac 1931

Magnetic monopoles and Dirac's quantization condition

Suppose $\psi_0(\mathbf{r})$ is the wavefunction of a charge in a region without fields and suppose it has a nodal line with winding number

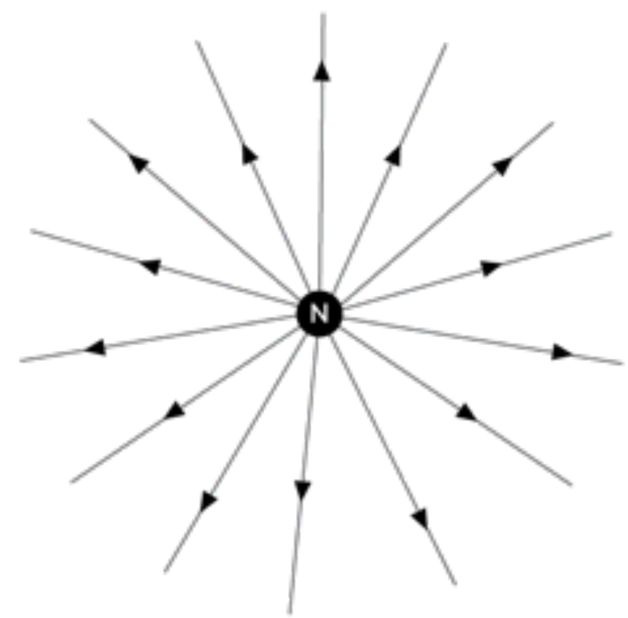
$$n = \frac{1}{2\pi}\oint dS = \frac{1}{2\pi}\oint \nabla S \cdot d\mathbf{r}$$

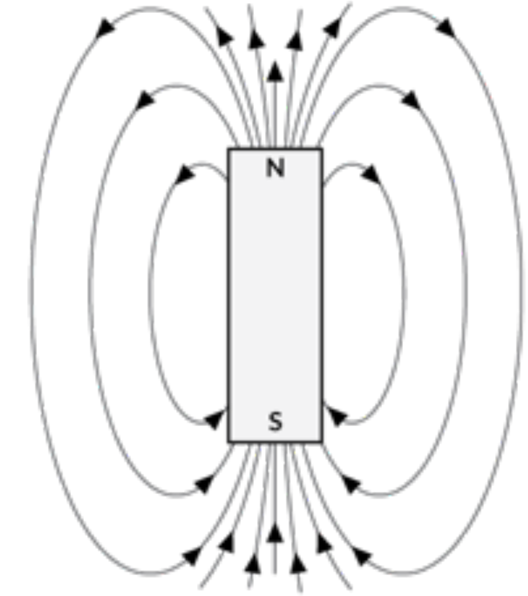
When an electromagnetic field is turned on the wavefunction becomes

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) e^{i\frac{e}{\hbar c}\int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{A}\cdot d\mathbf{x}}$$

Change in phase around a circuit is

$$\begin{aligned}\Delta S &= 2\pi n + \frac{e}{\hbar c}\oint_C \mathbf{A}\cdot d\mathbf{r} \\ &= 2\pi n + \frac{e}{\hbar c}\int_S \mathbf{B}\cdot d\mathbf{S}\end{aligned}$$





For a closed surface $\Delta S = 0$

$$\Rightarrow \quad \Phi_B = \frac{2\pi\hbar c}{e} = 4\pi g$$

$$g = \frac{n\hbar c}{2e} \;\Rightarrow\; g_0 = \frac{\hbar c}{2e}$$

Dirac 1931

From Berry curvature to topological invariants

$$\int_M K dS = 2\pi\chi(M)$$

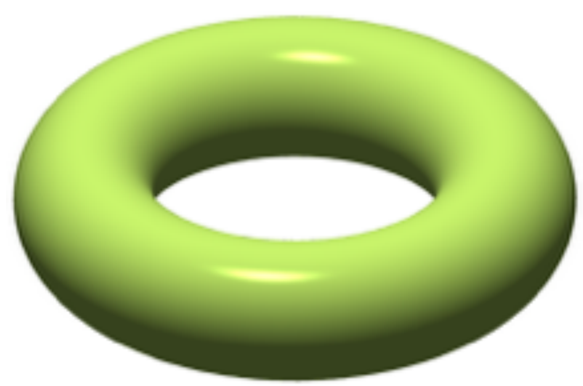
$K =$ Gaussian curvature

$\chi =$ Euler characteristic

$$\chi = 2 - 2g$$

$g =$ genus

$g = 0, \chi = 2$



$g = 1, \chi = 0$

$g = 2, \chi = -2$

Figures from wikipedia.com

From Berry curvature to topological invariants

Berry phase

$$\gamma(C) = -\iint_S \mathbf{B} \cdot d\mathbf{S}$$
$$= -\iint_S B_\perp dQ_2 dQ_3$$

Berry curvature

$$B_\perp = 2\mathrm{Im}\left\langle \frac{d\Phi_{\underline{\underline{\mathbf{R}}}}}{dQ_2} \middle| \frac{d\Phi_{\underline{\underline{\mathbf{R}}}}}{dQ_3} \right\rangle$$

The integral of the Berry curvature over a closed manifold is a topological invariant called the Chern number.

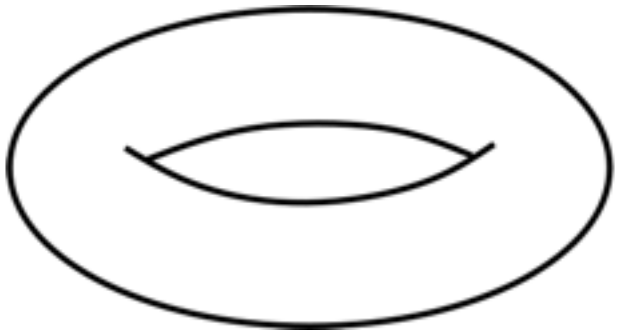
Example: Quantum Hall effect

*Thouless, Kohmoto, Nightingale, den Nijs Phys. Rev. Lett. 49, 405 (1982)

$$\sigma_{xy} = C\frac{e^2}{h}$$

$$C = \frac{1}{2\pi}\iint_{BZ} B_{k_1 k_2} dk_1 dk_2$$

TKNN integer*
(Chern number)

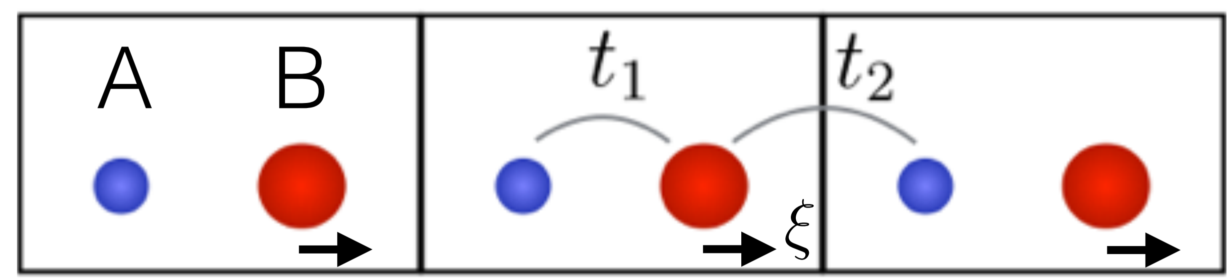


Edge states in one-dimensional systems

Su-Schrieffer-Heeger model $\hat{H} = \sum_{n\sigma} t_{n,n+1}(c^\dagger_{n\sigma}c_{n+1\sigma} + c^\dagger_{n+1\sigma}c_{n\sigma})$

dimerized hopping $t_1 = t_0 - \alpha\xi$

$t_2 = t_0 + \alpha\xi$



$\xi =$ displacement of B sublattice

Internal space $|A\rangle, |B\rangle \rightarrow$ pseudospin $\vec{\tau} = (\tau_x, \tau_y, \tau_z)$

$t_1 c^\dagger_{n\sigma}c_{n+1\sigma} \rightarrow t_1 c^\dagger_{lA}c_{lB}$ $\quad n =$ site index

$t_2 c^\dagger_{n+1\sigma}c_{n+2\sigma} \rightarrow t_2 c^\dagger_{lb}c_{l+1A}$ $\quad l =$ cell index

$$\hat{H} = t_1 \sum_{l\sigma} c^\dagger_{l\sigma}c_{l\sigma} \otimes \hat{\tau}_x + t_2 \sum_{l\sigma}\left(c^\dagger_{l+1\sigma}c_{l\sigma} \otimes \frac{\hat{\tau}_x + i\hat{\tau}_y}{2} + H.c.\right)$$

Su Schrieffer Heeger, Phys. Rev. Lett. 42, 1698 (1979)

Edge states in one-dimensional systems

Su-Schrieffer-Heeger model

$$\hat{H} = t_1 \sum_{l\sigma} c^\dagger_{l\sigma} c_{l\sigma} \otimes \hat{\tau}_x + t_2 \sum_{l\sigma} \left(c^\dagger_{l+1\sigma} c_{l\sigma} \otimes \frac{\hat{\tau}_x + i\hat{\tau}_y}{2} + H.c. \right)$$

k-space Hamiltonian $\hat{h}(k) = \langle k|\hat{H}|k\rangle = \vec{h}(k) \cdot \vec{\sigma}$

$$\begin{cases} h_x = t_1 + t_2 \cos k \\ h_y = t_2 \sin k \\ h_z = 0 \end{cases}$$

Bloch states $|\psi_{nk\sigma}\rangle = |u_{nk}\rangle \otimes |k\rangle \otimes |\sigma\rangle, \qquad |u_{nk}\rangle = a_{nk}|A\rangle + b_{nk}|B\rangle$

Chiral symmetry $\{\hat{H}, \hat{\Gamma}\} = 0 \qquad \hat{\Gamma}\hat{H}\hat{\Gamma}^\dagger = -\hat{H}$

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle \quad \Rightarrow \quad \hat{H}\hat{\Gamma}|\Psi_n\rangle = -\hat{\Gamma}\hat{H}|\Psi_n\rangle = -E_n|\Psi_n\rangle$$

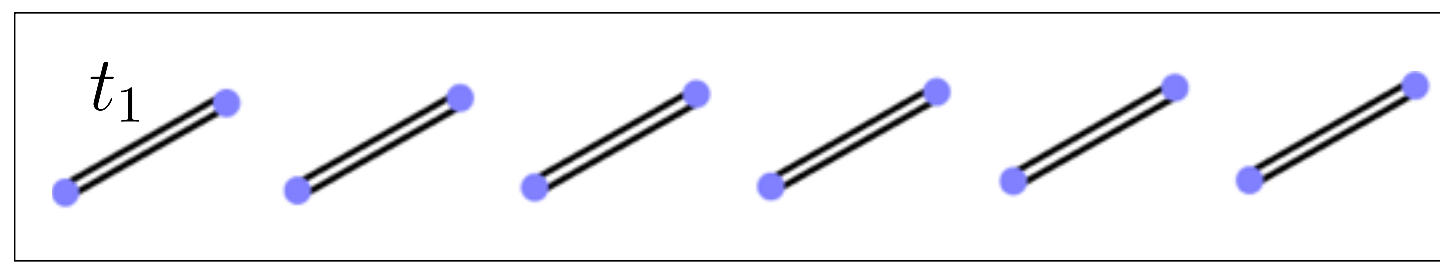
Asboth, Oroszlany, Palyi, A short course on topological insulators, 2016.

Edge states in one-dimensional systems

k-space Hamiltonian $\hat{h}(k) = \langle k|\hat{H}|k\rangle = \vec{h}(k)\cdot\vec{\sigma}$ $\quad \begin{cases} h_x = t_1 + t_2\cos k \\ h_y = t_2 \sin k \\ h_z = 0 \end{cases}$

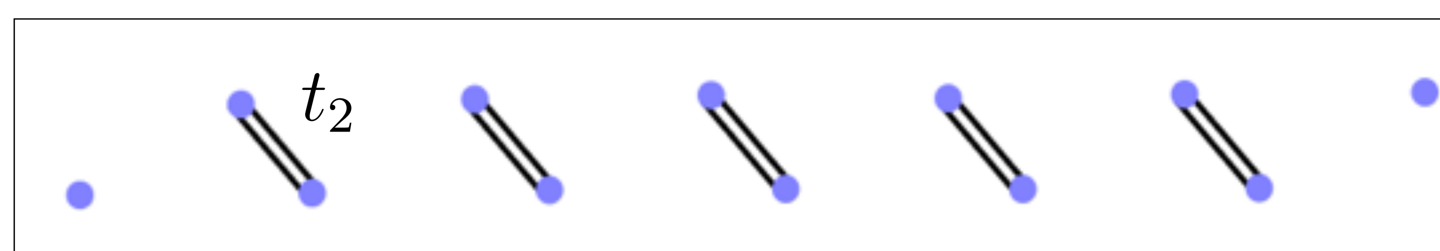
$$\hat{\sigma}_z \hat{h}(k)\hat{\sigma}_z = -h(k) \quad \Rightarrow \quad h_z = 0$$

Fully dimerized limit



1. No edge states

$t_1 = 1, t_2 = 0 \qquad \hat{h}(k) = \hat{\sigma}_x$

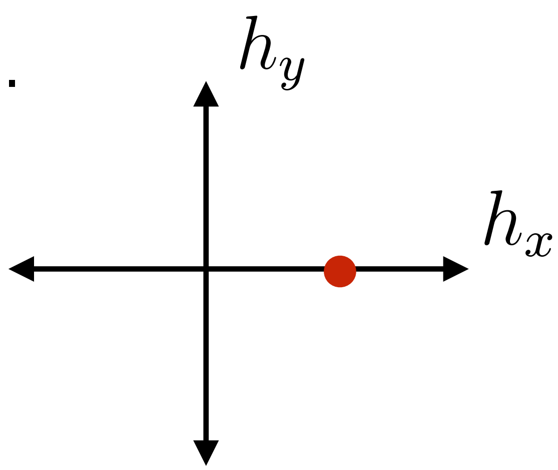


2. Zero-energy edge states

$t_1 = 0, t_2 = 1 \qquad \hat{h}(k) = \hat{\sigma}_x \cos k + \hat{\sigma}_y \sin k$

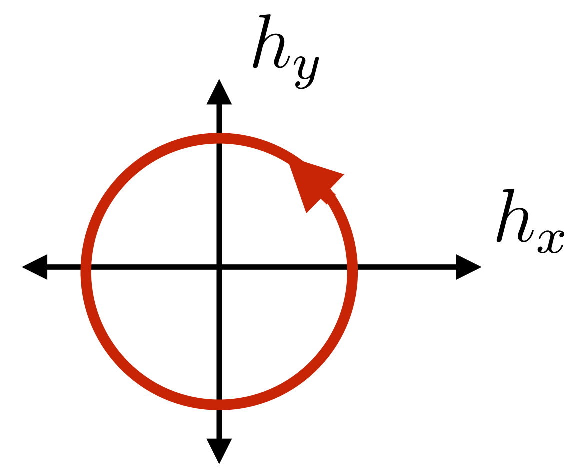
Edge states in one-dimensional systems

1.



winding number $\nu = 0$

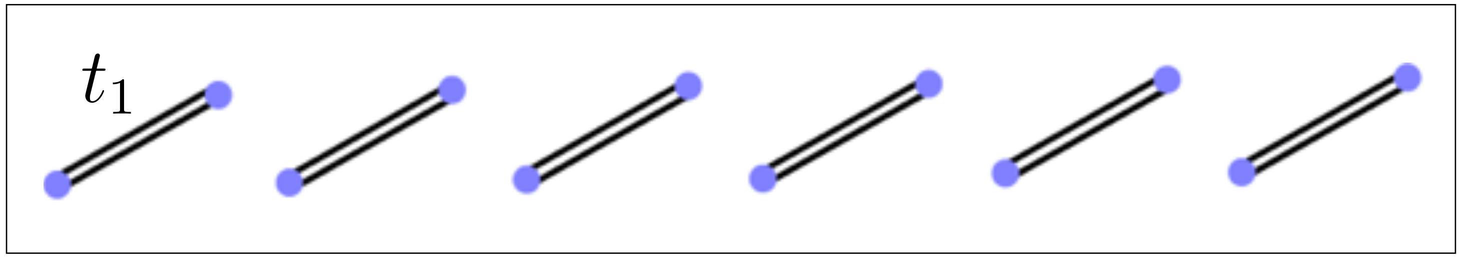
2.



winding number $\nu = 1$

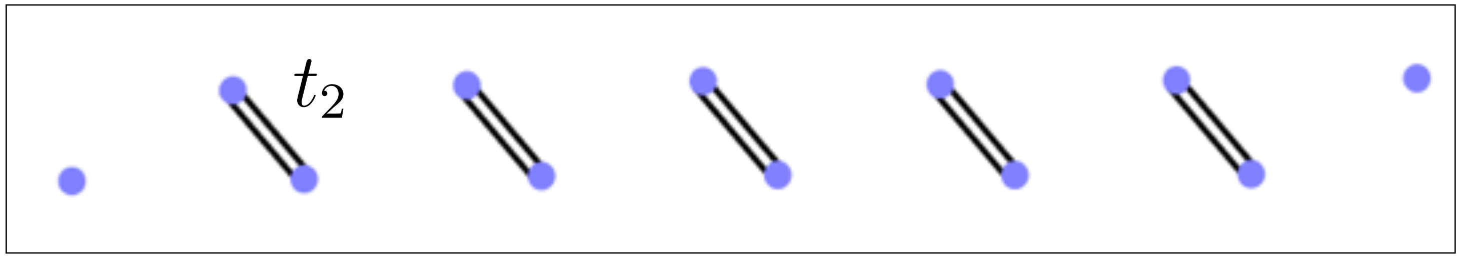
Fully dimerized limit

1. No edge states



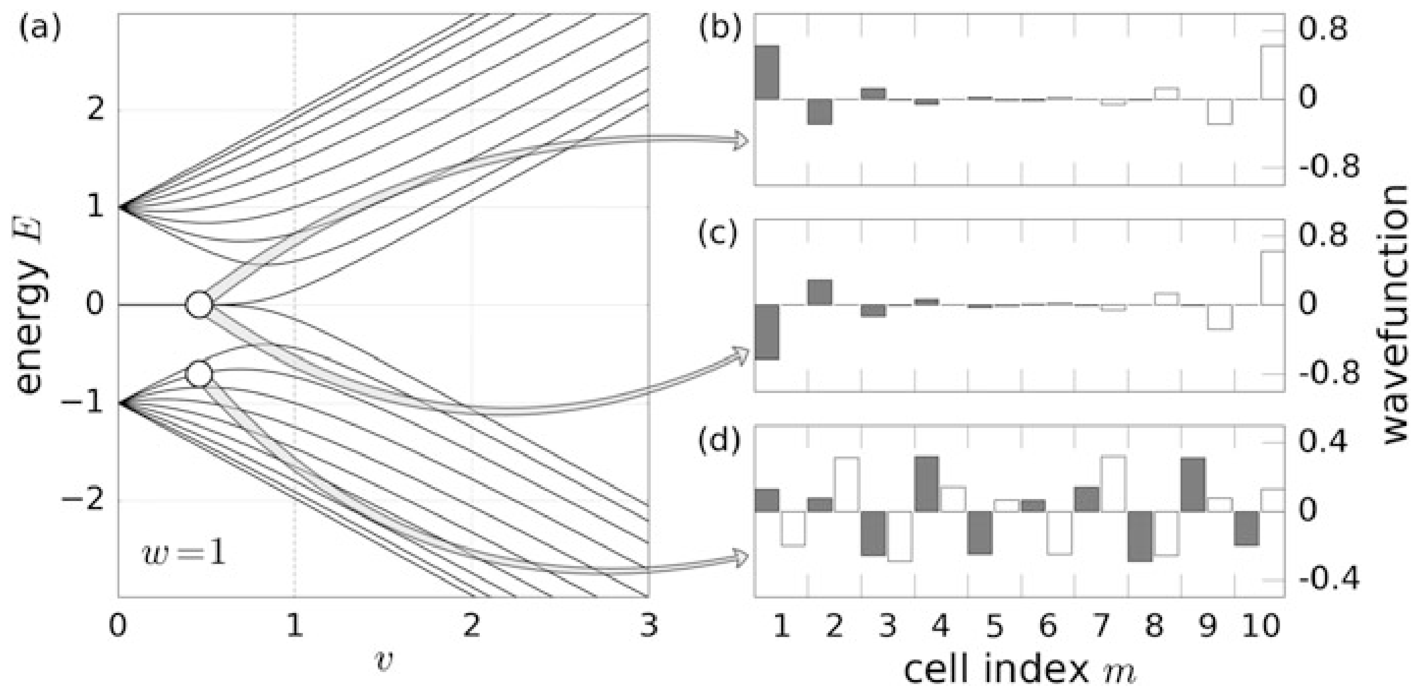
$t_1 = 1, t_2 = 0 \qquad \hat{h}(k) = \hat{\sigma}_x$

2. Zero-energy edge states



$t_1 = 0, t_2 = 1 \qquad \hat{h}(k) = \hat{\sigma}_x \cos k + \hat{\sigma}_y \sin k$

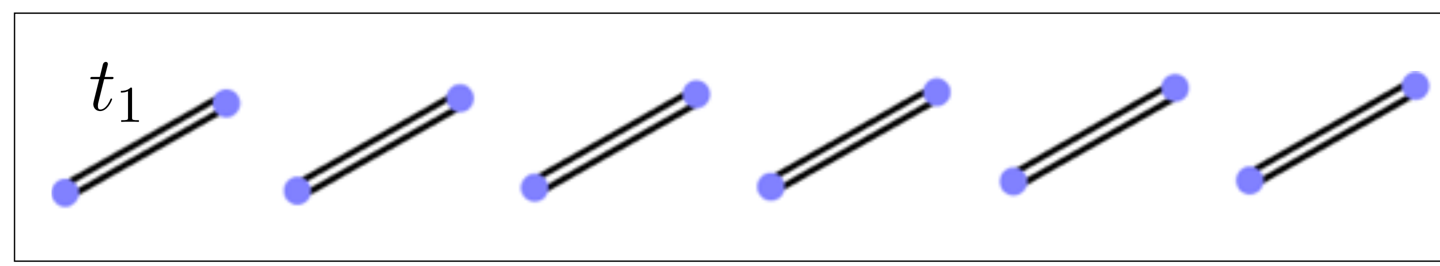
Edge states in one-dimensional systems



$\mu =$ number of zero-energy states at the left edge

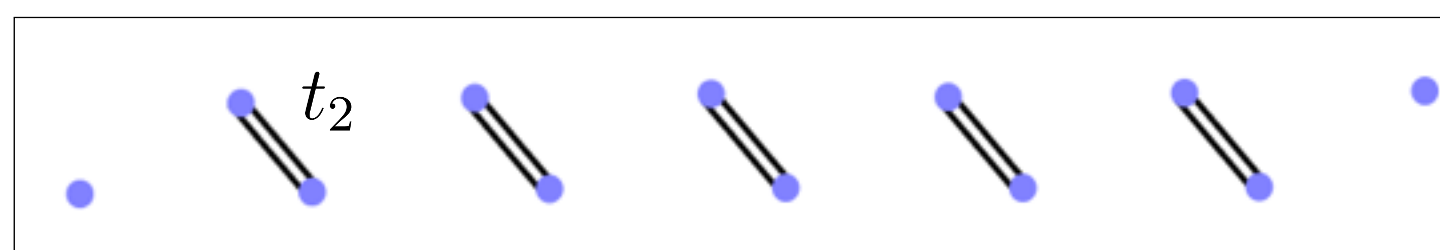
Fully dimerized limit

1. No edge states



$$t_1 = 1, t_2 = 0 \qquad \hat{h}(k) = \hat{\sigma}_x$$

2. Zero-energy edge states



$$t_1 = 0, t_2 = 1 \qquad \hat{h}(k) = \hat{\sigma}_x \cos k + \hat{\sigma}_y \sin k$$

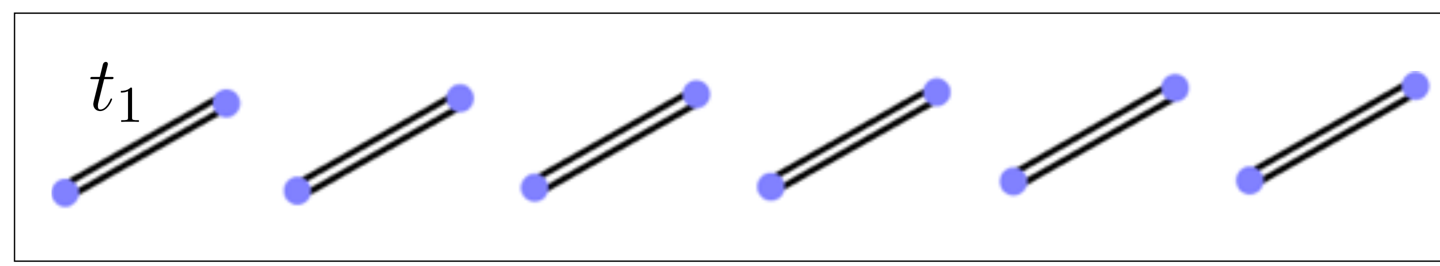
Asboth, Oroszlany, Palyi, A short course on topological insulators, 2016.

Edge states in one-dimensional systems

The notion of bulk-boundary correspondence allows one to make predictions about the boundary of a system (e.g. the existence of edge states) based on knowledge of a bulk topological invariant.

In the SSH model, one finds that the number (0 or 1) of left-edge states equals the winding number of $\vec{h}(k)$, i.e. $\mu = \nu$.

Fully dimerized limit



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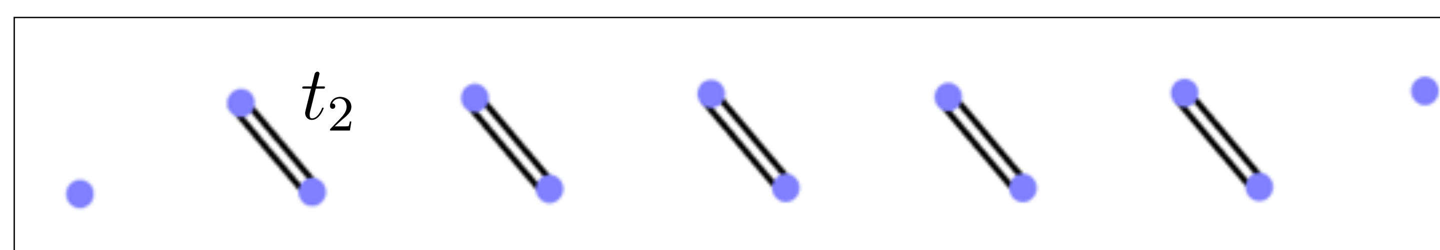

2. Zero-energy edge states

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Asboth, Oroszlany, Palyi, A short course on topological insulators, 2016.

Polarization in one-dimensional systems

Consider two types of centrosymmetric one-dimensional systems

1. Dimerized lattice 

2. Ionic lattice 

Geometric phase formula for the macroscopic polarization

$$P_{elec} = -\frac{e}{2\pi} \sum_{n}^{\mathrm{occ}} \int i \langle u_{nk} | \nabla_k u_{nk} \rangle dk \quad \mathrm{mod}\ e$$

Parity operator $\hat{\Pi}$ takes $P \to -P$

Centrosymmetric systems must have

$$P = 0 \mod e$$

or

$$P = \frac{e}{2} \mod e$$

Polarization in one-dimensional systems

Consider two types of centrosymmetric one-dimensional systems

1. Dimerized lattice 
2. Ionic lattice 

distinct topological phases

Geometric phase formula for the macroscopic polarization

$$P_{elec} = -\frac{e}{2\pi}\sum_{n}^{\mathrm{occ}} \int i\langle u_{nk}|\nabla_k u_{nk}\rangle dk \quad \mathrm{mod}\ e$$

$$P = P_{elec} + \frac{e}{a}\sum_n Z_n \mathbf{t}_n$$

1. Dimerized lattice $P_{elec} = \frac{e}{4} + \frac{e}{4} = \frac{e}{2} \ \mathrm{mod}\ e \quad \Rightarrow \quad P = 0 \ \mathrm{mod}\ e$

2. Ionic lattice $P_{elec} = \frac{e}{2} + \frac{e}{2} = 0 \ \mathrm{mod}\ e \quad \Rightarrow \quad P = \frac{e}{2} \ \mathrm{mod}\ e$

Thouless charge pumping

Spatially periodic time-dependent potential with time-period T

$$v(r, t + T) = v(r, t) \qquad v(r + a, t) = v(r, t)$$

Pumped charge per period is a topological invariant

$$Q = \frac{e}{2\pi} \int_0^T dt \int_{BZ} dk \, 2\mathrm{Im} \sum_n \langle \partial_t u_{nk} | \partial_k u_{nk} \rangle$$

Thouless Phys. Rev. B 27, 6083 (1983); Niu Thouless J. Phys. A: Math. Gen. 17, 2453 (1984)

Thouless charge pumping

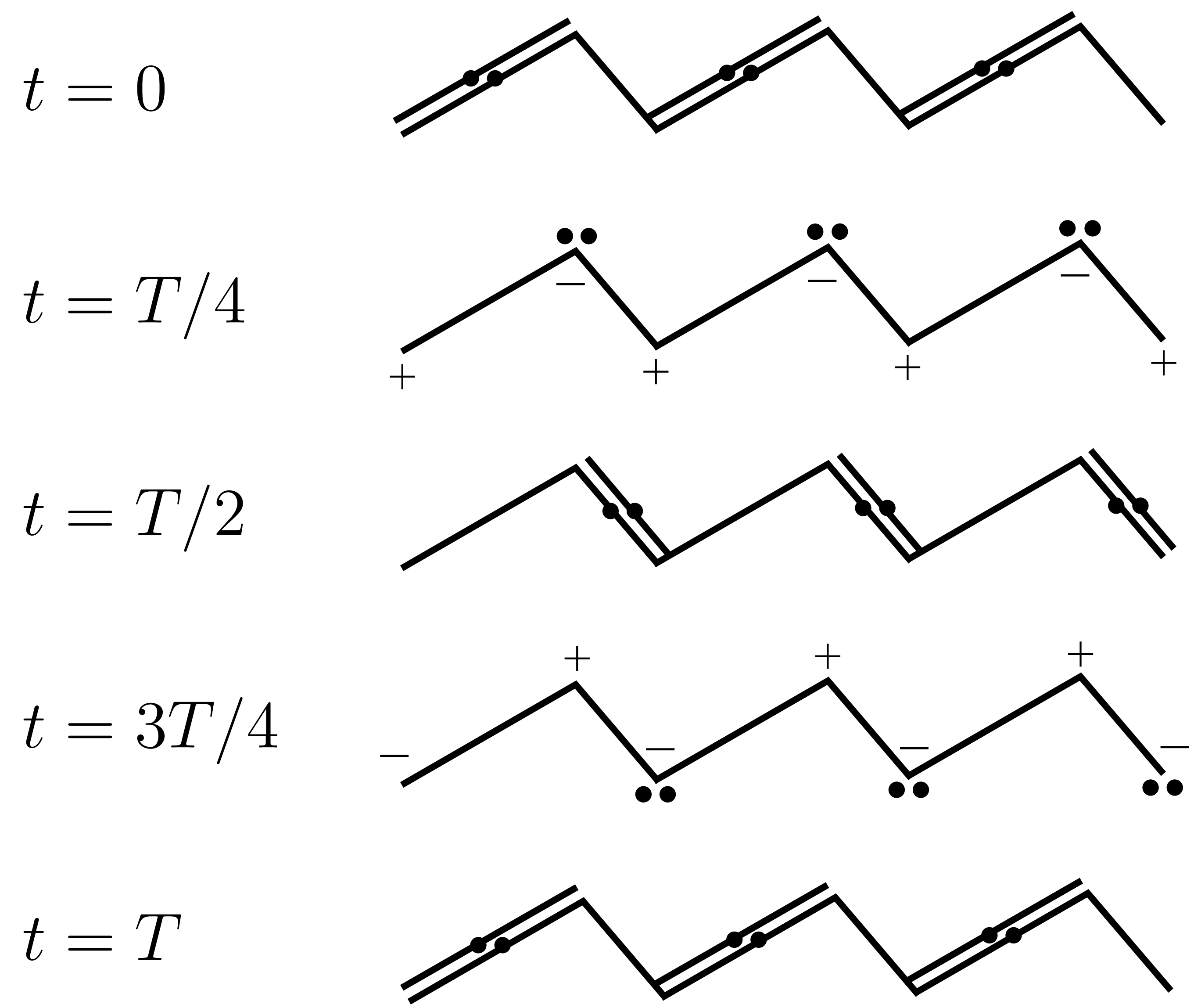
Rice-Mele-Hubbard model

$$\hat{H} = \sum_{n\sigma} \left[\epsilon_n c^\dagger_{n\sigma} c_{n\sigma} + t_{nn+1} (c^\dagger_{n\sigma} c_{n+1\sigma} + c^\dagger_{n+1\sigma} c_{n\sigma}) + U c^\dagger_{n\uparrow} c_{n\uparrow} c^\dagger_{n\downarrow} c_{n\downarrow} \right]$$

$$\epsilon_{2n} = -\Delta$$
$$\epsilon_{2n+1} = +\Delta$$

Driving protocol

$$t_1 = t_0 + \Delta_0 \cos(2\pi t/T)$$
$$t_2 = t_0 - \Delta_0 \cos(2\pi t/T)$$
$$\Delta = \Delta_0 \sin(2\pi t/T)$$



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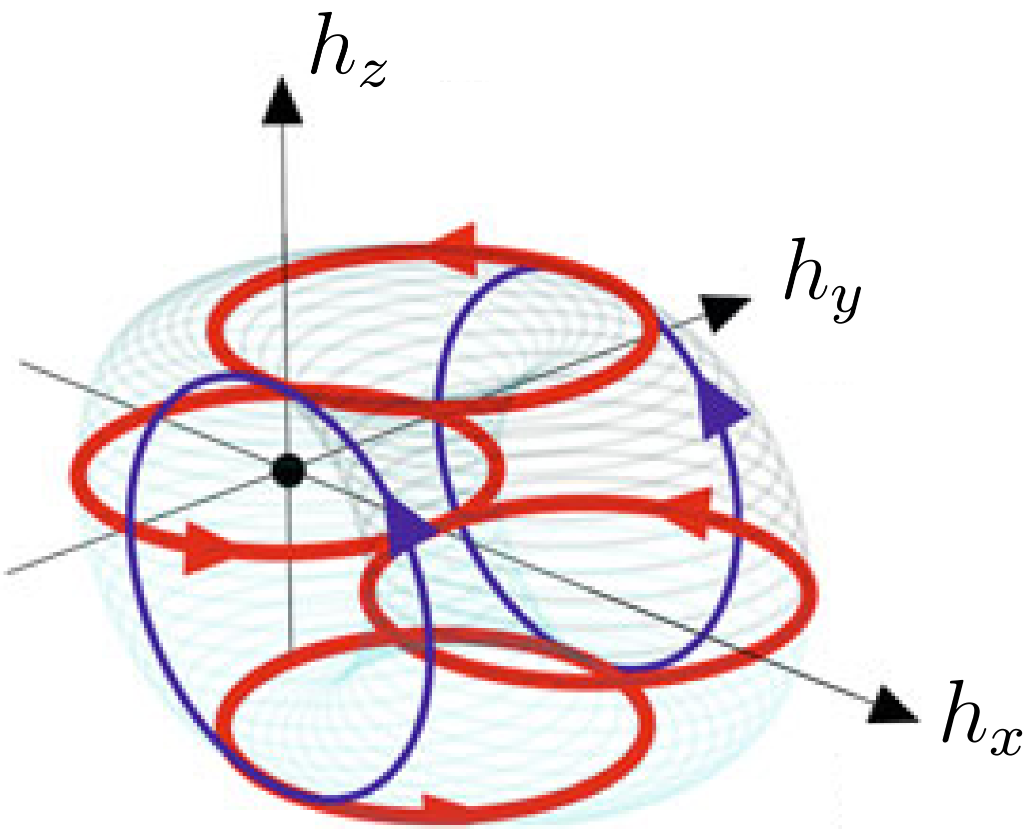
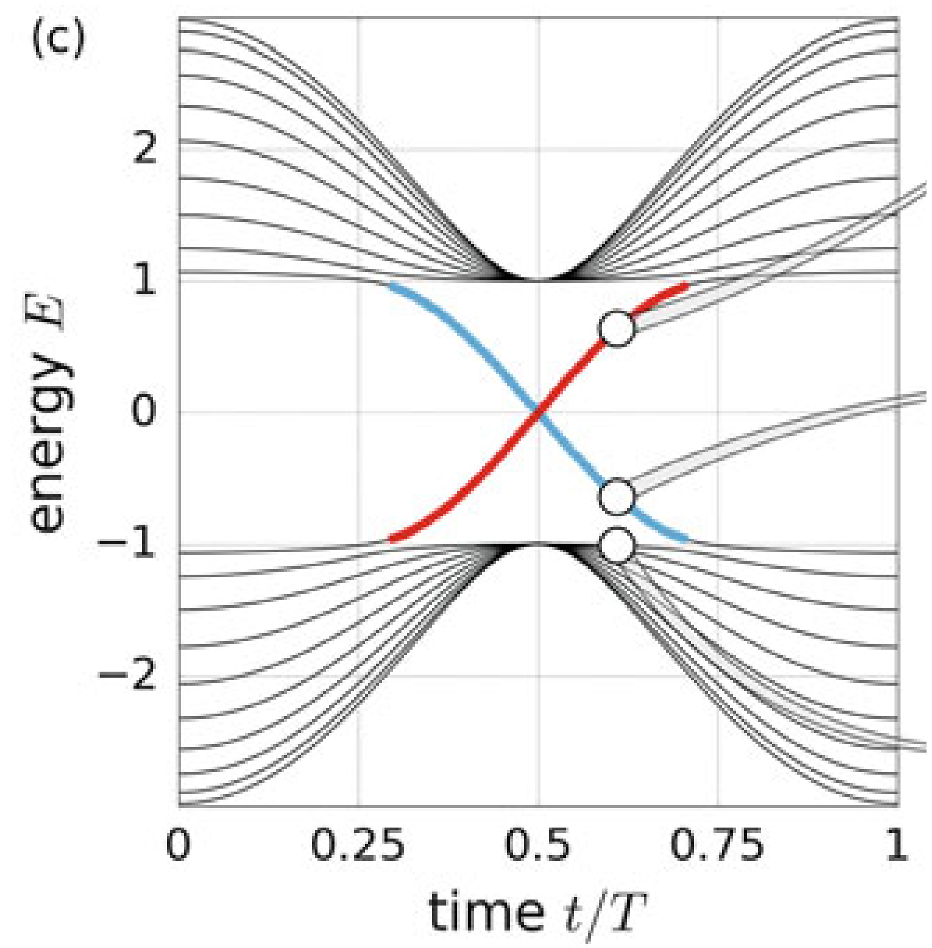
k-space Hamiltonian $\hat{h}(k) = \langle k|\hat{H}|k\rangle = \vec{h}(k) \cdot \vec{\sigma}$





Asboth, Oroszlany, Palyi, A short course on topological insulators, 2016.

Thouless charge pumping

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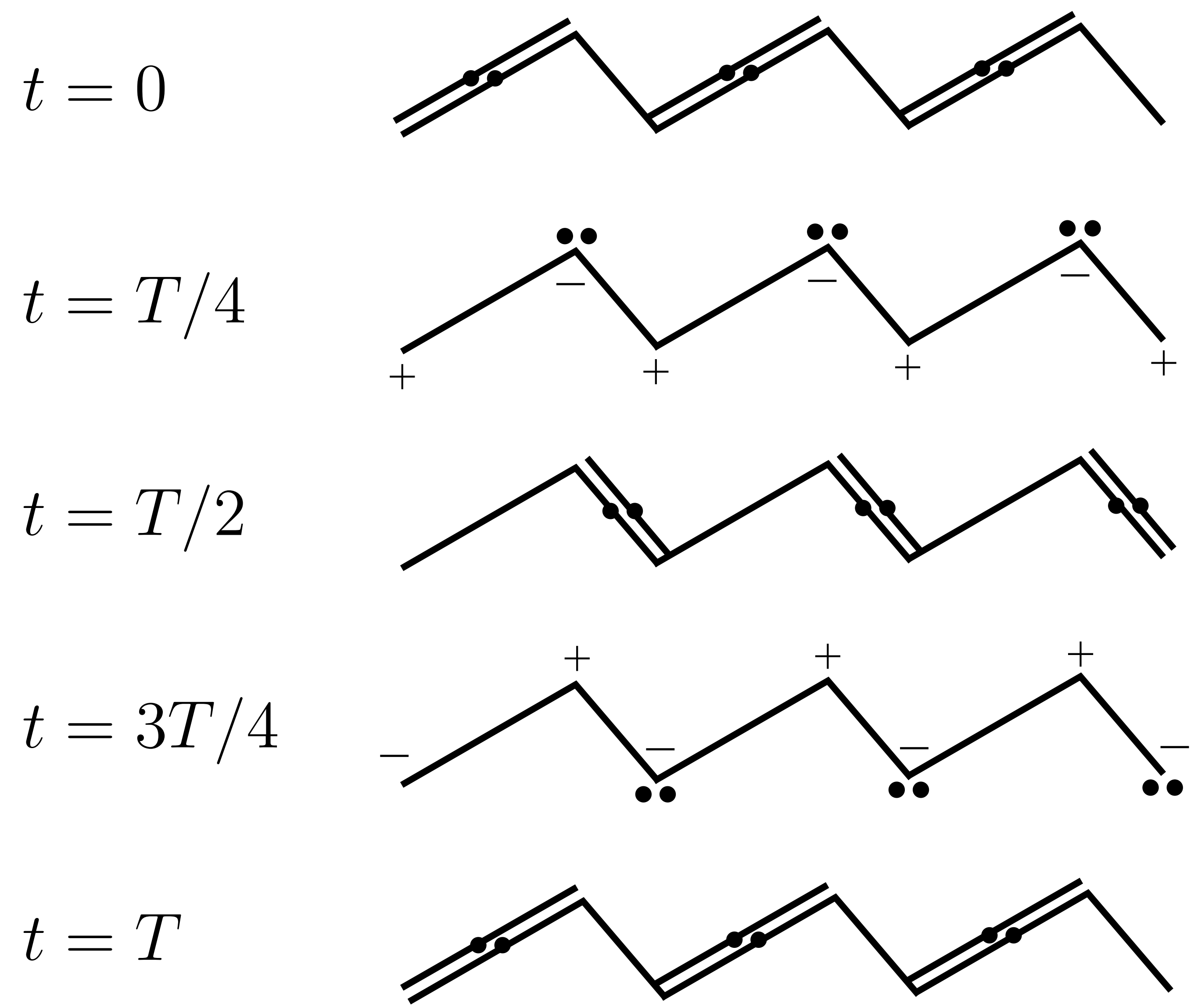
$$Q = 2e \to Q = 0e$$

at a critical U_c

For $\Delta_0 = \frac{t_0}{8}$,

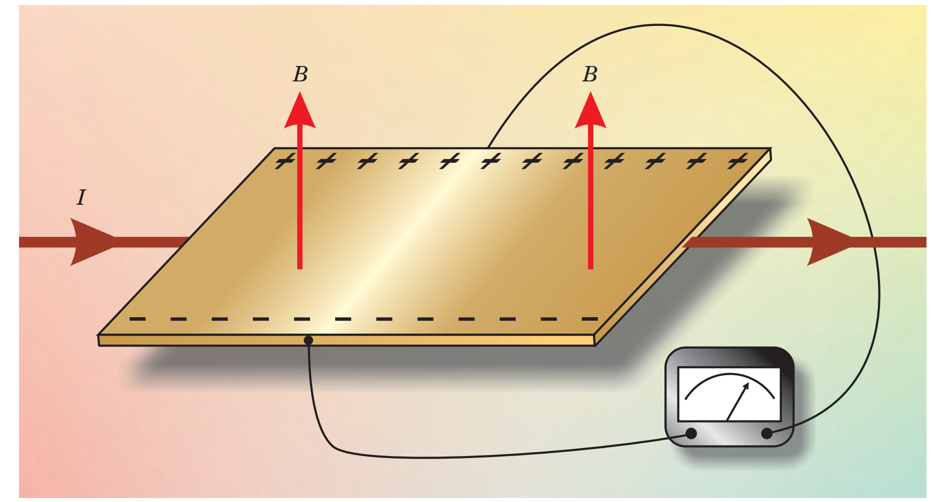
$$\boxed{U_c/t_0 = 0.630 \pm 0.001}$$



RR & Gross, arxiv:1709.03372

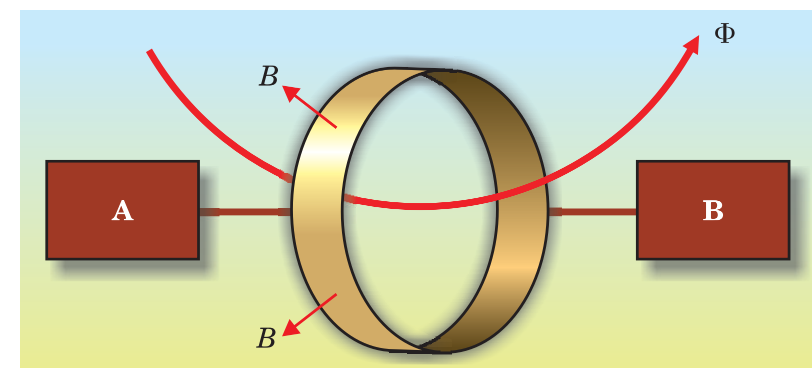
Two-dimensional topological insulators

Integer quantum Hall effect



$$\sigma_H = \frac{e^2}{h}\frac{1}{4\pi i}\int_{BZ} d^2k \sum_n^{\text{occ}} \left[\left\langle \frac{\partial u_n}{\partial k_1} \middle| \frac{\partial u_n}{\partial k_2} \right\rangle - \left\langle \frac{\partial u_n}{\partial k_2} \middle| \frac{\partial u_n}{\partial k_1} \right\rangle \right]$$

$$= \frac{e^2}{h} C \qquad C = \textbf{TKNN integer (Chern number)}$$



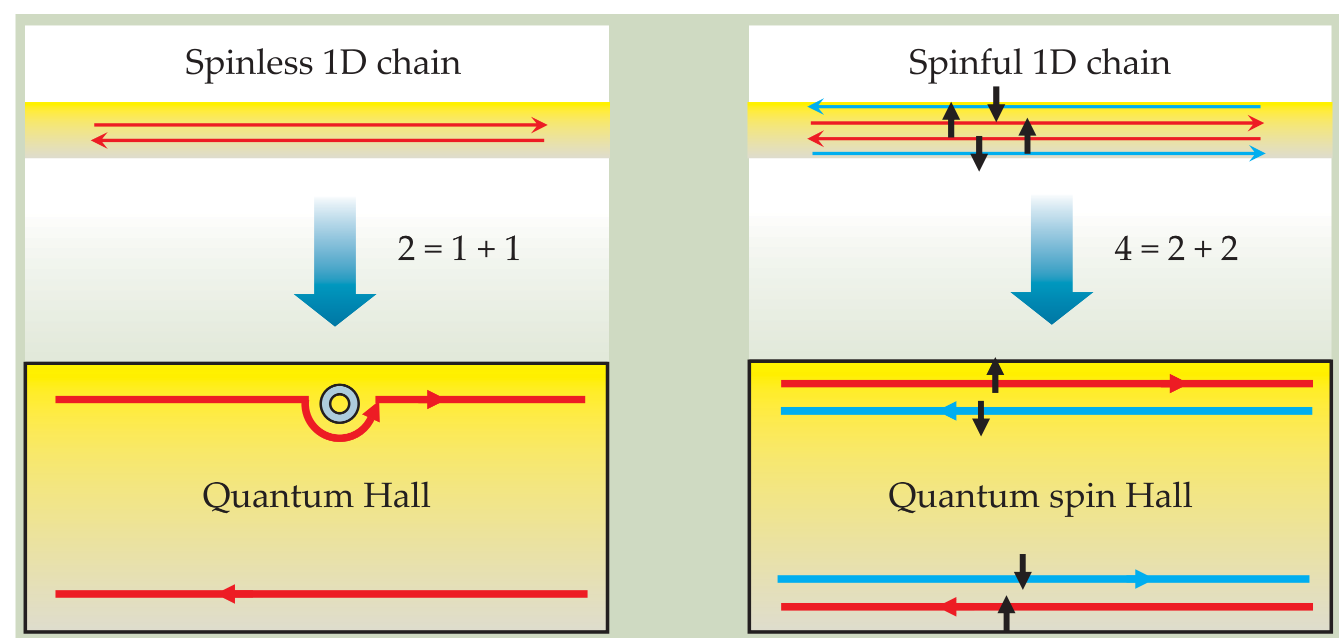
Thouless Kohmoto Nightingale den Nijs 1982; Avron Seiler Simon 1983; Niu Thouless Wu 1985; Avron Osadchy Seiler 2003.

Quantum spin Hall effect

$$I = \frac{1}{2\pi i}\oint_C d\mathbf{k}\cdot\nabla_{\mathbf{k}} \log[P(\mathbf{k}) + i\delta]$$

$$P(\mathbf{k}) = \mathrm{Pf}[\langle u_i(\mathbf{k})|\hat{\Theta}|u_j(\mathbf{k})\rangle]$$

Time-reversal op $\hat{\Theta}|u\rangle = i(\hat{I}\otimes\hat{s}^y)|u\rangle^*$



Kane Mele 2005

Qi Zhang, Physics Today 2010

Two-dimensional topological insulators

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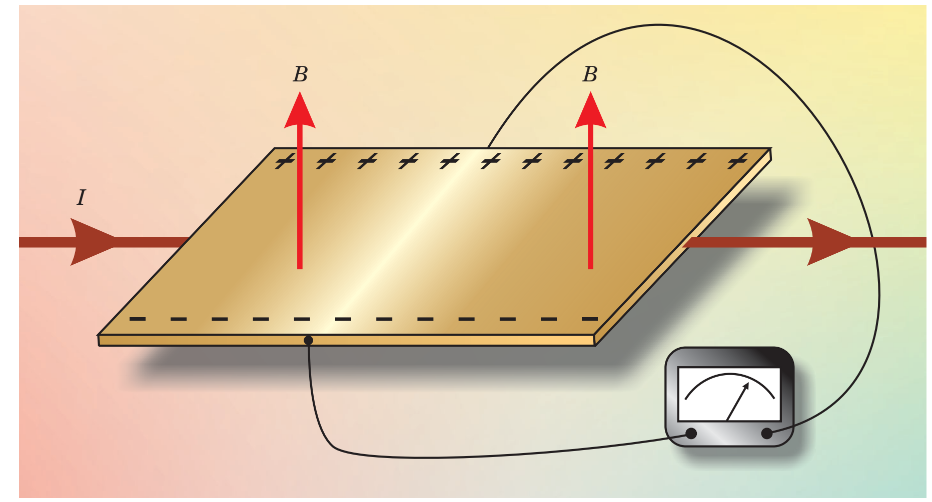
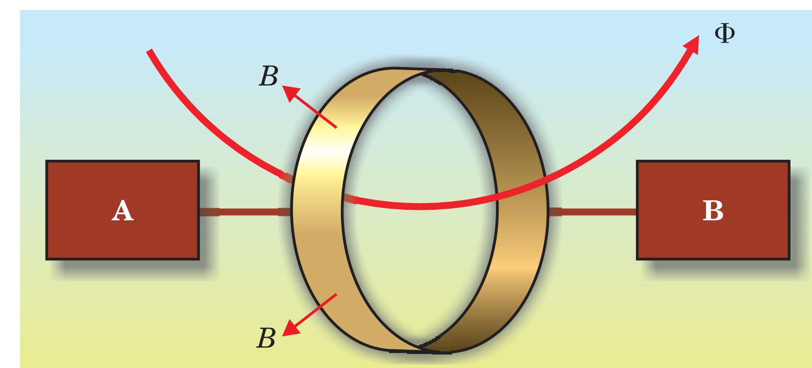
$$= \frac{e^2}{h} C \qquad\qquad C = \textbf{TKNN integer (Chern number)}$$





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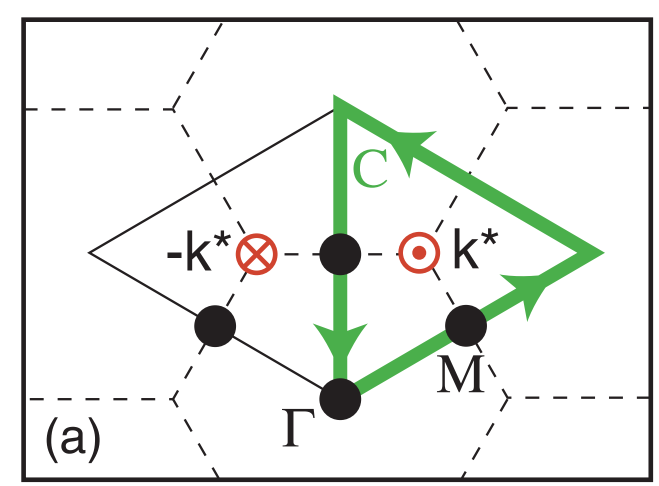

Kane Mele 2005

Qi Zhang, Physics Today 2010

Summary

- One-dimensional systems present several topological invariants
- Examples demonstrate the connections between Berry curvature, symmetry and topological invariants
- Bulk-boundary correspondence: Bulk topological invariants are connected to properties at the boundary
- Many-body interactions can induce transitions between distinct topological phases