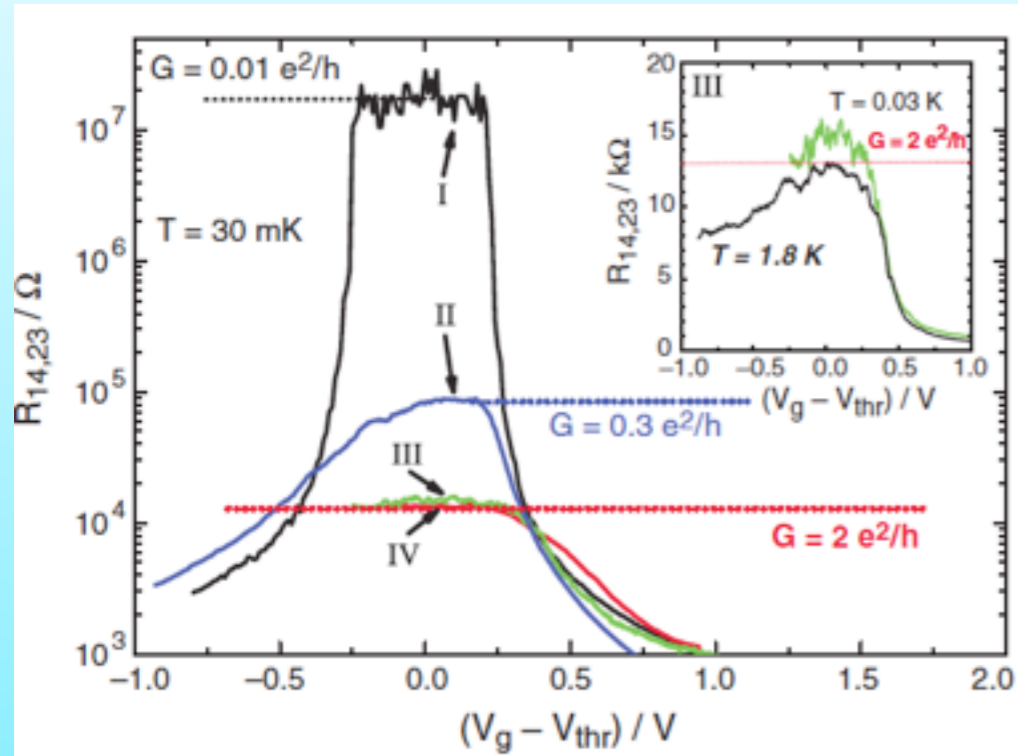


# Topological Insulator

**Topological insulator** : Quantum Spin Hall state



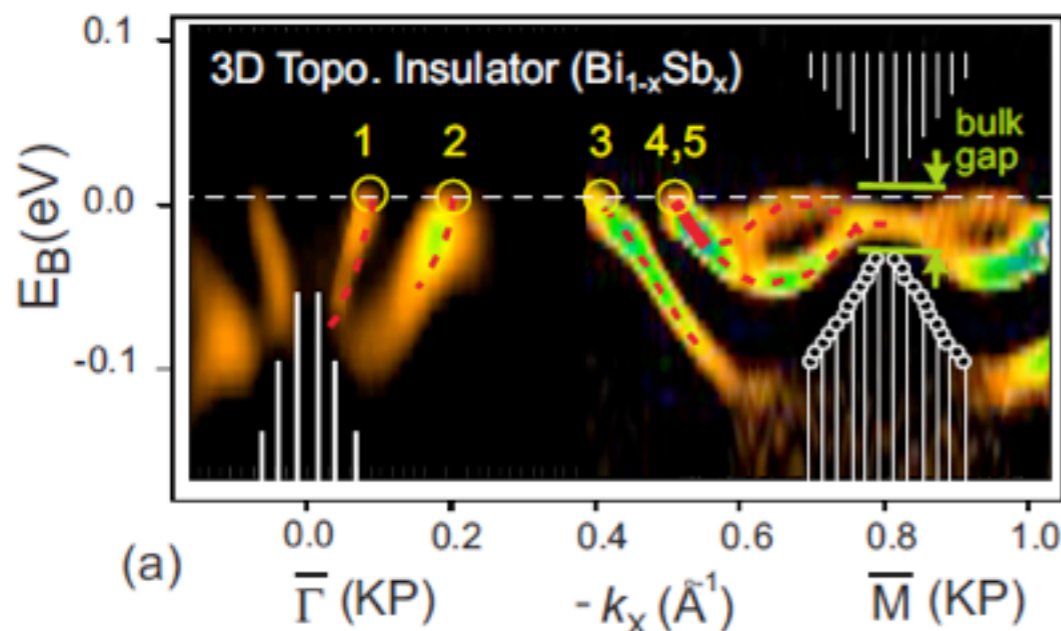
## Quantum Spin Hall Insulator State in HgTe Quantum Wells

Markus König,<sup>1</sup> Steffen Wiedmann,<sup>1</sup> Christoph Brüne,<sup>1</sup> Andreas Roth,<sup>1</sup> Hartmut Buhmann,<sup>1</sup> Laurens W. Molenkamp,<sup>1\*</sup> Xiao-Liang Qi,<sup>2</sup> Shou-Cheng Zhang<sup>2</sup>

*Science* **318**, 766 (2007)

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TOPOLOGICAL INSULATORS 378 NATURE PHYSICS | VOL 5 | JUNE 2009 |

## The next generation

Spin-orbit coupling in some materials leads to the formation of surface states that are immune to backscattering. Theory and experiments have found an important new family of such materials.

Joel Moore

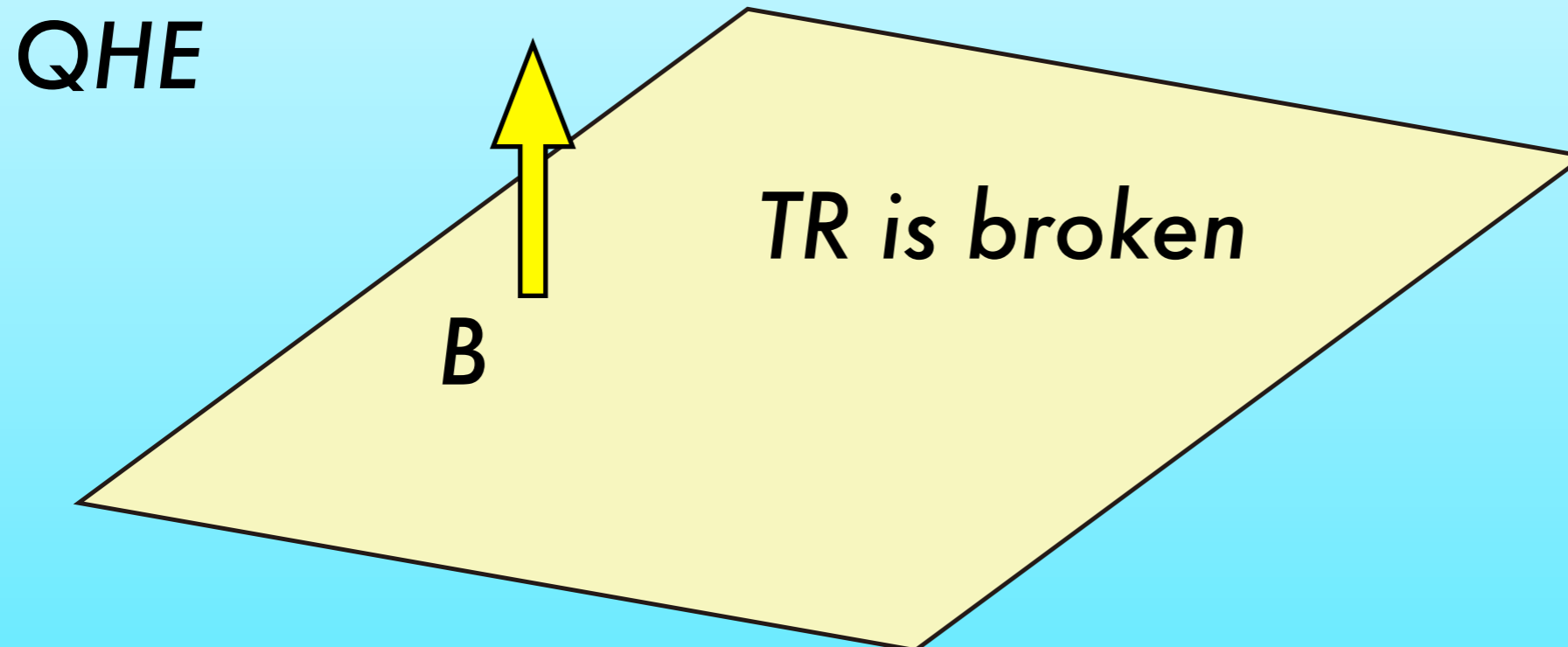
3D

Hsieh, D., D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava, and M. Z. Hasan, 2008, *Nature (London)* **452**, 970.

# "Quantum" *Spin* Hall Effect

= Quantum Hall Effect *without magnetic field*

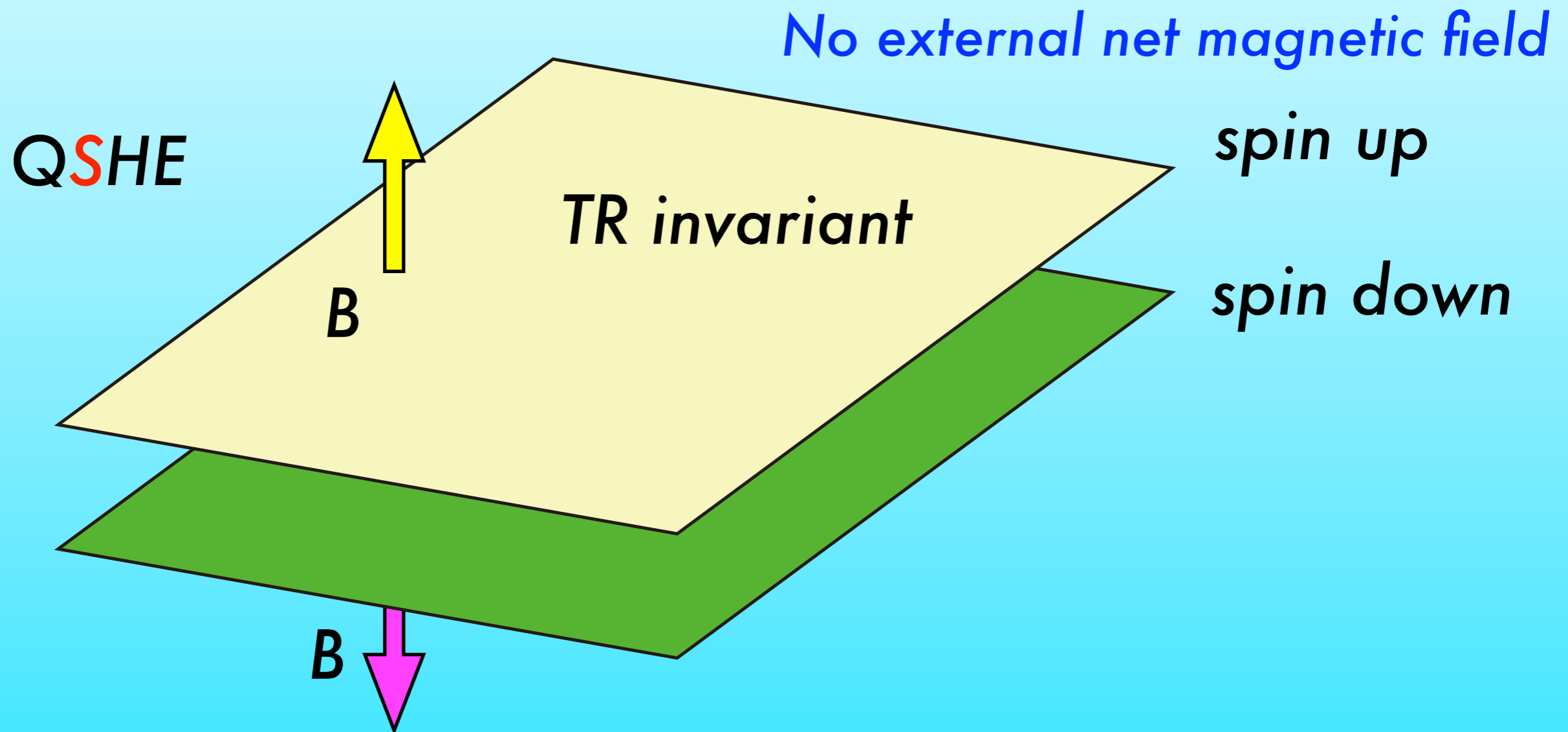
= Quantum Hall Effect *with time-reversal invariance*



# "Quantum" Spin Hall Effect

= Quantum Hall Effect *without magnetic field*

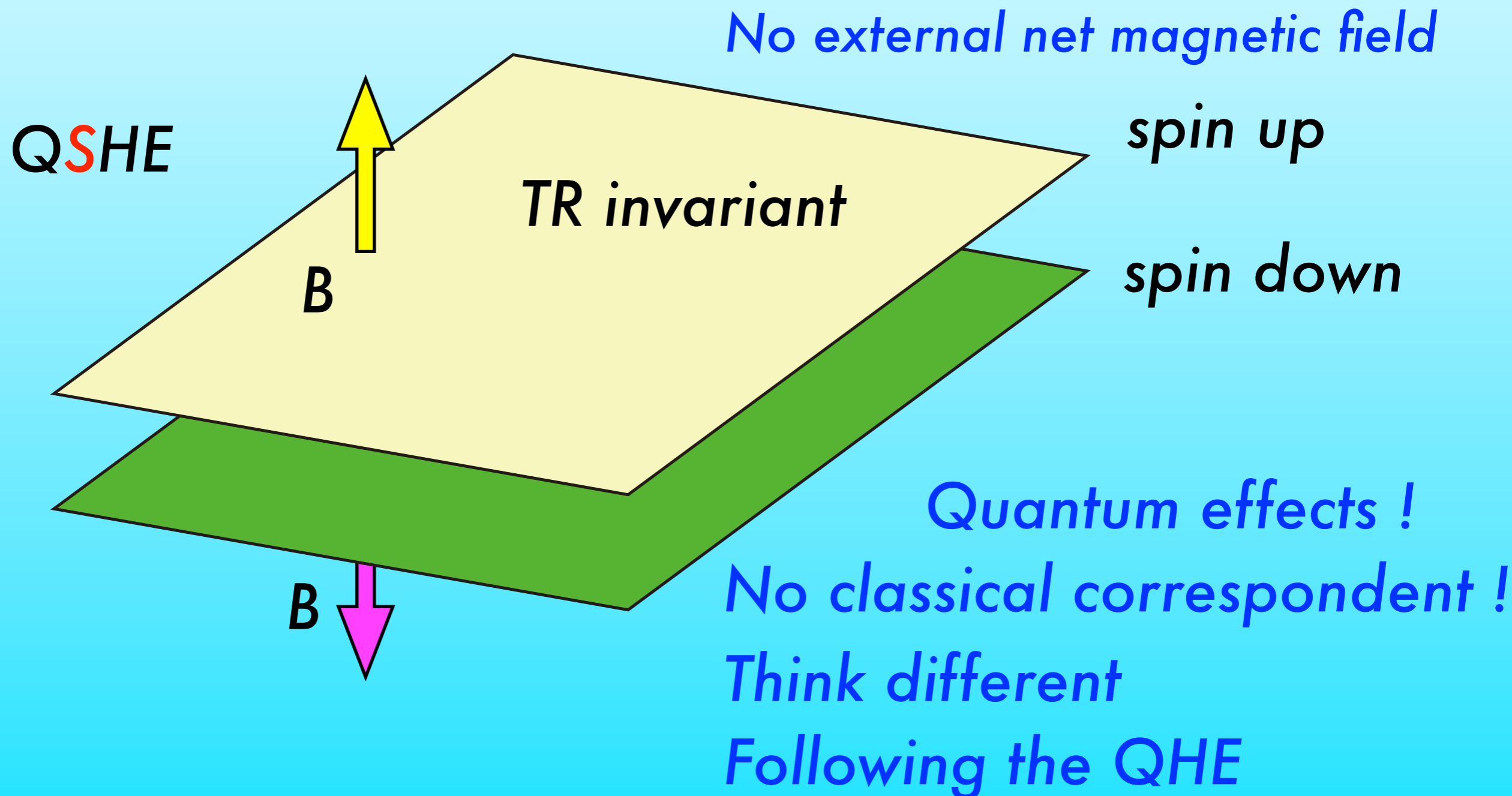
= Quantum Hall Effect *with time-reversal invariance*



# "Quantum" Spin Hall Effect

= Quantum Hall Effect *without magnetic field*

= Quantum Hall Effect *with time-reversal invariance*



so-called **Topological Insulator**

**Topological insulator** : Quantum Spin Hall state

*Need to understand !*

**Time Reversal**

**Kramers  
degeneracy**

*Let me explain !*

*Spin Hall conductance is not quantized*

*Spin is not conserved (spin-orbit)*

# Time-Reversal (TR) symmetry & Kramers degeneracy

**TR: Anti-Unitary  $\Theta$**  :  $c_i = \begin{bmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{bmatrix} \rightarrow \begin{bmatrix} c_{i\downarrow} \\ -c_{i\uparrow} \end{bmatrix} = J c_i$

$$\mathcal{H} = c_i^\dagger H_{ij} c_j$$

& complex conjugate

$$J = i\sigma_y = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

**TR invariance**

$$[\Theta, \mathcal{H}] = 0$$

$$\xrightarrow{J} J H^* J^{-1} = H \quad \{H\}_{ij} = H_{ij}$$

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix}^* \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} c^* & d^* \\ -a^* & -b^* \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} d^* & -c^* \\ -b^* & a^* \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$a = d^*, \quad b = -c^*$$

$$H = \begin{bmatrix} t & \Delta \\ -\Delta^* & t^* \end{bmatrix}$$

$t$  : Spin independent hopping

$\Delta$  : Spin-orbit, Rashba term, etc.

# Time-Reversal (TR) symmetry & Kramers degeneracy

**TR: Anti-Unitary  $\Theta$**  :  $c_i = \begin{bmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{bmatrix} \rightarrow \begin{bmatrix} c_{i\downarrow} \\ -c_{i\uparrow} \end{bmatrix} = J c_i$

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**TR invariance**  
 $[\Theta, \mathcal{H}] = 0$

$\rightarrow J H^* J^{-1} = H \quad \{H\}_{ij} = H_{ij}$

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix}^* \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

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$$a = d^*, \quad b = -c^*$$

$$H = \begin{bmatrix} t & \Delta \\ -\Delta^* & t^* \end{bmatrix}$$

**& hermiticity**  $t^\dagger = t$  **hermite**  
 $\Delta^\dagger = -\Delta^* \rightarrow \tilde{\Delta} = -\Delta$  **anti-symmetric**

# Time-Reversal (TR) symmetry & Kramers degeneracy

## Schrödinger Equation

$$\begin{bmatrix} t & \Delta \\ -\Delta^* & t^* \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = E \begin{bmatrix} u \\ v \end{bmatrix}$$



$$\begin{array}{l} tu + \Delta v = Eu \\ -\Delta^* u + t^* v = Ev \end{array} \begin{array}{c} \nearrow \\ \searrow \end{array} \begin{array}{l} tv^* + \Delta(-u^*) = Ev^* \\ -\Delta^* v^* + t^*(-u^*) = E(-u^*) \end{array}$$



# Time-Reversal (TR) symmetry & Kramers degeneracy

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**Ah !**

$$H \begin{bmatrix} v^* \\ -u^* \end{bmatrix} = E \begin{bmatrix} v^* \\ -u^* \end{bmatrix}, \quad \begin{bmatrix} v^* \\ -u^* \end{bmatrix} \text{ is also an eigen state with the same energy}$$

$$\rightarrow \begin{bmatrix} u_{\Theta} \\ v_{\Theta} \end{bmatrix} = \begin{bmatrix} v^* \\ -u^* \end{bmatrix} \quad \& \quad \begin{bmatrix} u \\ v \end{bmatrix} : \text{ the same energy, degenerate ?}$$

# Time-Reversal (TR) symmetry & Kramers degeneracy

## Schrödinger Equation

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**Not yet !**

**the same state ??**

# Time-Reversal (TR) symmetry & Kramers degeneracy

## Schrödinger Equation

$$\begin{bmatrix} t & \Delta \\ -\Delta^* & t^* \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = E \begin{bmatrix} u \\ v \end{bmatrix}$$



$$\begin{array}{l} tu + \Delta v = Eu \\ -\Delta^* u + t^* v = Ev \end{array} \quad \begin{array}{c} \nearrow \\ \searrow \end{array} \quad \begin{array}{l} tv^* + \Delta(-u^*) = Ev^* \\ -\Delta^* v^* + t^*(-u^*) = E(-u^*) \end{array}$$

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**Not yet !**

**OK ! surely different !**

**the same state ??**

**Orthogonal !**

$$\begin{bmatrix} u \\ v \end{bmatrix}^{\dagger} \begin{bmatrix} u_{\Theta} \\ v_{\Theta} \end{bmatrix} = u^* v^* + v^* (-u^*) = 0$$

# Time-Reversal (TR) symmetry & Kramers degeneracy

## Schrödinger Equation

$$\begin{bmatrix} t & \Delta \\ -\Delta^* & t^* \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = E \begin{bmatrix} u \\ v \end{bmatrix}$$

**Kramers degeneracy**

Any one particle state is doubly degenerate

$$\begin{array}{l} tu + \Delta v = Eu \\ -\Delta^* u + t^* v = Ev \end{array} \quad \begin{array}{l} \nearrow \\ \searrow \end{array} \quad \begin{array}{l} tv^* + \Delta(-u^*) = Ev^* \\ -\Delta^* v^* + t^*(-u^*) = E(-u^*) \end{array}$$

**Ah !**

$$H \begin{bmatrix} v^* \\ -u^* \end{bmatrix} = E \begin{bmatrix} v^* \\ -u^* \end{bmatrix}, \quad \begin{bmatrix} v^* \\ -u^* \end{bmatrix} \text{ is also an eigen state with the same energy}$$

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**Not yet !**

**OK ! surely different !**

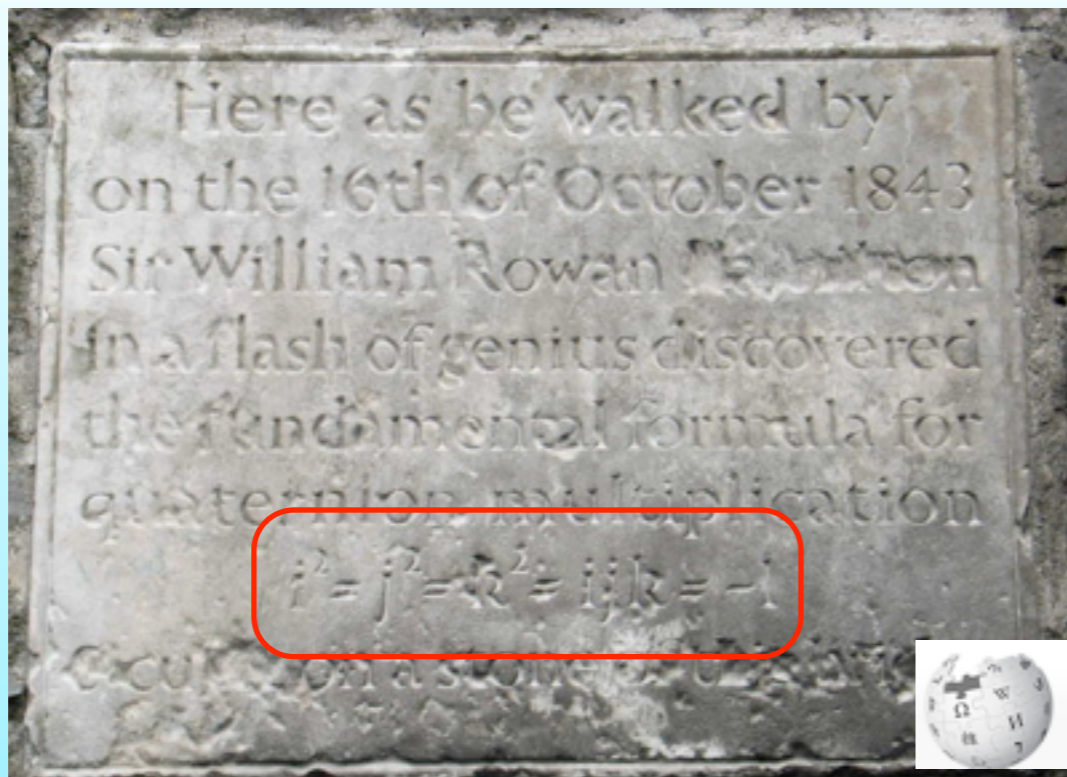
the same state ??

**Orthogonal !**

$$\begin{bmatrix} u \\ v \end{bmatrix}^{\dagger} \begin{bmatrix} u_{\Theta} \\ v_{\Theta} \end{bmatrix} = u^* v^* + v^* (-u^*) = 0$$

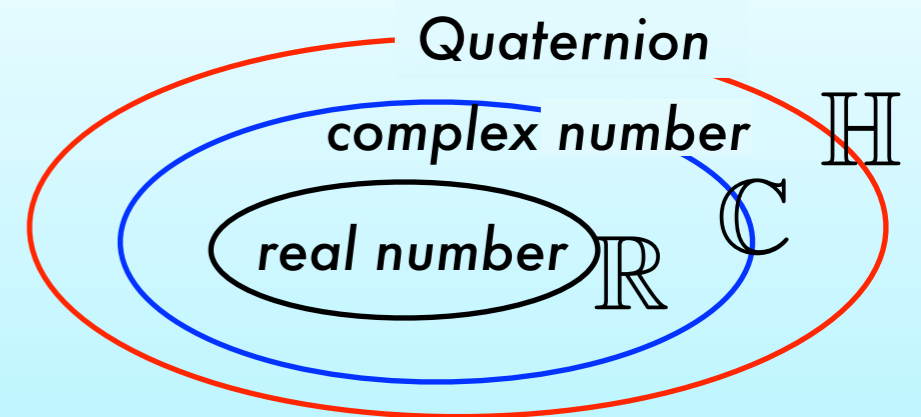
# Time Reversal & Quaternions

Classical to Quantum



Hamilton 四元数発見の碑

F.J.Dyson '61-



No magic, neither crazy  
just Pauli matrices

$$H = \begin{bmatrix} t & \Delta \\ -\Delta^* & t^* \end{bmatrix} = (\text{Re}t)I_2 + (\text{Im}t)i\sigma_z + (\text{Re}\Delta)i\sigma_y + (\text{Im}\Delta)i\sigma_x$$

$$\cong (\text{Re}t)1 + (\text{Im}t)i_{\mathbb{H}} + (\text{Re}\Delta)j_{\mathbb{H}} + (\text{Im}\Delta)k_{\mathbb{H}}$$

: Quaternion (四元数)

$$i_{\mathbb{H}} \cong i\sigma_z, j_{\mathbb{H}} \cong i\sigma_y, k_{\mathbb{H}} \cong i\sigma_x$$

$$i_{\mathbb{H}}^2 = j_{\mathbb{H}}^2 = k_{\mathbb{H}}^2 = i_{\mathbb{H}}j_{\mathbb{H}}k_{\mathbb{H}} = -1$$

Quaternion 2x2 Matrix, Yang Monopole & quantization: YH, NJP12, 065004 (2010)

# Time-Reversal, Spins & Spinors

$$\hat{S}^{\text{spin}} = \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} = \mathbf{c}^\dagger \mathbf{S} \mathbf{c}, \quad \mathbf{S} = \frac{\boldsymbol{\sigma}}{2}, \quad \mathbf{c}^{\text{spinor}} = \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

$$\Theta \hat{S} \Theta^{-1} = \mathbf{c}^\dagger \mathbf{S}^\Theta \mathbf{c} \qquad \Theta \mathbf{c} \Theta^{-1} = \mathbf{J} \mathbf{c}$$

$$\mathbf{S}^\Theta = \mathbf{J} \mathbf{S}^* \mathbf{J}^{-1}$$

$$\sigma_x^\Theta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^* \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -\sigma_x$$

$$\sigma_y^\Theta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}^* \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & -i \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -\sigma_y$$

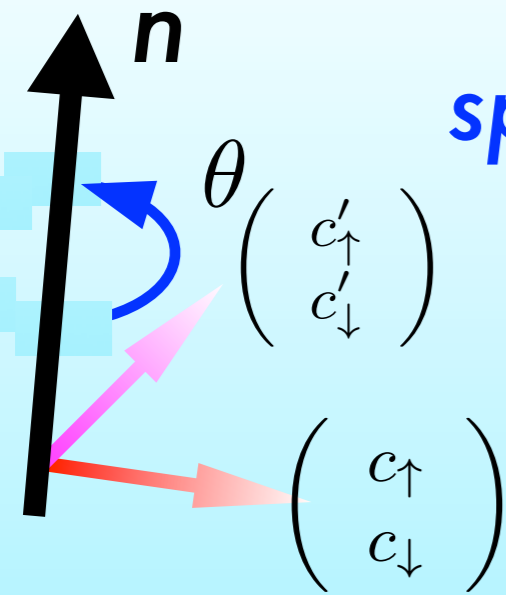
$$\sigma_z^\Theta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^* \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -\sigma_z$$

$$\mathbf{S}^\Theta = -\mathbf{S}$$

$$\mathbf{B} \cdot \mathbf{S} \rightarrow -\mathbf{B} \cdot \mathbf{S}$$

Magnetic field  
Zeeman term breaks TR

# Rotation: Spin & Spinor

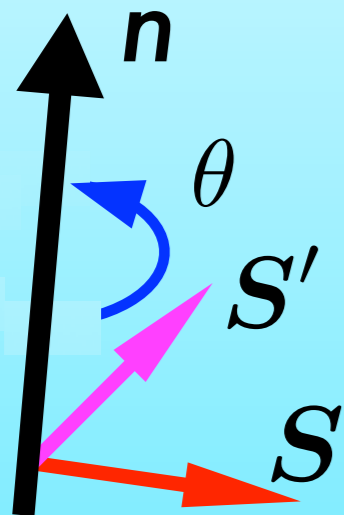


spinor

$$\begin{pmatrix} c'_\uparrow \\ c'_\downarrow \end{pmatrix} = U(\theta) \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} \quad U \in SU(2)$$

$$U(\theta) = e^{-i\mathbf{S} \cdot \mathbf{n} \theta} = \cos \frac{\theta}{2} - i\mathbf{n} \cdot \boldsymbol{\sigma} \sin \frac{\theta}{2}$$

$$\det U = e^{-i(\text{Tr } \mathbf{S}) \cdot \mathbf{n} \theta} = e^0 = 1$$



spin

$$\begin{pmatrix} S'_x \\ S'_y \\ S'_z \end{pmatrix} = U S U^\dagger = \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & Q(\theta) & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$$

$S'$  : hermite  $\text{Tr } S' = \text{Tr } S U^\dagger U = 0$

Expand by Pauli matrices with real coefficients

$$\text{Tr } S'_\alpha S'_\beta = \text{Tr } S_\alpha S_\beta = \frac{1}{2} \delta_{\alpha\beta}$$

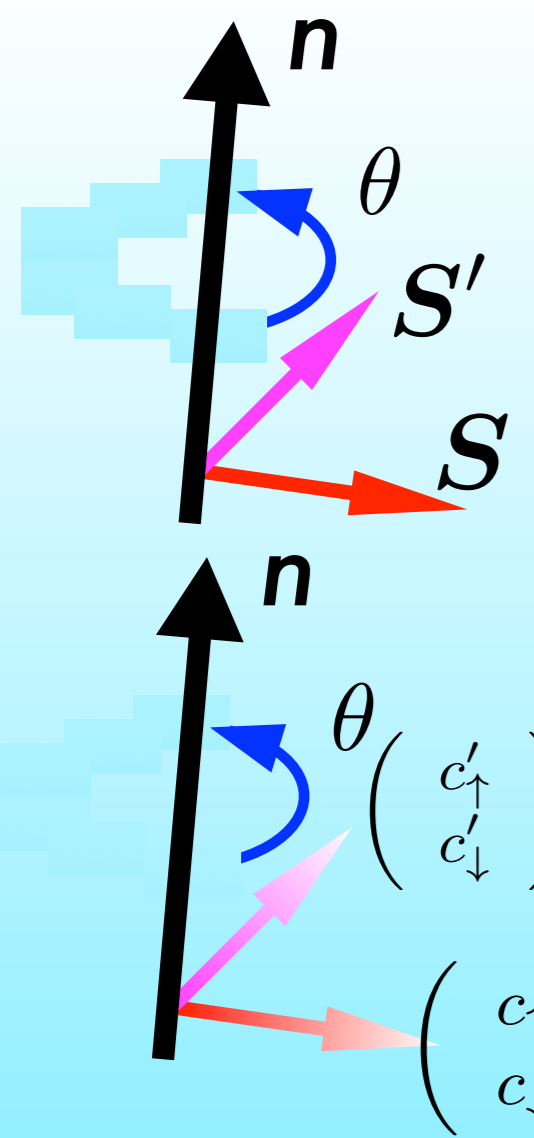
$$\text{Tr } S'_\alpha S'_\beta = Q_{\alpha\alpha'} Q_{\beta\beta'} \text{Tr } S_{\alpha'} S_{\beta'}$$

$$= \frac{1}{2} Q_{\alpha\gamma} Q_{\beta\gamma} = \frac{1}{2} (Q\tilde{Q})_{\alpha\beta}$$

$$Q\tilde{Q} = E_3 \quad Q \in SO(3)$$

continuously connected to  $E_3$

# Rotation: Spin & Spinor



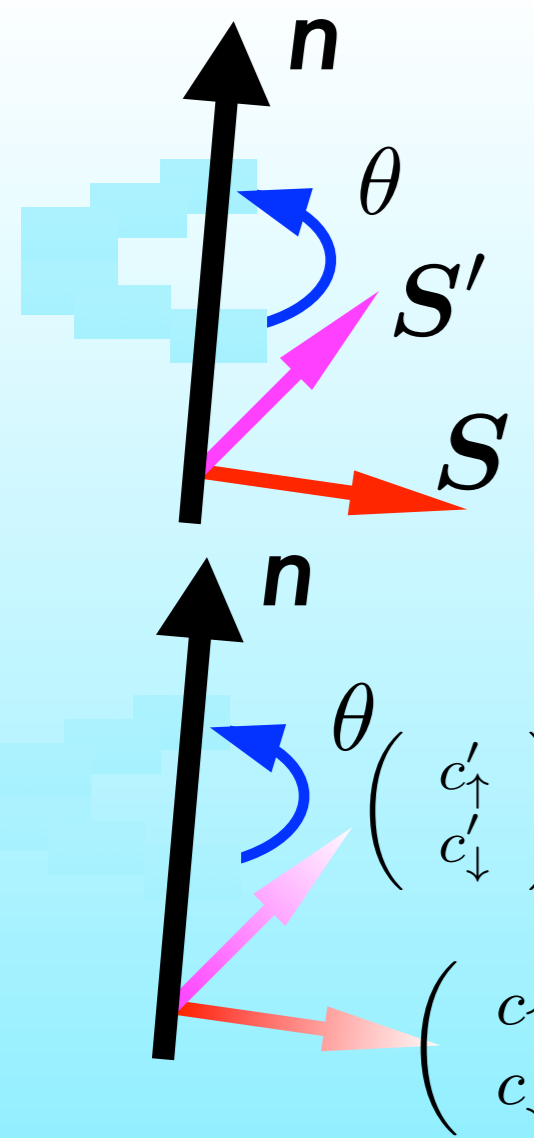
spin  $\begin{pmatrix} S'_x \\ S'_y \\ S'_z \end{pmatrix} = U S U^\dagger = \begin{pmatrix} & & \\ & Q(\theta) & \\ & & \end{pmatrix} \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$

spinor  $\begin{pmatrix} c'_{\uparrow} \\ c'_{\downarrow} \end{pmatrix} = U(\theta) \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix}$

$$U(\theta) = e^{-i\mathbf{S} \cdot \mathbf{n} \theta} = \cos \frac{\theta}{2} - i \mathbf{n} \cdot \boldsymbol{\sigma} \sin \frac{\theta}{2}$$



# Rotation: Spin & Spinor



spin  $\begin{pmatrix} S'_x \\ S'_y \\ S'_z \end{pmatrix} = U S U^\dagger = \begin{pmatrix} Q(\theta) \\ \vdots \\ \vdots \\ \vdots \end{pmatrix} \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$

spinor  $\begin{pmatrix} c'_\uparrow \\ c'_\downarrow \end{pmatrix} = U(\theta) \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$

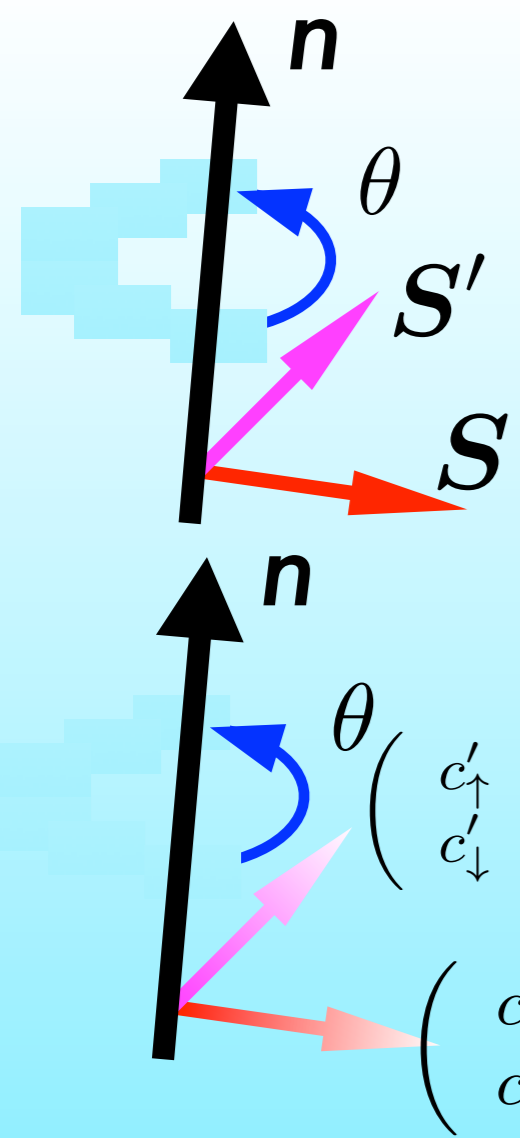
$$U(\theta) = e^{-i\mathbf{S} \cdot \mathbf{n} \theta} = \cos \frac{\theta}{2} - i \mathbf{n} \cdot \boldsymbol{\sigma} \sin \frac{\theta}{2}$$

Spin goes back by  $2\pi$  rotation  
 Spinor does not go

$$Q(\theta + 2\pi) = + Q(\theta)$$

$$U(\theta + 2\pi) = - U(\theta)$$

# Rotation: Spin & Spinor



spin  $\begin{pmatrix} S'_x \\ S'_y \\ S'_z \end{pmatrix} = U S U^\dagger = \begin{pmatrix} Q(\theta) \\ \vdots \\ \vdots \\ \vdots \end{pmatrix} \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$

spinor  $\begin{pmatrix} c'_\uparrow \\ c'_\downarrow \end{pmatrix} = U(\theta) \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$

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Spinor does not go

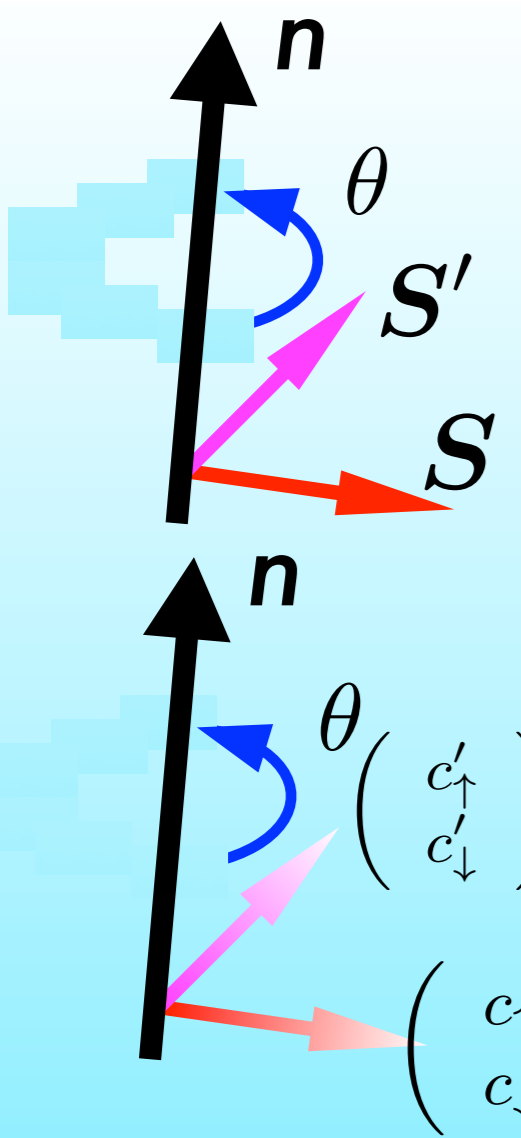
back by  $2\pi$  rotation

$$Q(\theta + 2\pi) = + Q(\theta)$$

$$U(\theta + 2\pi) = - U(\theta)$$

$4\pi$  is always OK :  
continuously deformed  
to 0 rotation c.f. 2D

# Rotation: Spin & Spinor



**spin**  $\begin{pmatrix} S'_x \\ S'_y \\ S'_z \end{pmatrix} = U S U^\dagger = \begin{pmatrix} Q(\theta) \end{pmatrix} \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$

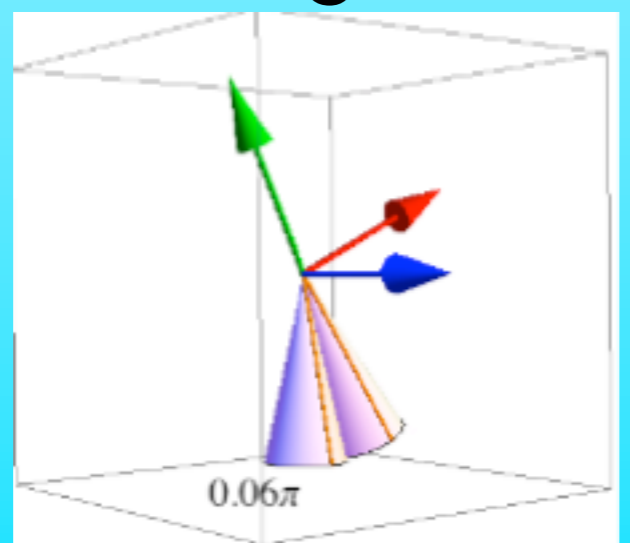
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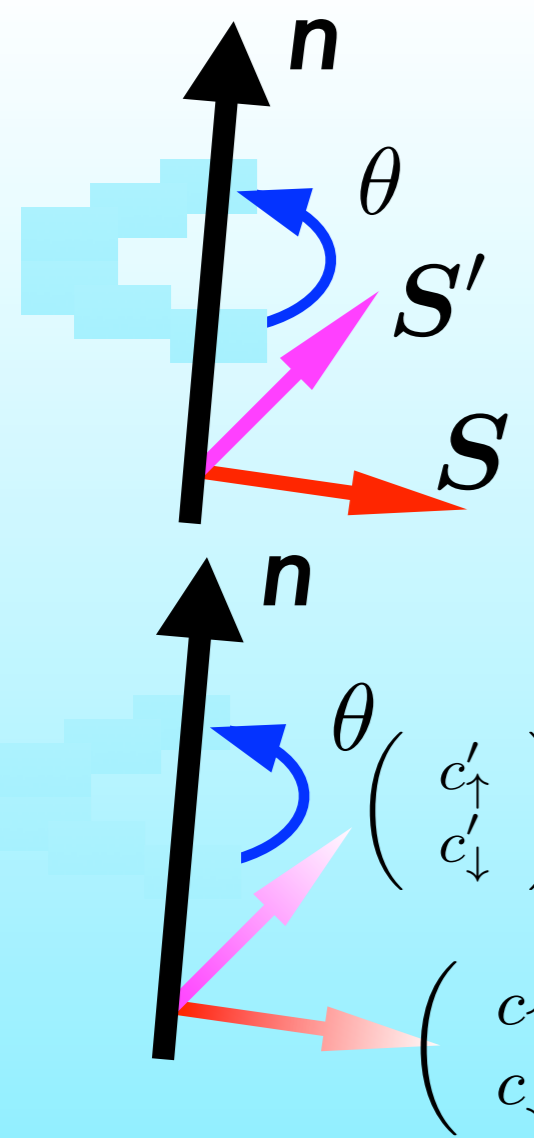
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# Rotation: Spin & Spinor



spin  $\begin{pmatrix} S'_x \\ S'_y \\ S'_z \end{pmatrix} = U S U^\dagger = \begin{pmatrix} Q(\theta) \\ \vdots \\ \vdots \\ \vdots \end{pmatrix} \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$

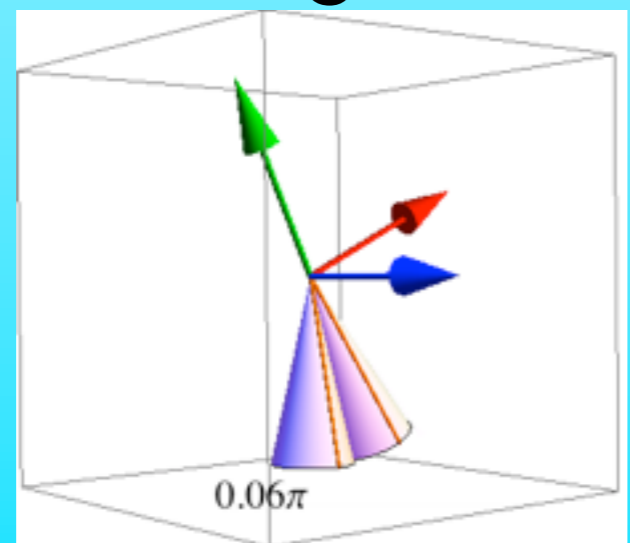
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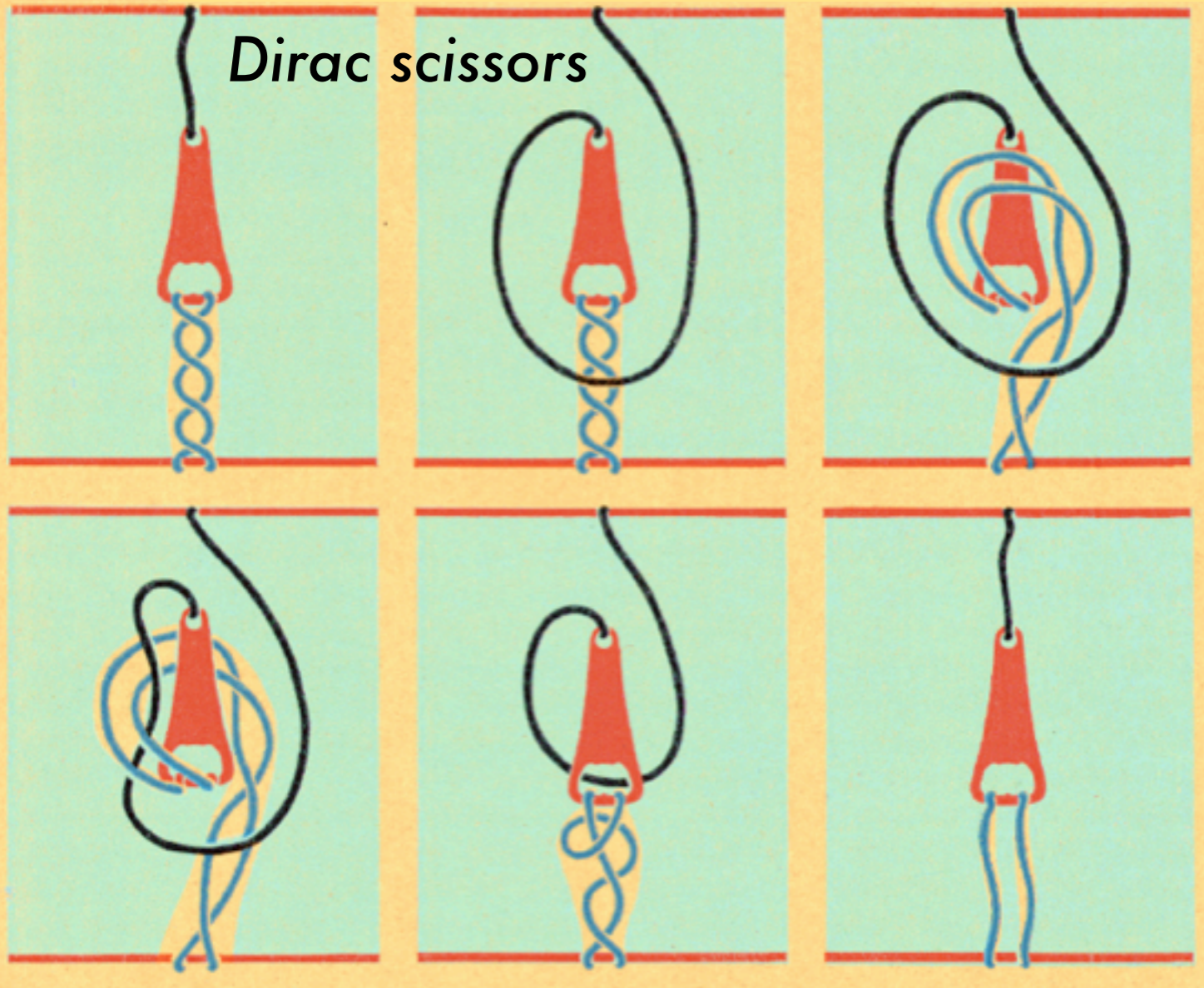
$$Q(\theta + 2\pi) = + Q(\theta)$$

$$U(\theta + 2\pi) = - U(\theta)$$



$4\pi$  is always OK :  
 continuously deformed  
 to 0 rotation c.f. 2D

# & Spinor



$$U^\dagger = \begin{pmatrix} & & \\ & Q(\theta) & \\ & & \end{pmatrix} \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$$

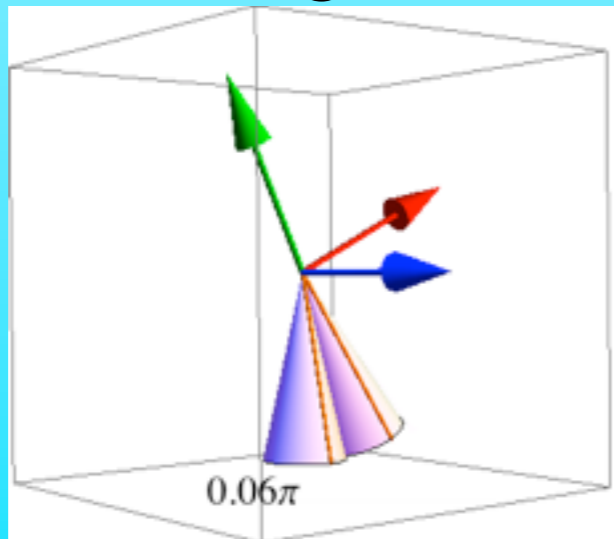
$$\begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

$$U(\theta) = \cos \frac{\theta}{2} - i \mathbf{n} \cdot \boldsymbol{\sigma} \sin \frac{\theta}{2}$$

$$Q(\theta + 2\pi) = + Q(\theta)$$

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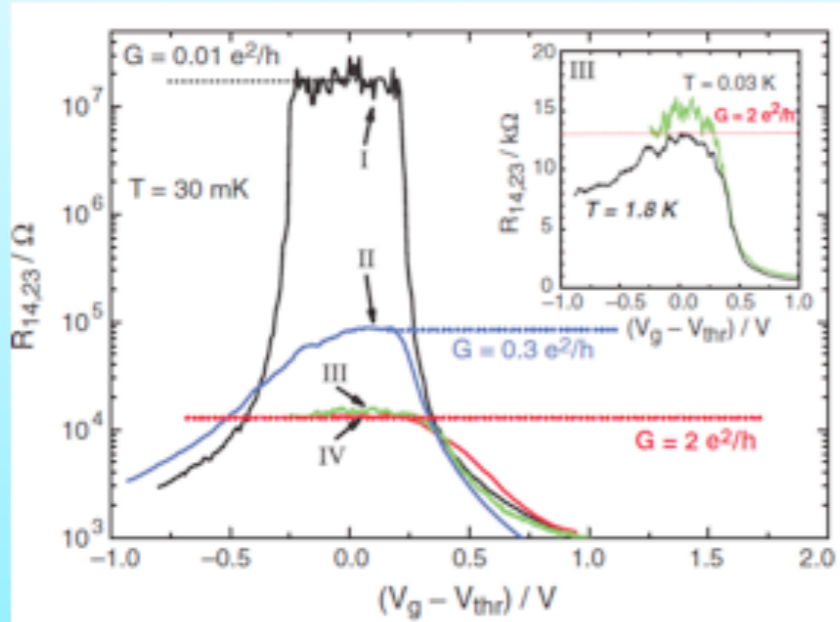
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# Quantum Spin Hall effect ??

*Topological insulator* : Quantum *Spin* Hall state



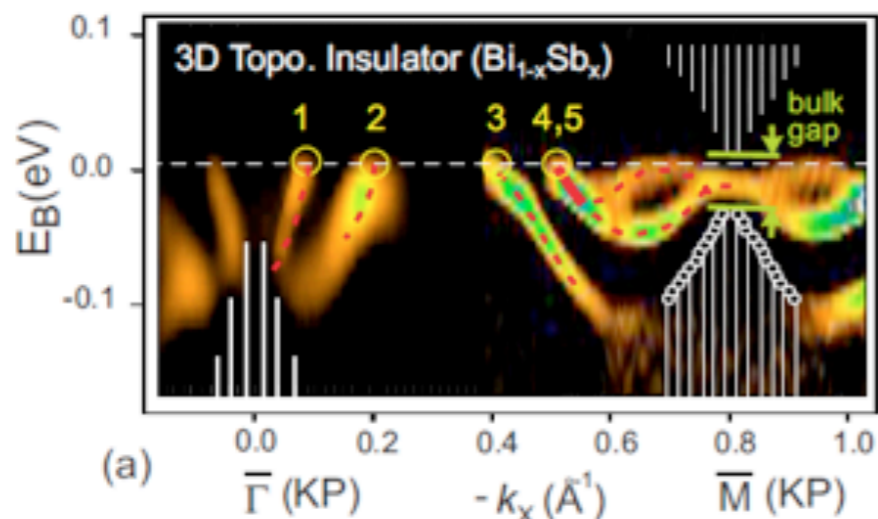
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*Science* **318**, 766 (2007)

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TOPOLOGICAL INSULATORS 378 NATURE PHYSICS | VOL 5 | JUNE 2009

## The next generation

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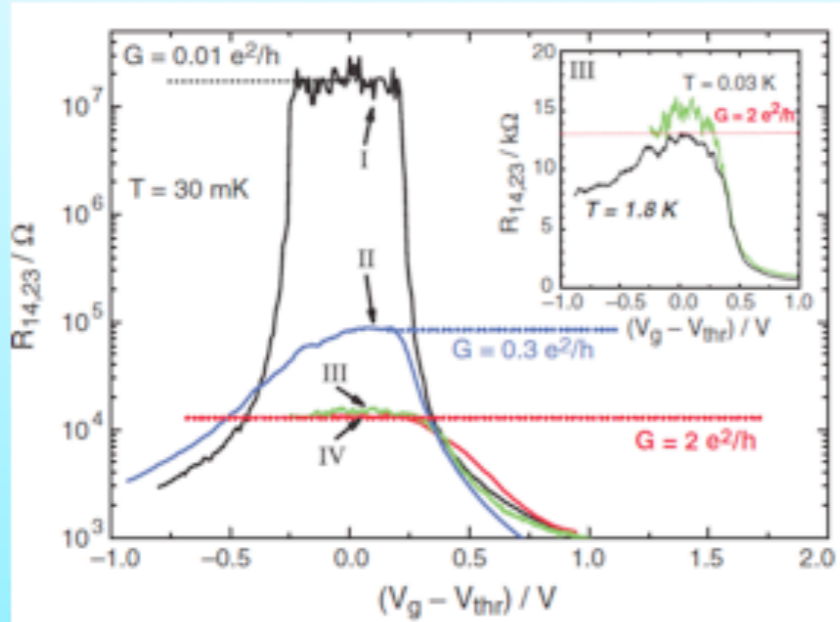
Joel Moore

3D

Hsieh, D., D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava, and M. Z. Hasan, 2008, *Nature (London)* **452**, 970.

# Quantum Spin Hall effect ??

*Topological insulator* : Quantum "Spinor" Hall state



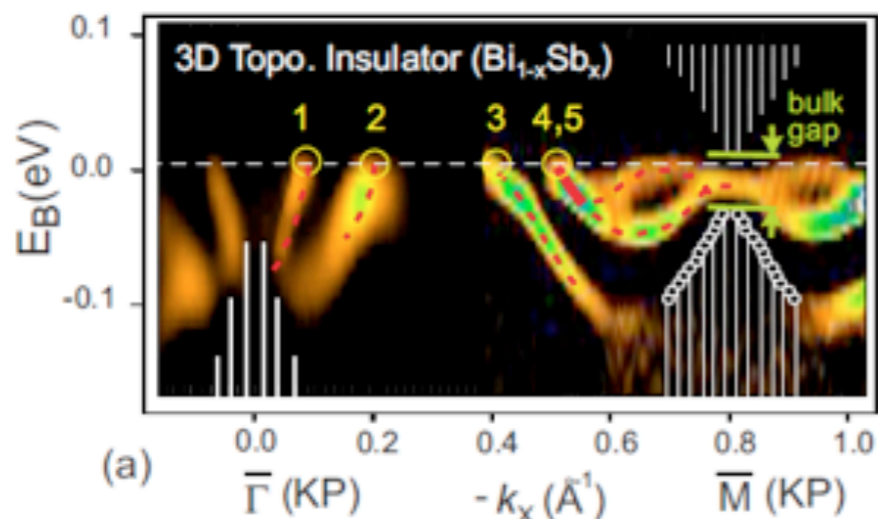
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*Science* **318**, 766 (2007)

2D

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## The next generation

Spin-orbit coupling in some materials leads to the formation of surface states that are immune to backscattering. Theory and experiments have found an important new family of such materials.

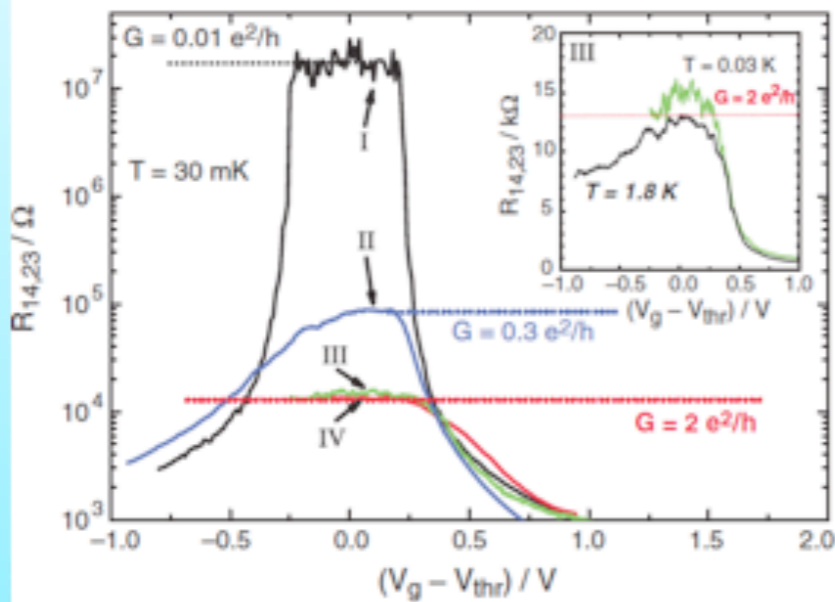
Joel Moore

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Hsieh, D., D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava, and M. Z. Hasan, 2008, *Nature (London)* **452**, 970.

# Quantum Spin Hall effect ??

*Topological insulator* : Quantum "Spinor" Hall state



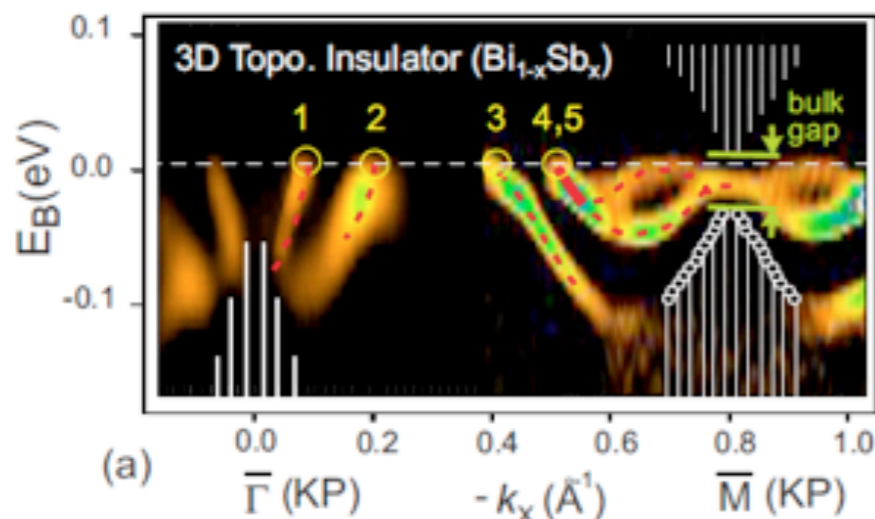
## Quantum Spin Hall Insulator State in HgTe Quantum Wells

Markus König,<sup>1</sup> Steffen Wiedmann,<sup>1</sup> Christoph Brüne,<sup>1</sup> Andreas Roth,<sup>1</sup> Hartmut Buhmann,<sup>1</sup> Laurens W. Molenkamp,<sup>1\*</sup> Xiao-Liang Qi,<sup>2</sup> Shou-Cheng Zhang<sup>2</sup>

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*Purely quantum mechanical !*