DIRAC MATERIALS
IN CONDENSED MATTER

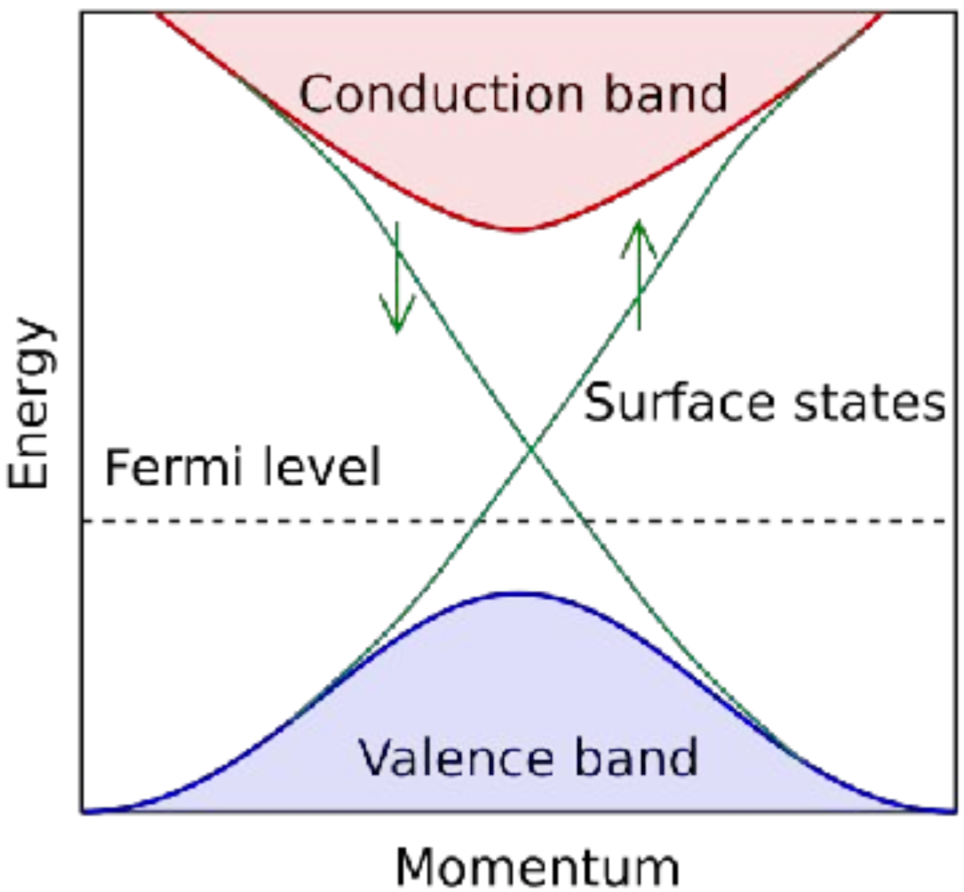
PART I: Dirac equation

Alberto Cortijo

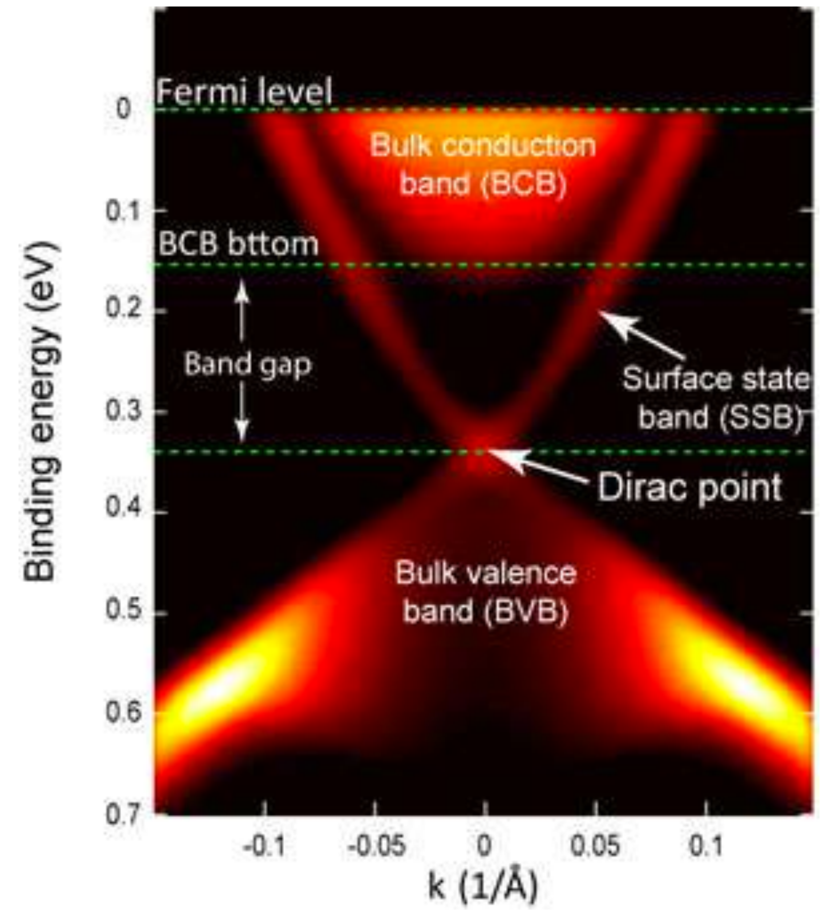
OUTLINE

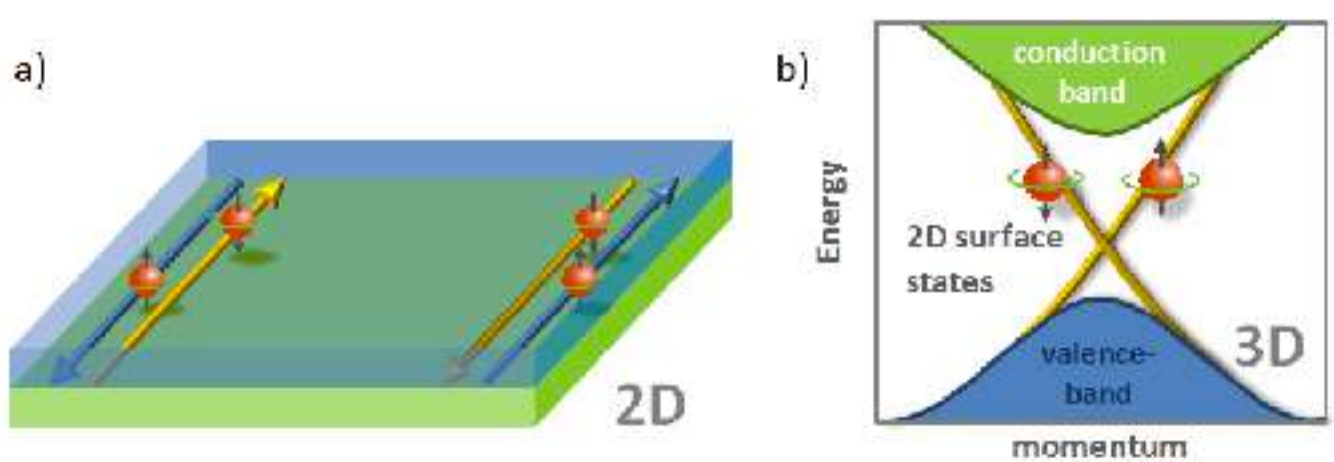
1. The Dirac equation: Origins, definition and the concept of spin.
2. Bloch theorem. Symmetries with and without spin.
3. Dirac equation on a lattice: graphene, Germanene (Kane-Mele model), TMDC, the BHZ model, Bi2Se3…
4. Conclusions to part I

1. The Dirac equation.



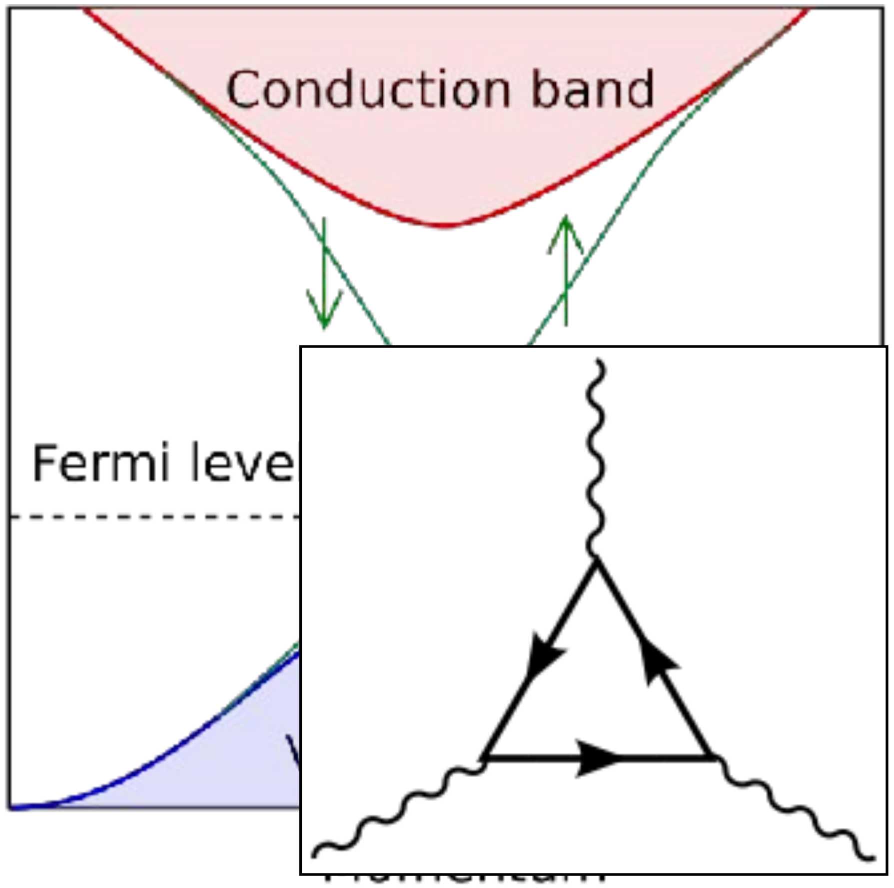
Symmetry Protected Topological Phases



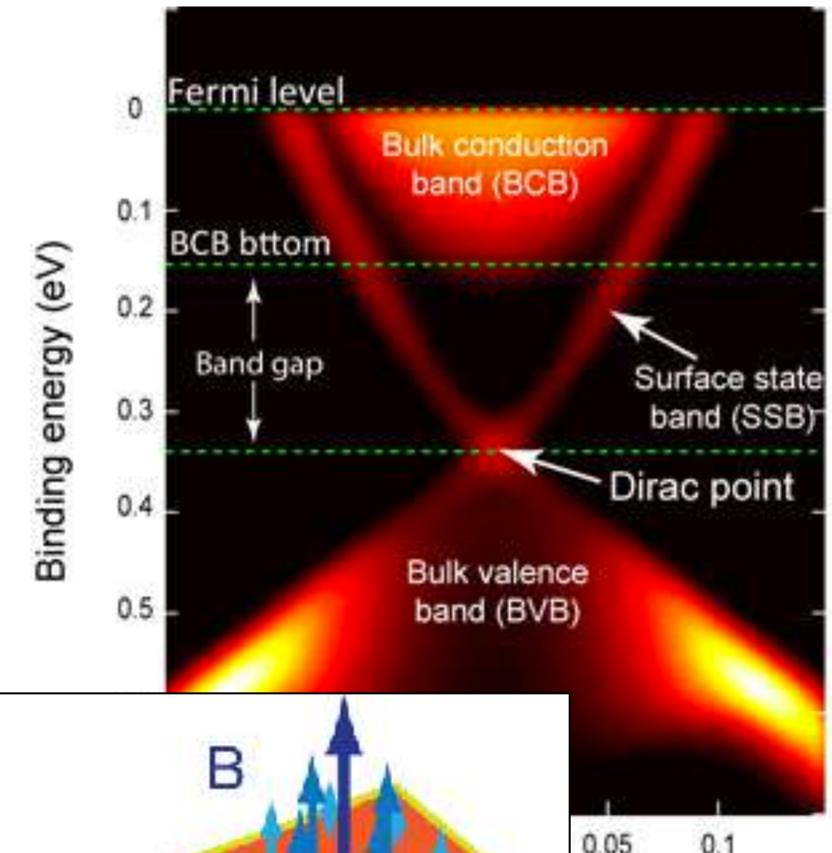


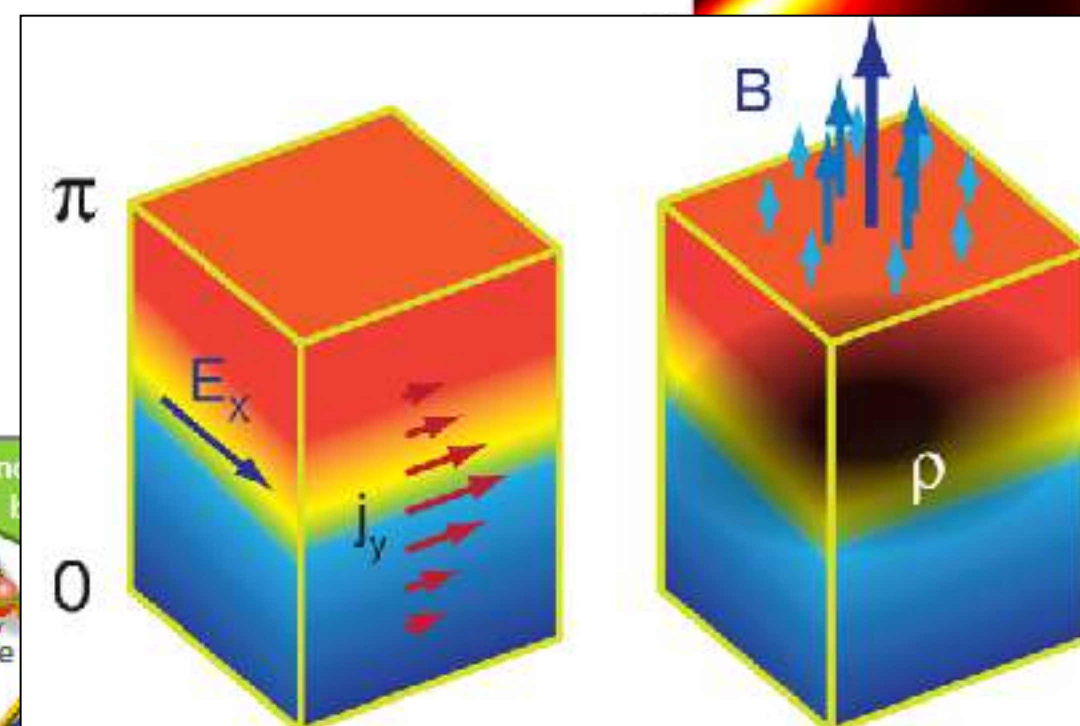
Quantum spin Hall effect

1. The Dirac equation.

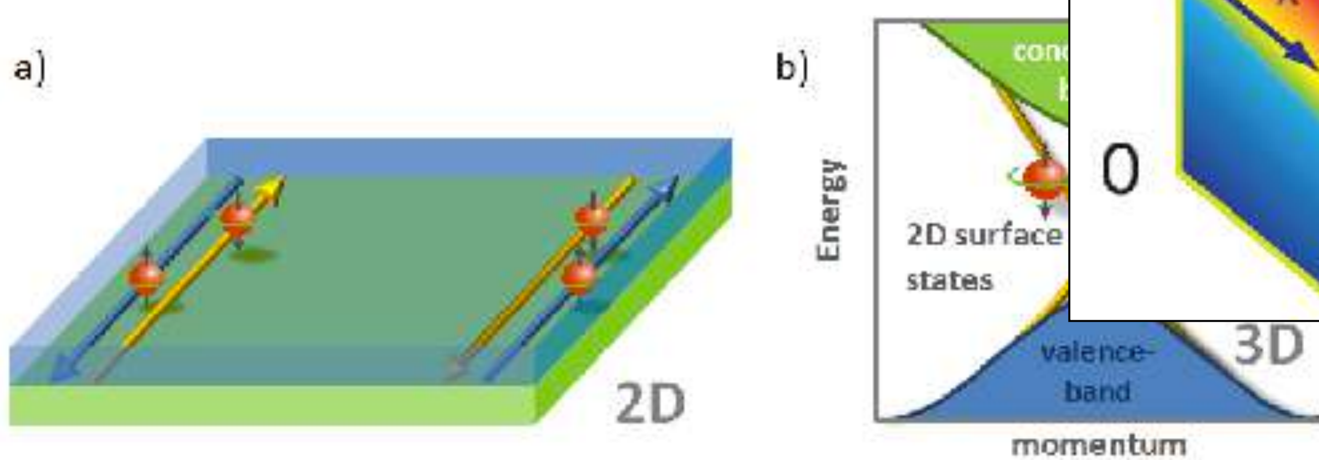


Topological magneto-electric effect

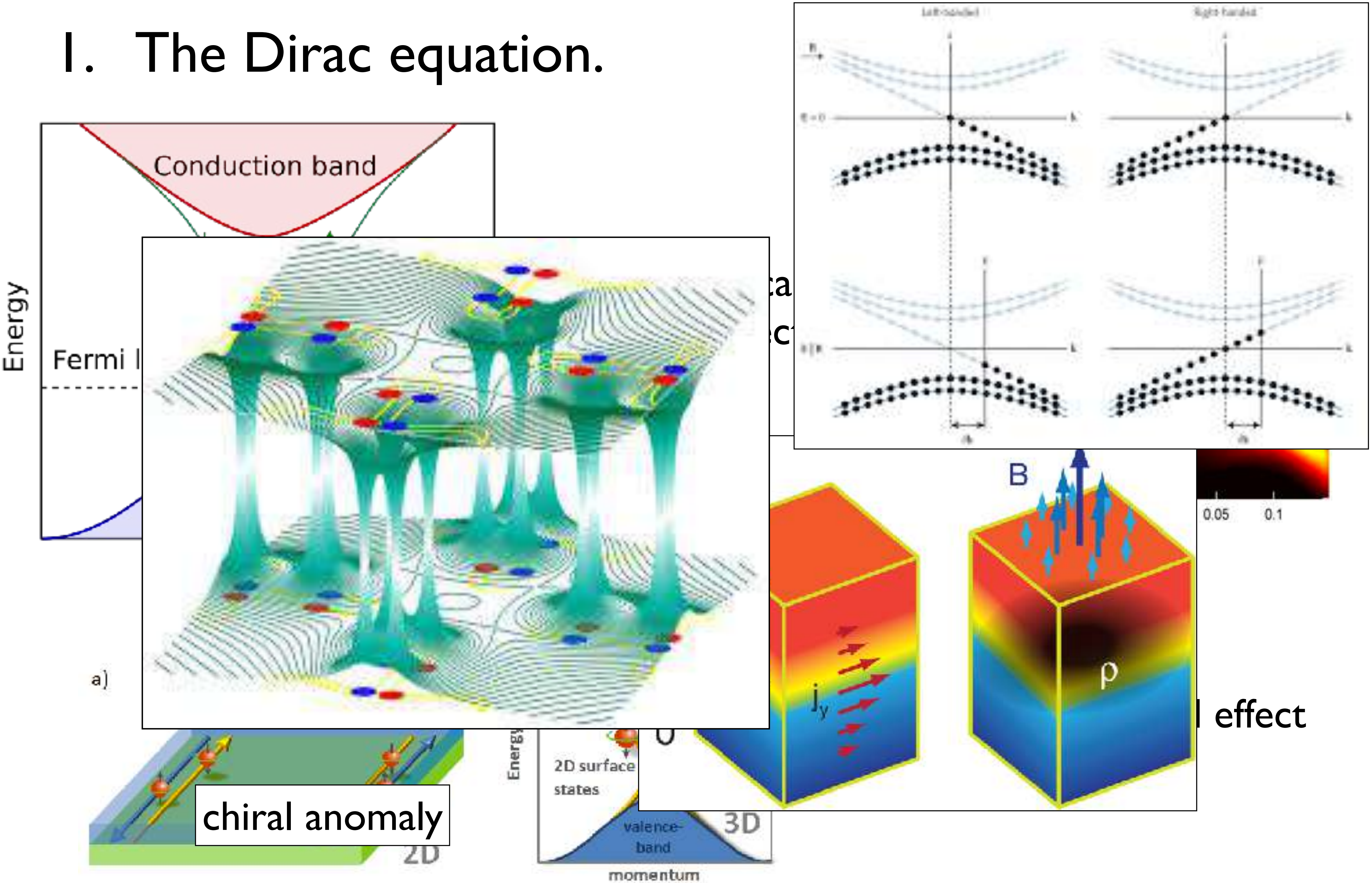




l effect



1. The Dirac equation.



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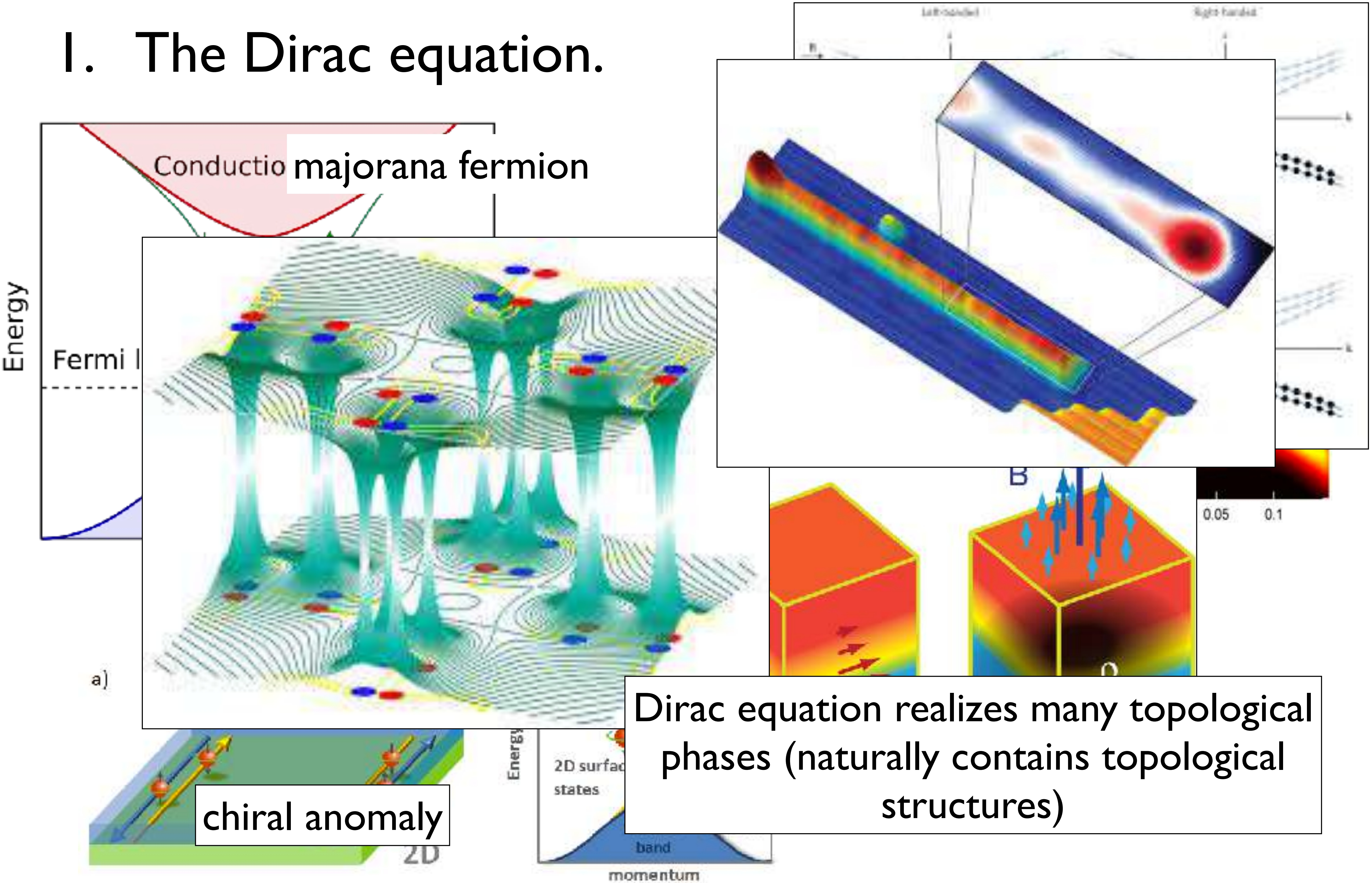


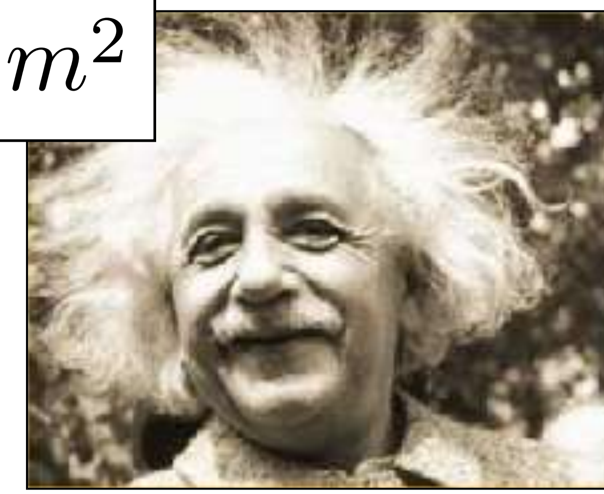
Dirac equation realizes many topological phases (naturally contains topological structures)

1. The Dirac equation.

$$\varepsilon = \frac{\boldsymbol{k}^2}{2m}$$

G Galilei (1564-1642)

$$\varepsilon = \sqrt{\boldsymbol{k}^2 + m^2}$$



A Einstein (1879-1955)

$$i\partial_t \leftrightarrow \varepsilon$$

$$\boldsymbol{k} \leftrightarrow -i\partial_{\boldsymbol{r}}$$

$$\varepsilon\psi = \frac{\boldsymbol{k}^2}{2m}\psi$$

E. Schrödinger
(1887-1961)

$$\varepsilon^2\phi = (\boldsymbol{k}^2 + m^2)\phi$$

Klein-Gordon equation
Troublesome

O Klein (1894-1977)

I. The Dirac equation.

PAM Dirac (1902-1984)

$$H\psi = \varepsilon\psi \qquad i\partial_t \leftrightarrow \varepsilon$$

$$\boldsymbol{k} \leftrightarrow -i\partial_{\boldsymbol{r}}$$

$$\boldsymbol{\sigma} \cdot \boldsymbol{k} \leftrightarrow \sqrt{k_1^2 + k_2^2 + k_3^2}$$

$$\varepsilon\psi = \boldsymbol{\sigma} \cdot \boldsymbol{k}\psi$$

We need more matrices as we have a mass

$$\sqrt{\boldsymbol{k}^2 + m^2} \leftrightarrow \boldsymbol{\gamma} \cdot \boldsymbol{k} + \gamma_4 m$$

$$\begin{pmatrix} -m & \boldsymbol{\sigma} \cdot \boldsymbol{k} \\ -\boldsymbol{\sigma} \cdot \boldsymbol{k} & m \end{pmatrix} \begin{pmatrix} \phi_a \\ \phi_b \end{pmatrix} = E \begin{pmatrix} \phi_a \\ \phi_b \end{pmatrix}$$

Dirac equation

1. The Dirac equation.

$$H = \boldsymbol{\alpha} \cdot \hat{\boldsymbol{k}} + m\beta$$

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \qquad \{\alpha_i, \beta\} = 0 \qquad \beta^2 = 1$$

Pauli matrices almost do the job

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

(α_i, β) are 4x4 matrices

In 3D or if the particle is massless, with the Pauli matrices is enough

1. The Dirac equation.

W Pauli (1900-1958)

$$E^2 - \boldsymbol{k}^2 = m^2$$

$$(E - \boldsymbol{\sigma} \cdot \boldsymbol{k})(E + \boldsymbol{\sigma} \cdot \boldsymbol{k}) = m^2$$

$$(E - \boldsymbol{\sigma} \cdot \boldsymbol{k})\phi_1 = m\phi_2$$

$$(E + \boldsymbol{\sigma} \cdot \boldsymbol{k})\phi_2 = m\phi_1$$

$$\psi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$$

$$\begin{pmatrix} m & E + \boldsymbol{\sigma} \cdot \boldsymbol{k} \\ E - \boldsymbol{\sigma} \cdot \boldsymbol{k} & m \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = 0$$

1. The Dirac equation.

W Pauli (1900-1958)

$$\begin{pmatrix} E+m & -\boldsymbol{\sigma}\cdot\boldsymbol{\pi} \\ -\boldsymbol{\sigma}\cdot\boldsymbol{\pi} & E-m \end{pmatrix} \begin{pmatrix} \phi_a \\ \phi_b \end{pmatrix} = 0$$

$\boldsymbol{\pi} = \boldsymbol{k} - e\boldsymbol{A}$

$$E = m + E_{NR}$$

$$E_{NR}\phi_b = \boldsymbol{\sigma}\cdot\boldsymbol{\pi}\phi_a$$

$$\phi_a = \frac{1}{E_{NR}+2m}\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\phi_b$$

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$$\phi_a = \frac{1}{E_{NR}+2m}\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\phi_b \sim \frac{1}{2m}(1-\frac{E_{NR}}{2m})\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\phi_b$$

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$$E_{NR}\phi_b = \frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\phi_a$$

1. The Dirac equation.

$$E_{NR}\phi_b = \frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\phi_a$$

$$H_{NR} = \frac{1}{2m}(\boldsymbol{k} - e\boldsymbol{A})^2 - \frac{1}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{B}$$

Pauli Hamiltonian

W Pauli (1900-1958)

1. The Dirac equation.

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$$H_{NR} = \frac{1}{2m}(\boldsymbol{k} - e\boldsymbol{A})^2 - \frac{1}{2m}\boldsymbol{\sigma} \cdot \boldsymbol{B}$$

Pauli Hamiltonian

$$H_{NR} = \frac{1}{2m}\boldsymbol{\pi}^2 - \frac{\boldsymbol{\pi}^4}{8m^3} - \frac{1}{2m}\boldsymbol{\sigma} \cdot \boldsymbol{B} - \frac{1}{4m^2}\boldsymbol{\sigma} \cdot (\boldsymbol{E} \times \boldsymbol{\pi}) - \frac{1}{8m^2}\boldsymbol{\nabla} \cdot \boldsymbol{E}$$

Spin-orbit term   Darwin term

1. The Dirac equation.

W Pauli (1900-1958)

$$E_{NR}\phi_b = \frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\phi_a$$

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Pauli Hamiltonian

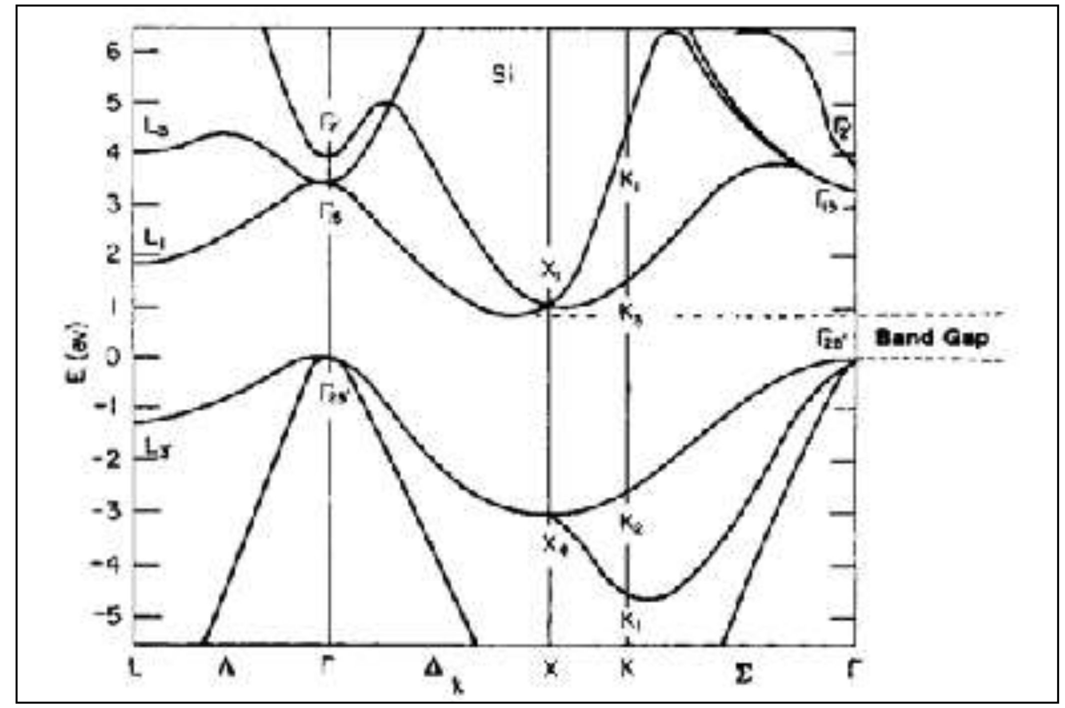
$$H_{NR} = \frac{1}{2m}\boldsymbol{\pi}^2 - \frac{\boldsymbol{\pi}^4}{8m^3} - \frac{1}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{B} - \frac{1}{4m^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{\pi}) - \frac{1}{8m^2}\boldsymbol{\nabla}\cdot\boldsymbol{E}$$

Spin-orbit term Darwin term

$$\boldsymbol{E} = -\frac{1}{r}\frac{\partial V}{\partial r}\boldsymbol{r} \qquad \boldsymbol{\sigma}\cdot(\boldsymbol{r}\times\boldsymbol{\pi}) \sim \boldsymbol{S}\cdot\boldsymbol{L}$$

3. Dirac equation on a lattice.

$$\begin{pmatrix} E + \boldsymbol{\sigma}\cdot\boldsymbol{k} & m \\ m & E - \boldsymbol{\sigma}\cdot\boldsymbol{k} \end{pmatrix}\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = 0$$

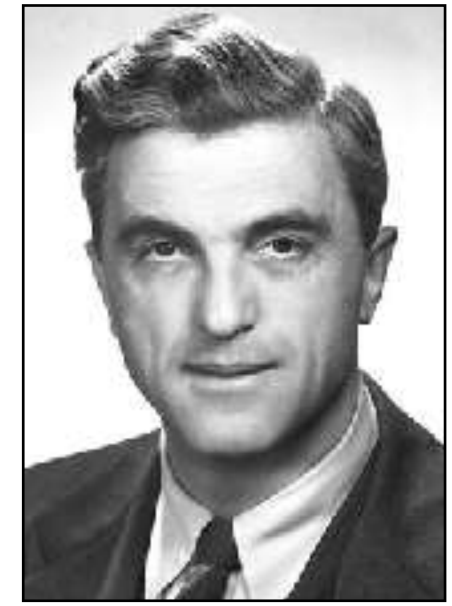


In Condensed Matter Physics, any particular form of the Hamiltonian possibly comes from symmetries of the lattice (through the Bloch theorem) and the constraints of inversion and time reversal invariance, not from Lorentz (relativistic) invariance

2. The Bloch theorem.

$$H = H_{\boldsymbol{k}} + V$$

$$V(\boldsymbol{r}) = V(\boldsymbol{r} + \boldsymbol{a})$$



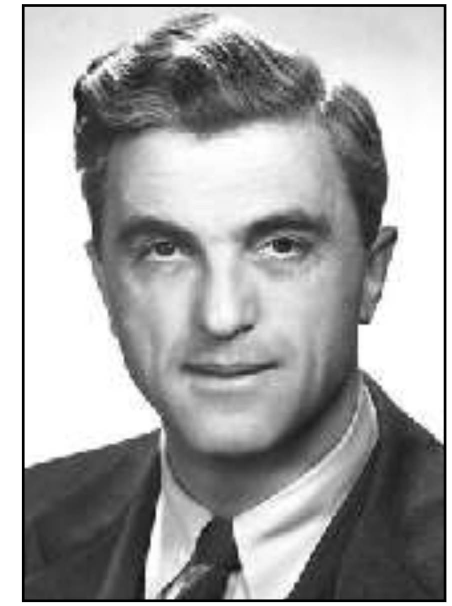
F Bloch (1905-1983)

$$|\psi\rangle = e^{i\boldsymbol{k}\boldsymbol{r}}\,|u_{\boldsymbol{k}}(\boldsymbol{r})\rangle \qquad |u_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{a})\rangle = e^{i\boldsymbol{k}\boldsymbol{a}}\,|u_{\boldsymbol{k}}(\boldsymbol{r})\rangle$$

2. The Bloch theorem.

$$H = H_{\boldsymbol{k}} + V \qquad V(\boldsymbol{r}) = V(\boldsymbol{r} + \boldsymbol{a})$$

$$\psi = e^{i\boldsymbol{k}\boldsymbol{r}} u_{\boldsymbol{k}}(\boldsymbol{r}) \qquad u_{\boldsymbol{k}}(\boldsymbol{r} + \boldsymbol{a}) = e^{i\boldsymbol{k}\boldsymbol{a}} u_{\boldsymbol{k}}(\boldsymbol{r})$$



F Bloch (1905-1983)

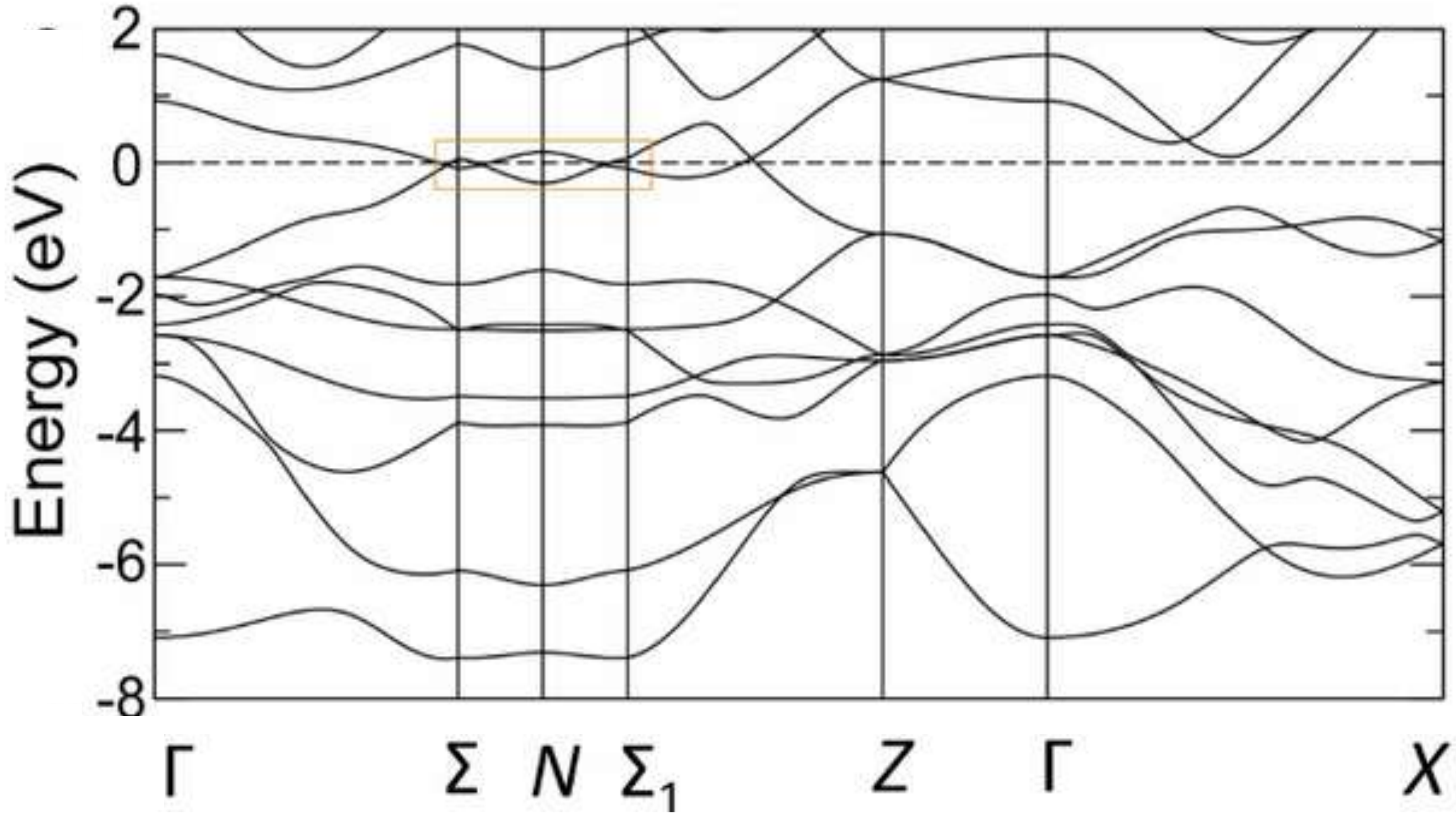
$$\varepsilon_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}+\boldsymbol{G}}$$

$$\boldsymbol{G} \cdot \boldsymbol{a} = 2\pi n$$

$\boldsymbol{k}$

Not only the Bloch state is periodic
but the band structure is as well

2. The Bloch theorem.



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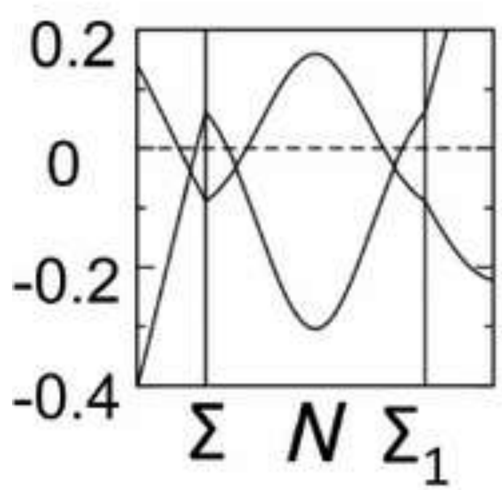
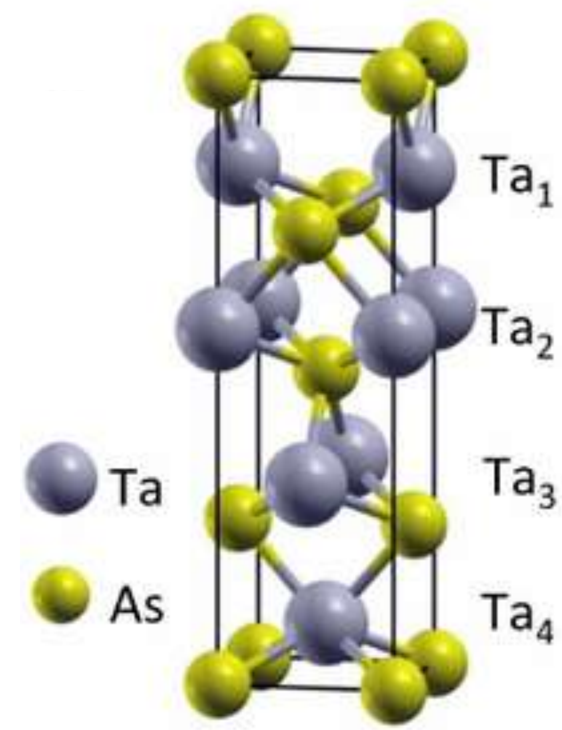


Discrete symmetries control this spaghetti

But sometimes bands go close or intersect around the Fermi level:

<u>Multicomponent wave functions</u>



2. The Bloch theorem. Symmetries

$$H = \frac{1}{2m}\boldsymbol{k}^2 + V - \frac{1}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{B} + \frac{1}{4m^2}\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}V \times \boldsymbol{k}) + \ldots$$

Time reversal operation: $T : t \to -t$ $\qquad T\psi(t) = \psi(-t)$

$$T^{-1}\boldsymbol{k}T = -\boldsymbol{k} \qquad T^{-1}\boldsymbol{\sigma}T = -\boldsymbol{\sigma} \qquad T^{-1}\boldsymbol{r}T = \boldsymbol{r}$$

$$[\boldsymbol{r},\boldsymbol{k}] = i \qquad T^{-1}(i)T = T^{-1}[\boldsymbol{r},\boldsymbol{k}]T = -[\boldsymbol{r},\boldsymbol{k}] = -i$$

flips i

$$T = U\mathcal{K} \qquad (\mathcal{K}f = f^*)$$

2. The Bloch theorem. Symmetries

$T = U\mathcal{K}$ For spinless particles $U = I$

$$T^2 = U\mathcal{K}U\mathcal{K} = U^2\mathcal{K}^2 = I$$

For spinful particles $T^{-1}\boldsymbol{\sigma}T = -\boldsymbol{\sigma}$ spin is also reversed

$$T^{-1}\sigma_1 T = U^{-1}\mathcal{K}\sigma_1 U\mathcal{K} = U^{-1}\sigma_1 U = -\sigma_1$$

$$T^{-1}\sigma_2 T = U^{-1}\mathcal{K}\sigma_2 U\mathcal{K} = -U^{-1}\sigma_2 U = -\sigma_2$$

$$T^{-1}\sigma_3 T = U^{-1}\mathcal{K}\sigma_3 U\mathcal{K} = U^{-1}\sigma_3 U = -\sigma_3$$

2. The Bloch theorem. Symmetries

$T = U\mathcal{K}$ For spinless particles $U = I$

$$T^2 = U\mathcal{K}U\mathcal{K} = U^2\mathcal{K}^2 = I$$

Unitary operator

For spinful particles $T^{-1}\boldsymbol{\sigma}T = -\boldsymbol{\sigma}$

$$U = i\sigma_2 \qquad U^{-1} = -i\sigma_2$$

$$T^2 = i\sigma_2\mathcal{K}(i\sigma_2)\mathcal{K} = (i\sigma_2)^2 = -I$$

anti-unitary operator

2. The Bloch theorem. Symmetries

$$T^2 = i\sigma_2 \mathcal{K}(i\sigma_2)\mathcal{K} = (i\sigma_2)^2 = -I$$

anti-unitary operator

$$T^2\psi = -\psi$$

Kramer's theorem: $[T, H] = 0$ $\quad H|\psi\rangle = E|\psi\rangle$

$$HT|\psi\rangle = ET|\psi\rangle$$

assume $T|\psi\rangle = e^{i\alpha}|\psi\rangle$

$$T^2|\psi\rangle = Te^{i\alpha}|\psi\rangle = e^{-i\alpha}T|\psi\rangle = |\psi\rangle$$

2. The Bloch theorem. Symmetries

$$T^2 = i\sigma_2 \mathcal{K}(i\sigma_2)\mathcal{K} = (i\sigma_2)^2 = -I$$

anti-unitary operator

$$T^2\psi = -\psi$$

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assume $T|\psi\rangle = e^{i\alpha}|\psi\rangle$

$$T^2|\psi\rangle = Te^{i\alpha}|\psi\rangle = e^{-i\alpha}T|\psi\rangle = |\psi\rangle$$

$$T^2 = I$$

2. The Bloch theorem. Symmetries

$$T^2 = i\sigma_2 \mathcal{K} (i\sigma_2) \mathcal{K} = (i\sigma_2)^2 = -I$$

anti-unitary operator

$$T^2 \psi = -\psi$$

Kramer's theorem: $[T, H] = 0$ $\qquad H\left|\psi\right\rangle = E\left|\psi\right\rangle$

$$HT\left|\psi\right\rangle = ET\left|\psi\right\rangle$$

assume $T\left|\psi\right\rangle \neq e^{i\alpha}\left|\psi\right\rangle$

$$T^2\left|\psi\right\rangle = Te^{i\alpha}\left|\psi\right\rangle = e^{-i\alpha}T\left|\psi\right\rangle = \left|\psi\right\rangle$$

The spectrum is doubly degenerate $\qquad T^2 \neq I$

$$\boxed{\langle T\psi|\psi\rangle = 0}$$

2. The Bloch theorem. Symmetries

Now, with the presence of the momentum

$$T^{-1}\boldsymbol{k}T = -\boldsymbol{k} \qquad T\left|\boldsymbol{k}, s\right\rangle = \left|-\boldsymbol{k}, -s\right\rangle$$

$$H_{\boldsymbol{k}}\left|-\boldsymbol{k}, -s\right\rangle = \varepsilon_{-\boldsymbol{k}}^{-s}\left|-\boldsymbol{k}, -s\right\rangle$$

$$\varepsilon_{\boldsymbol{k}}^{s} = \varepsilon_{-\boldsymbol{k}}^{-s}$$

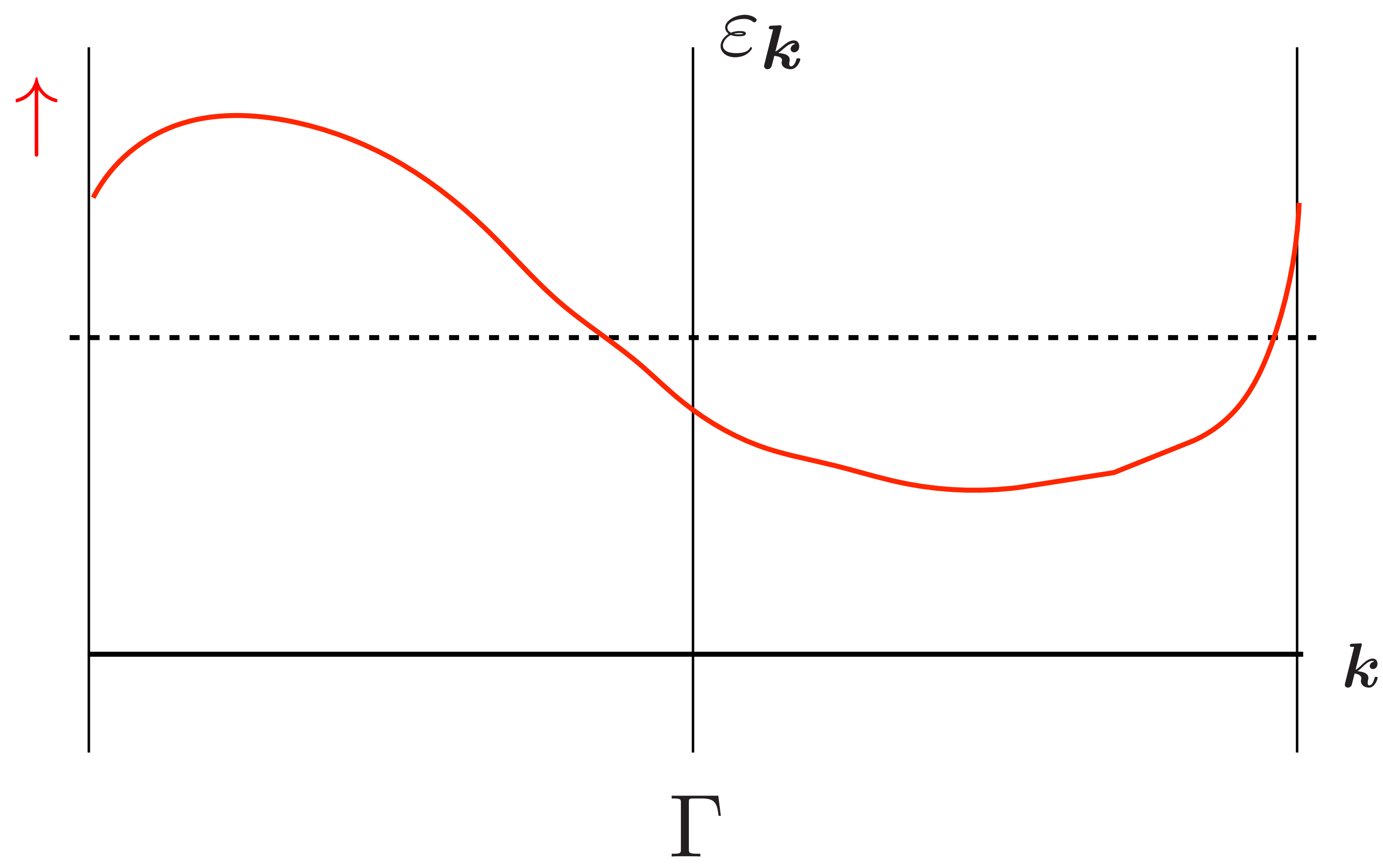
The spectrum is doubly degenerate, but the degeneracy occurs for different spins and momenta

$$\left|\boldsymbol{k}, \uparrow\right\rangle \qquad \left|-\boldsymbol{k}, \downarrow\right\rangle \qquad \qquad \left|\boldsymbol{k}, \downarrow\right\rangle \qquad \left|-\boldsymbol{k}, \uparrow\right\rangle$$

2. The Bloch theorem. Symmetries

Now, with the presence of the momentum

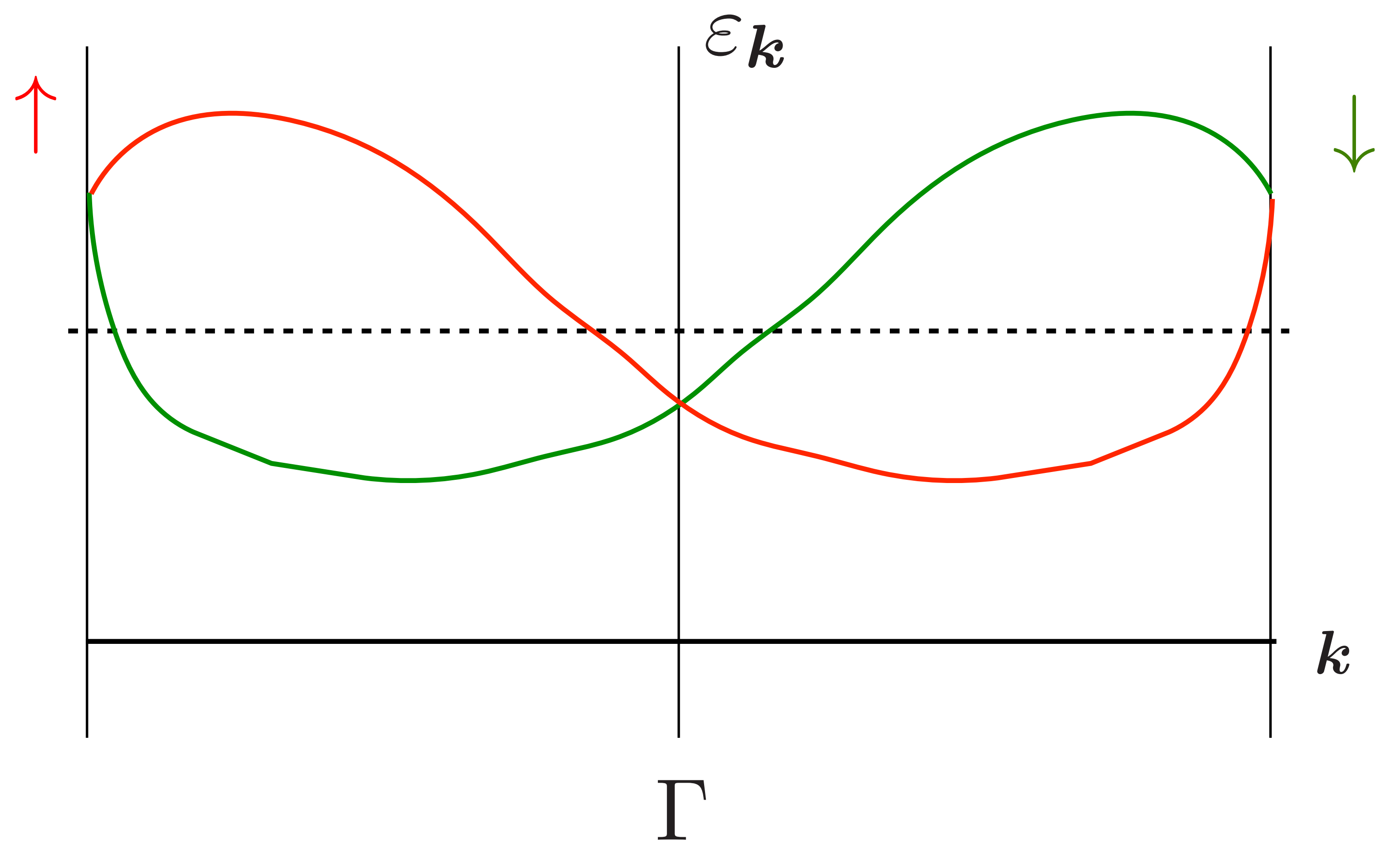
$$|\boldsymbol{k}, \uparrow\rangle \qquad |-\boldsymbol{k}, \downarrow\rangle \qquad \varepsilon_{\boldsymbol{k}}^{s} = \varepsilon_{-\boldsymbol{k}}^{-s} \qquad |\boldsymbol{k}, \downarrow\rangle \qquad |-\boldsymbol{k}, \uparrow\rangle$$



2. The Bloch theorem. Symmetries

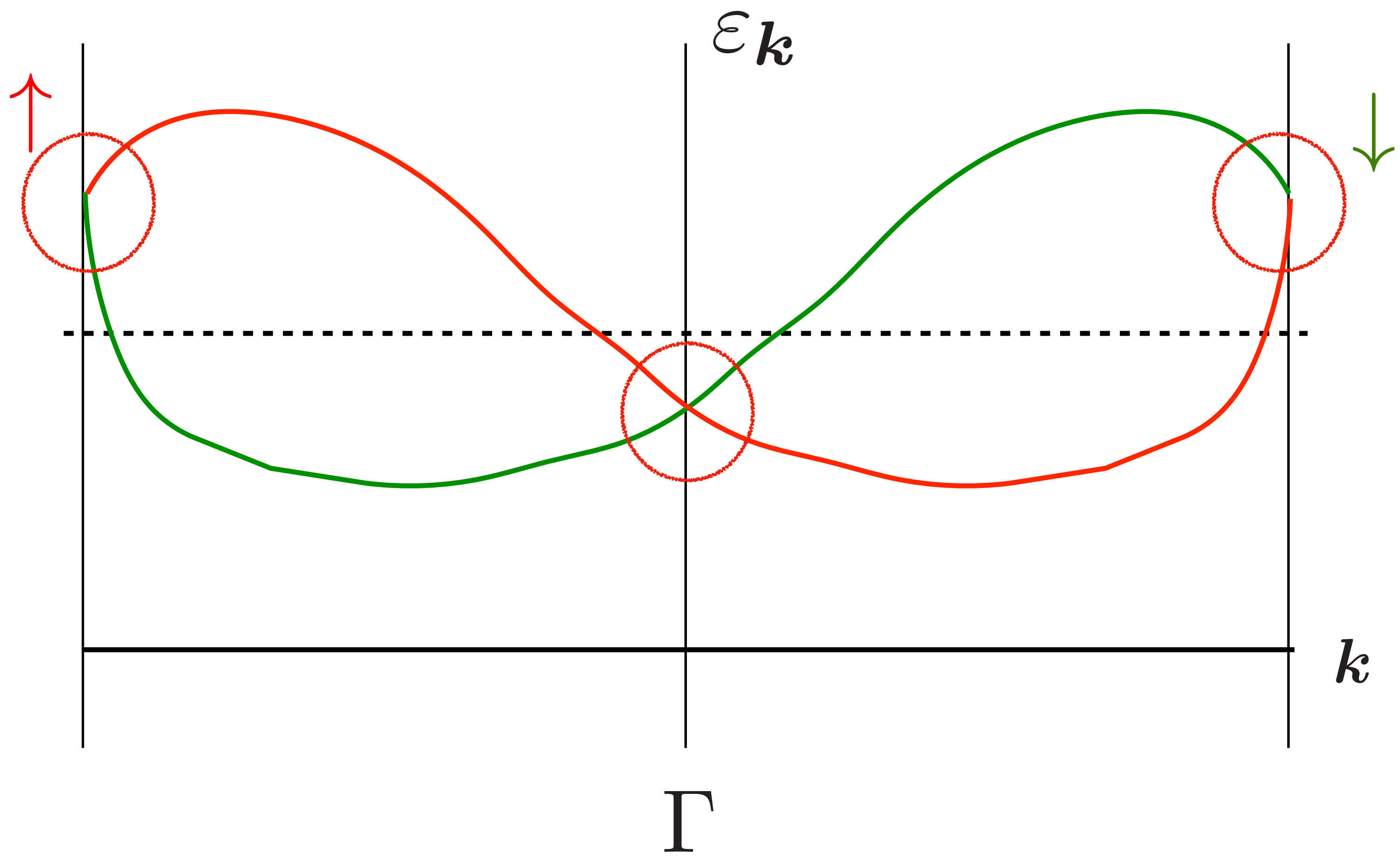
Now, with the presence of the momentum

$|\boldsymbol{k}, \uparrow\rangle \qquad |-\boldsymbol{k}, \downarrow\rangle \qquad \varepsilon^{s}_{\boldsymbol{k}} = \varepsilon^{-s}_{-\boldsymbol{k}} \qquad |\boldsymbol{k}, \downarrow\rangle \qquad |-\boldsymbol{k}, \uparrow\rangle$



2. The Bloch theorem. Symmetries

time reversal symmetry $\varepsilon_{\boldsymbol{k}}^{s} = \varepsilon_{-\boldsymbol{k}}^{-s}$

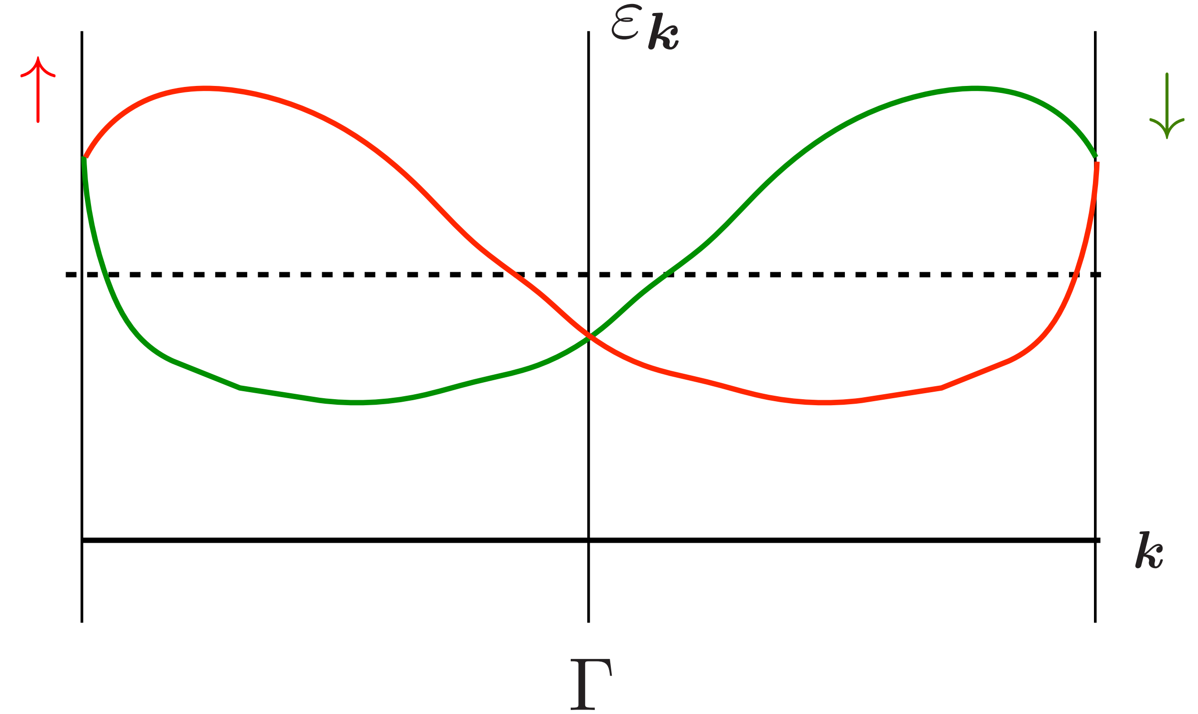


$$\varepsilon_{\boldsymbol{k}}^{s} = \varepsilon_{-\boldsymbol{k}}^{-s} = \varepsilon_{\boldsymbol{k}+\boldsymbol{G}}^{-s} = \varepsilon_{\boldsymbol{k}}^{-s}$$

$$-\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{G}$$

TRIMs

2. The Bloch theorem. Symmetries



Just imposing time reversal symmetry, we conclude that the system is always a metal

two ways out: breaking T (can or not open)
adding extra degrees of freedom: extra bands and extra symmetries

2. The Bloch theorem. Symmetries

Inversion operation:

$$P^{-1}\boldsymbol{r}P = -\boldsymbol{r} \qquad P^{-1}\boldsymbol{k}P = -\boldsymbol{k} \qquad P^{-1}\boldsymbol{\sigma}P = \boldsymbol{\sigma}$$

$$P^2 = I$$

for inversion symmetric systems: $[P, H] = 0$

$$\varepsilon^s_{\boldsymbol{k}} = \varepsilon^s_{-\boldsymbol{k}}$$

2. The Bloch theorem. Symmetries

for time reversal and inversion symmetric systems:

$$[P, H] = 0 \qquad\qquad [T, H] = 0$$

$$\varepsilon_{\boldsymbol{k}}^{s} = \varepsilon_{-\boldsymbol{k}}^{s} \qquad\qquad \varepsilon_{\boldsymbol{k}}^{s} = \varepsilon_{-\boldsymbol{k}}^{-s}$$

$$\varepsilon_{\boldsymbol{k}}^{s} = \varepsilon_{\boldsymbol{k}}^{-s}$$

The two bands are totally degenerated
not only at TRIMs

2. The Bloch theorem. Symmetries

$$[P, H] = 0 \qquad\qquad [T, H] = 0$$

$$\varepsilon^s_{\boldsymbol{k}} = \varepsilon^s_{-\boldsymbol{k}} \qquad\qquad \varepsilon^s_{\boldsymbol{k}} = \varepsilon^{-s}_{-\boldsymbol{k}}$$

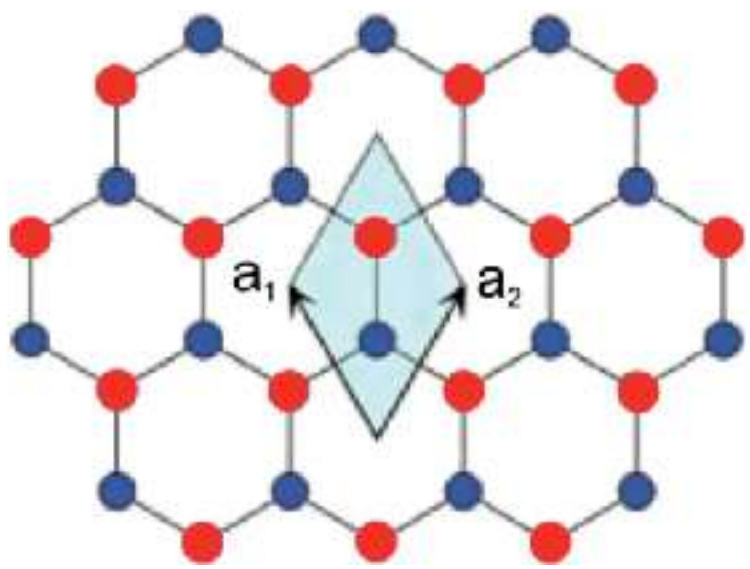
$$\varepsilon^s_{\boldsymbol{k}} = \varepsilon^{-s}_{\boldsymbol{k}}$$

for time reversal and inversion symmetric systems,
we cannot scape from being a metal
but inversion can be implemented in several ways:

$P^2 = I$ but $P \neq I$

3. Dirac equation on a lattice.

massless Dirac fermions in 2D:



graphene

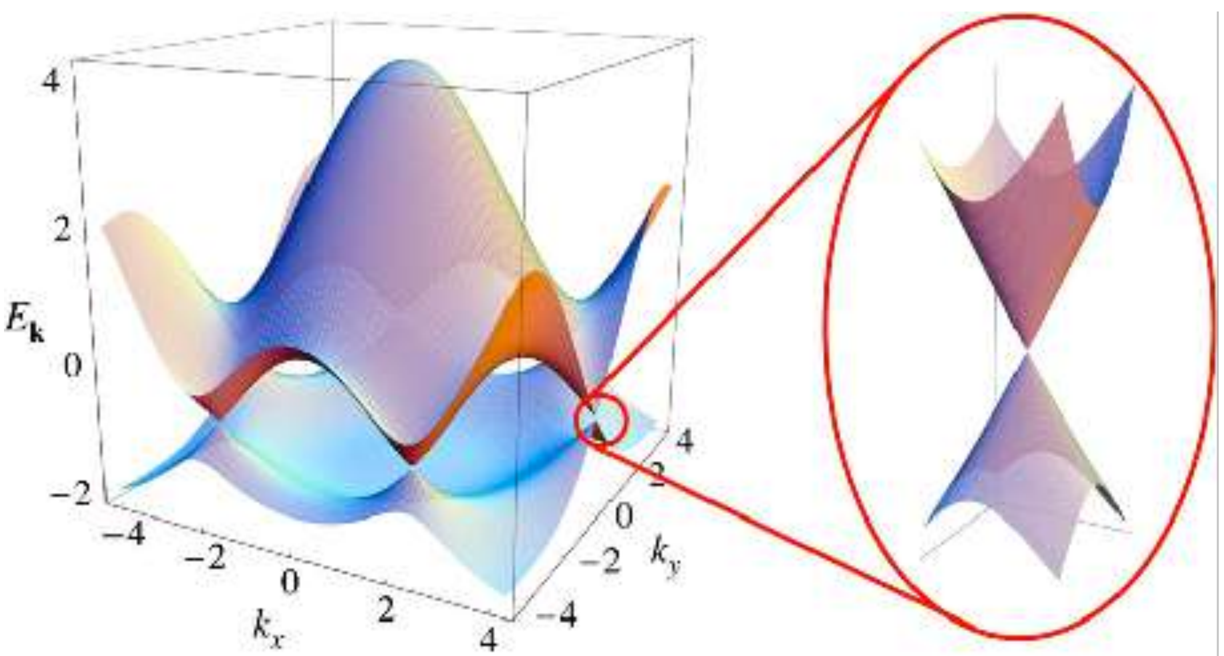
Two atoms per unit cell: two triangular interpenetrating sublattices

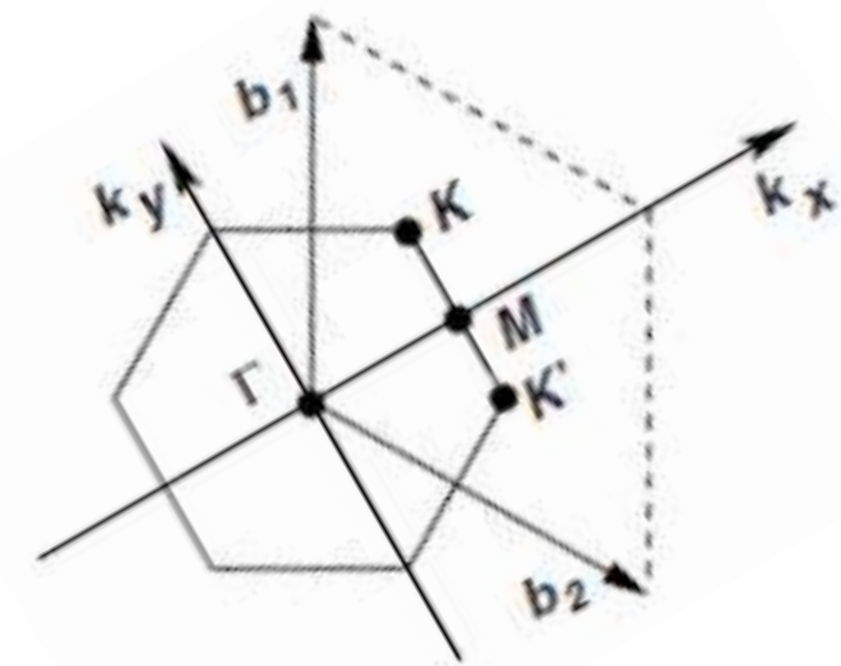
“Diracness” comes from the fact that each atom couples to its neighbours that belong to the other sub lattice

$$|\psi\rangle = \begin{pmatrix} \phi_a \\ \phi_b \end{pmatrix}$$

3. Dirac equation on a lattice.

massless Dirac fermions in 2D: graphene





Two valleys

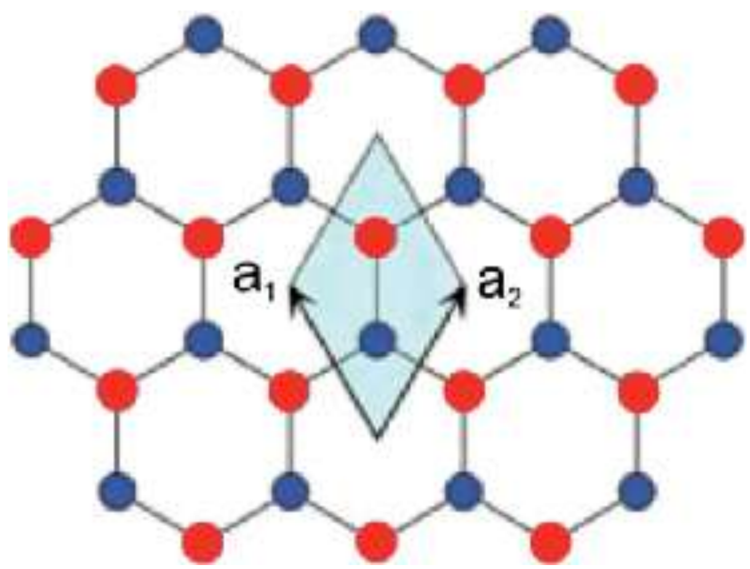
(K and K' are NOT TRIMs!)

$$H(\eta \boldsymbol{K} + \boldsymbol{k})$$

$$(\eta \tau_1 k_1 + \tau_2 k_2)\psi_\eta(\boldsymbol{k}) = E\psi_\eta(\boldsymbol{k})$$

3. Dirac equation on a lattice.

massless Dirac fermions:



Graphene is inversion symmetric and time reversal invariant (no spin-orbit) pz orbital are real

$$T^2 = 1 \qquad T = \mathcal{K}$$

$$H(\boldsymbol{k}) = H^*(-\boldsymbol{k})$$

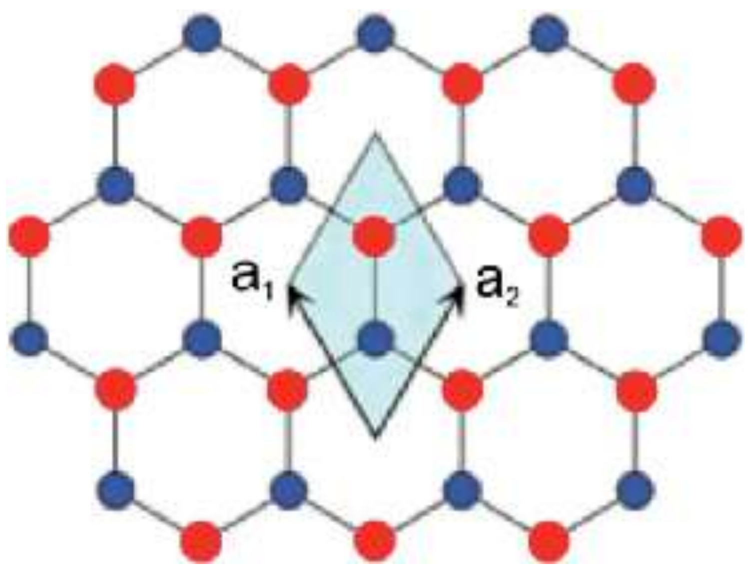
$$P = \tau_1 \qquad \boldsymbol{k} \to -\boldsymbol{k}$$

but inversion operation sends the pz orbital to the other

$$H^P(\eta \boldsymbol{K} + \boldsymbol{k}) = \tau_1 H(-\eta \boldsymbol{K} - \boldsymbol{k})\tau_1$$

3. Dirac equation on a lattice.

massless Dirac fermions:



inversion operation sends the pz orbital to the other

Graphene is inversion symmetric and time reversal invariant (no spin-orbit)
pz orbital are real

$$H^P = (-\eta)\tau_1\tau_1\tau_1(-k_1) + \tau_1\tau_2\tau_1(-k_2)$$

$$H^P(\eta \boldsymbol{K} + \boldsymbol{k}) = \tau_1 H(-\eta \boldsymbol{K} - \boldsymbol{k})\tau_1 = \eta\tau_1 k_1 + \tau_2 k_2$$

$$H^P = H$$

3. Dirac equation on a lattice.

giving a mass to massless Dirac fermions in graphene:

$m(\boldsymbol{k}) \sim m + ...$

$m(\boldsymbol{k}) \sim \eta m + ...$

$$H = \eta\tau_1 k_1 + \tau_2 k_2 + \tau_3 m$$

$$H = \eta\tau_1 k_1 + \tau_2 k_2 + \eta\tau_3 m$$

inversion:

$$H^P = (-\eta)\tau_1\tau_1\tau_1(-k_1) + \tau_1\tau_2\tau_1(-k_2) + \tau_1\tau_3\tau_1 m$$

$$H^P = \eta\tau_1 k_1 + \tau_2 k_2 - \tau_3 m$$

breaks inversion

$$H^P = (-\eta)\tau_1\tau_1\tau_1(-k_1) + \tau_1\tau_2\tau_1(-k_2) + (-\eta)\tau_1\tau_3\tau_1 m$$

$$H^P = \eta\tau_1 k_1 + \tau_2\ k_2 + \eta\tau_3 m$$

opposite masses for each valley preserves inversion

3. Dirac equation on a lattice.

giving a mass to massless Dirac fermions in graphene:

$$m(\boldsymbol{k}) \sim m + ...$$

$$m(\boldsymbol{k}) \sim \eta m + ...$$

TR inversion:

$$H = \eta\tau_1 k_1 + \tau_2 k_2 + \tau_3 m$$

$$H = \eta\tau_1 k_1 + \tau_2 k_2 + \eta\tau_3 m$$

$$H^T = (-\eta)\tau_1(-k_1) - \tau_2(-k_2) + \tau_3 m = H$$

preserves TR inversion

$$H^T = (-\eta)\tau_1(-k_1) - \tau_2(-k_2) + (-\eta)\tau_3 m$$

opposite masses for each valley breaks TR inversion

3. Dirac equation on a lattice.

giving a mass to massless Dirac fermions in graphene:

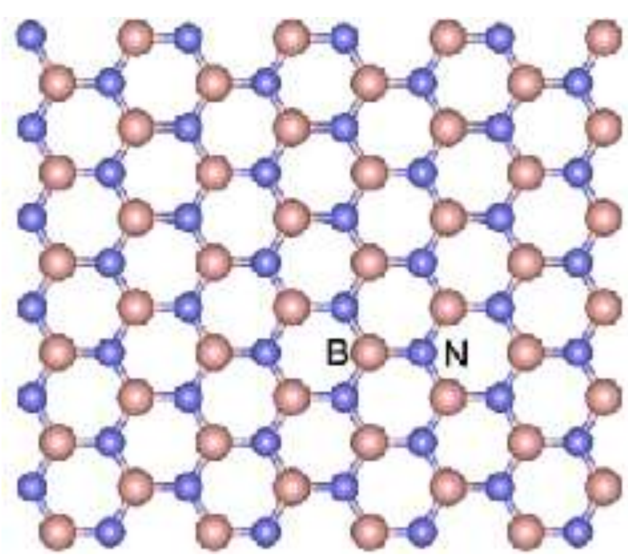
$$H = \eta \tau_1 k_1 + \tau_2 k_2 + \tau_3 m \qquad H = \eta \tau_1 k_1 + \tau_2 k_2 + \eta \tau_3 m$$

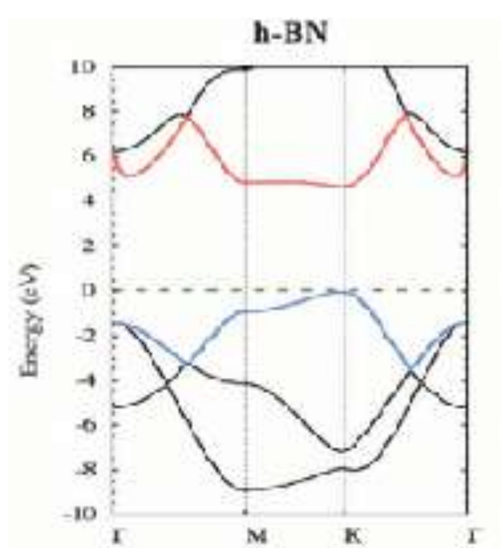
preserves TR inversion

breaks inversion

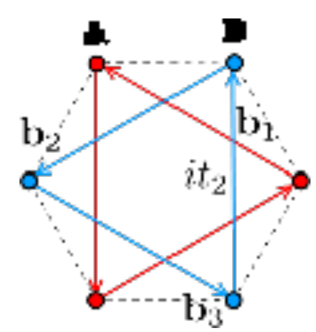
breaks TR inversion

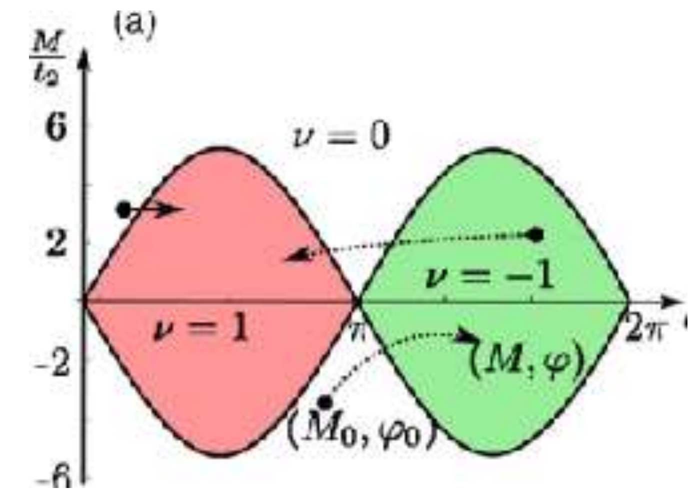
preserves inversion





Boron nitride



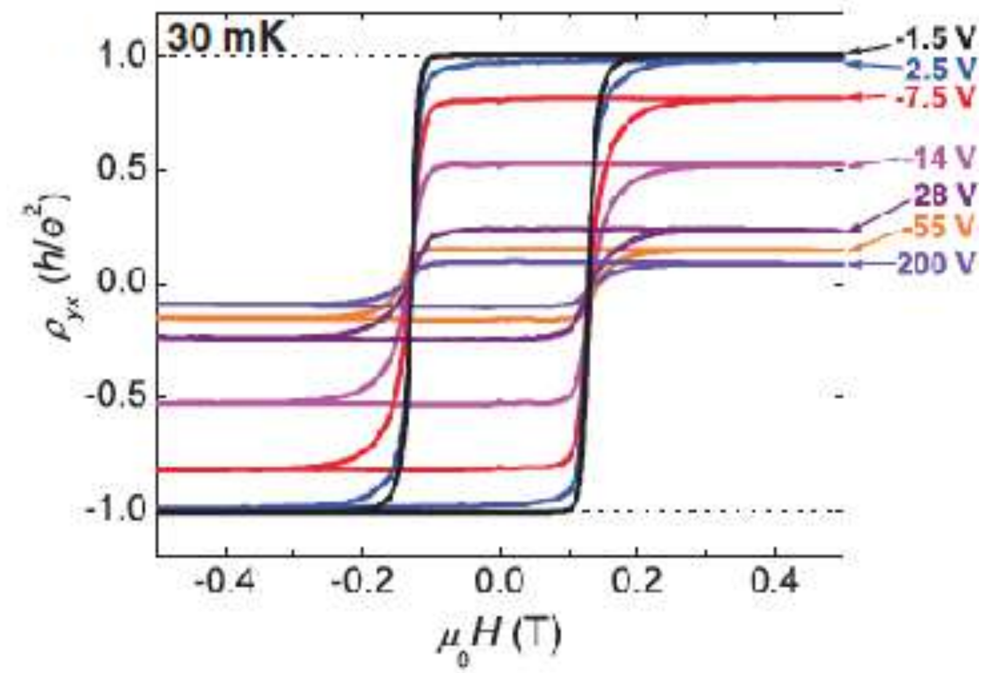


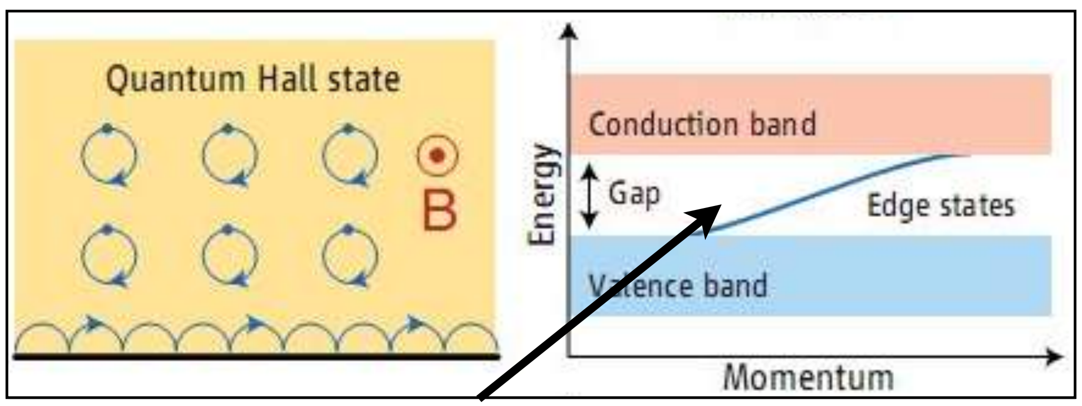
D. Haldane

Haldane model: anomalous Hall insulator

3. Dirac equation on a lattice.

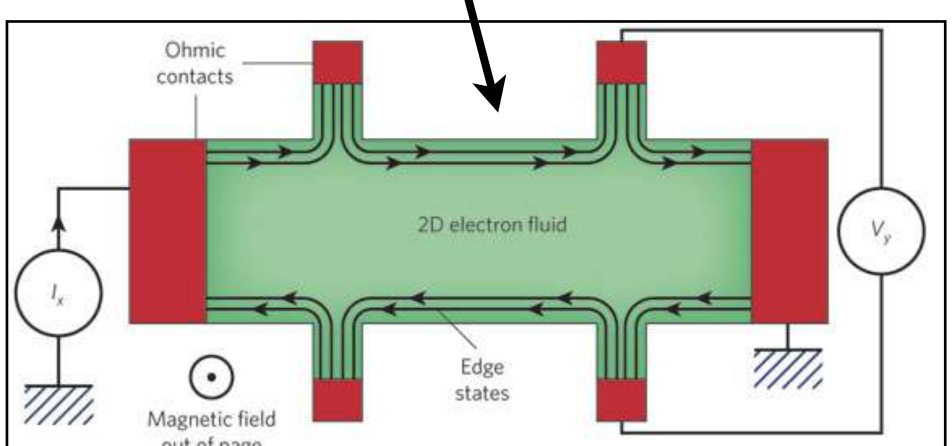
Experimental Observation of the Quantum Anomalous Hall Effect in a Magnetic Topological Insulator

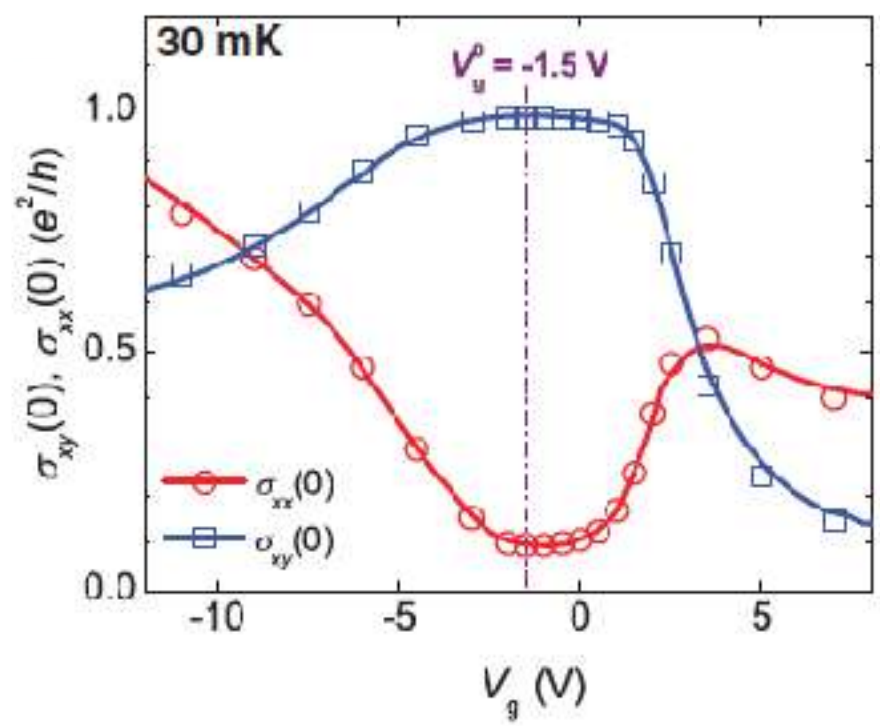




insulating bulk

conducting edge channels





CZ Chang et al Science 340, 167 (2013)

3. Dirac equation on a lattice.

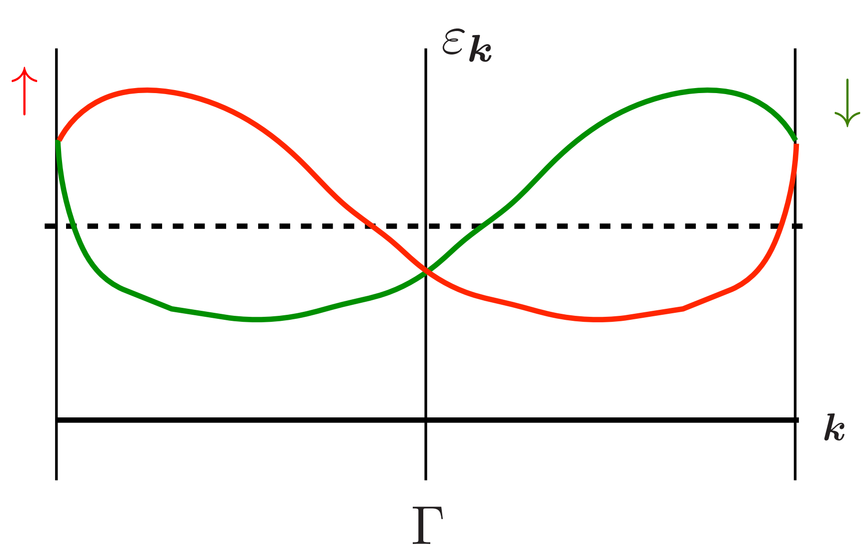
giving a mass to massless Dirac fermions in graphene with spin orbit:

$$T^2 = 1 \quad T = \mathcal{K} \qquad P^2 = 1 \qquad P = \tau_1$$

$$\boldsymbol{k} \to -\boldsymbol{k}$$

$$H_{NR} = \frac{1}{2m}\boldsymbol{\pi}^2 - \frac{\boldsymbol{\pi}^4}{8m^3} - \frac{1}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{B} - \frac{1}{4m^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{\pi}) - \frac{1}{8m^2}\boldsymbol{\nabla}\cdot\boldsymbol{E}$$

$$\boldsymbol{E} = -\frac{1}{r}\frac{\partial V}{\partial r}\boldsymbol{r} \qquad \boldsymbol{\sigma}\cdot(\boldsymbol{r}\times\boldsymbol{\pi}) \sim \boldsymbol{S}\cdot\boldsymbol{L}$$



many orbital degrees of freedom
more bands

3. Dirac equation on a lattice.

giving a mass to massless Dirac fermions in graphene with spin orbit:

$$T^2 = -1 \qquad T = i\sigma_2 \mathcal{K} \qquad P^2 = 1 \qquad P = \tau_1$$

$$\boldsymbol{k} \to -\boldsymbol{k}$$

Min et al PRB 74, 165310 (2006)

$$H = \eta\sigma_0\tau_1 k_1 + \sigma_0\tau_2 k_2 + \eta\sigma_3\tau_3 m$$

Inversion is the same as before, since it jumps over spin

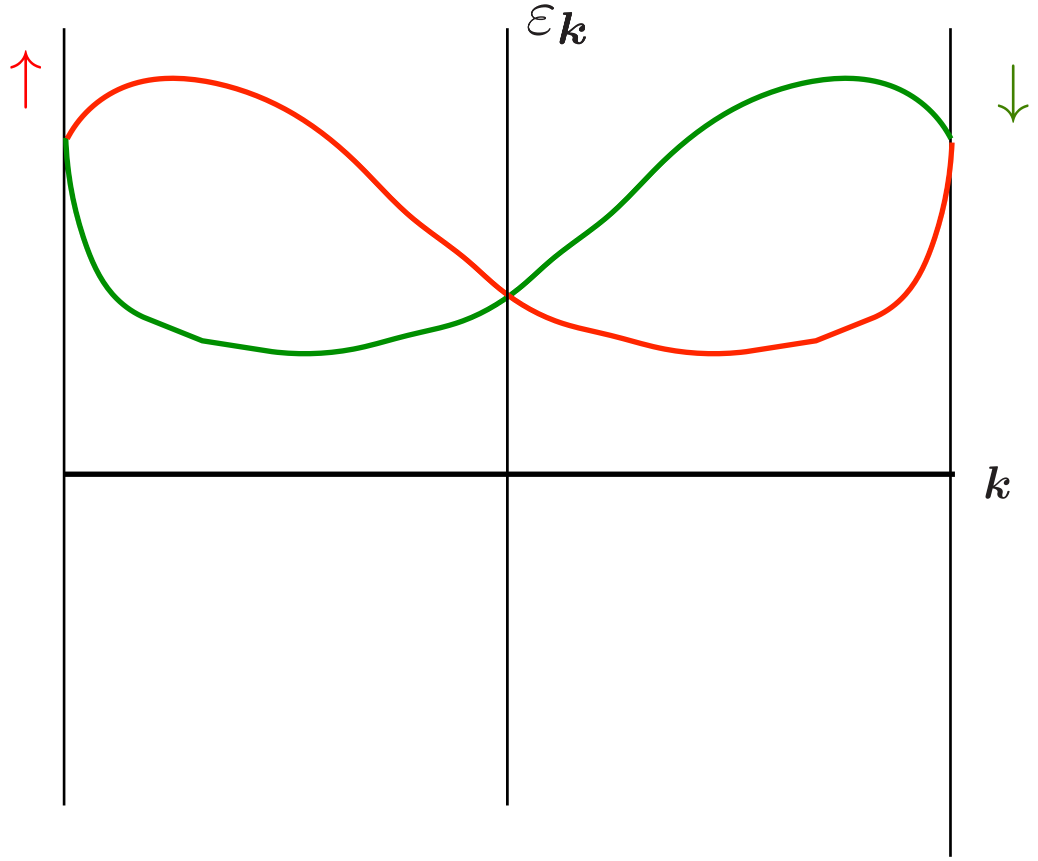
$$T^{-1}H(\boldsymbol{K}+\boldsymbol{k})T = (-i\sigma_2)H^*(-\boldsymbol{K}-\boldsymbol{k})(-i\sigma_2) =$$

$$= \tau_1 k_1 + \tau_2 k_2 + \sigma_3\tau_3 m$$

Inversion symmetric AND time reversal symmetric

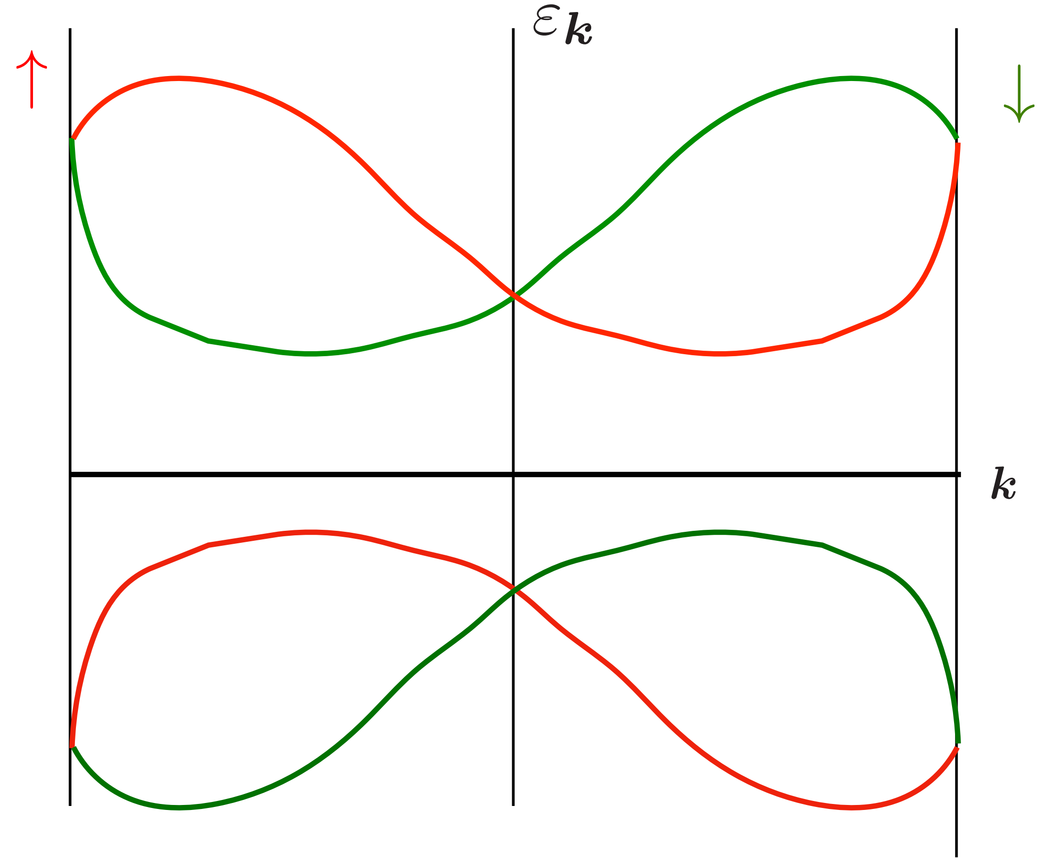
3. Dirac equation on a lattice.

giving a mass to massless Dirac fermions in graphene with spin orbit:



3. Dirac equation on a lattice.

giving a mass to massless Dirac fermions in graphene with spin orbit:

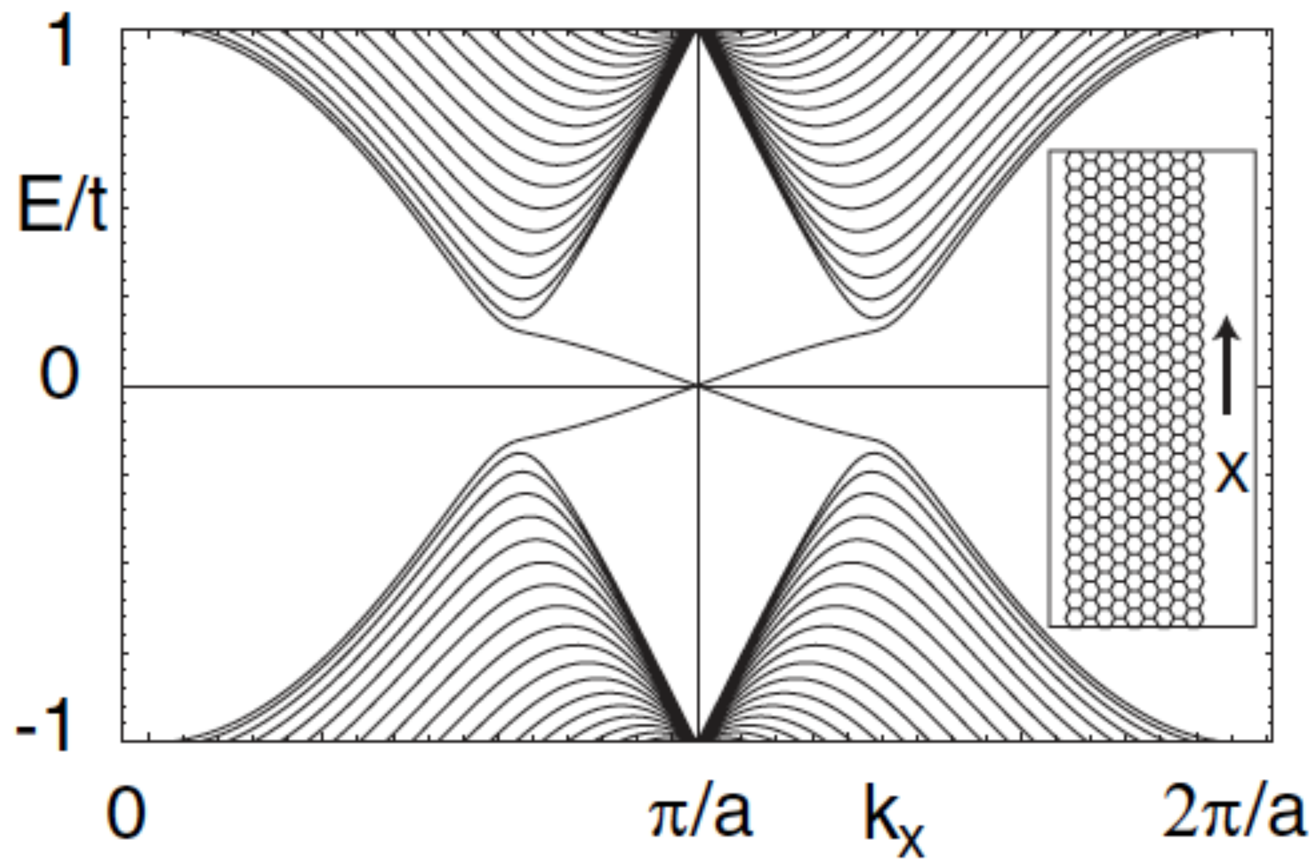


there are band crossing as dictated by TRS, but we have doubled the spectrum and placed the Fermi level in the gap!

3. Dirac equation on a lattice.

giving a mass to massless Dirac fermions in graphene with spin orbit:

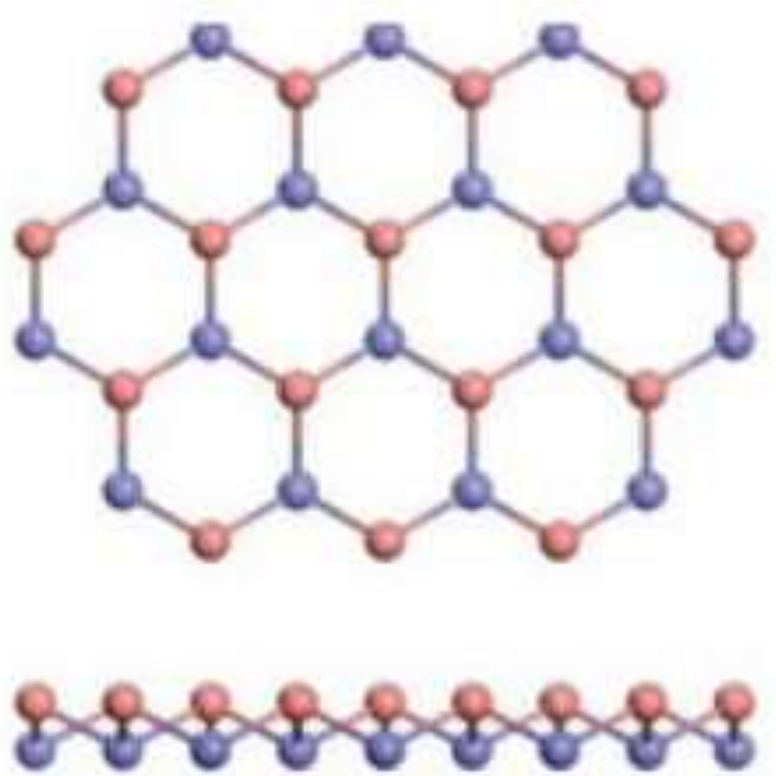
E. Mele, C. Kane



there are band crossing as dictated by TRS, but we have doubled the spectrum and placed the Fermi level in the gap!

3. Dirac equation on a lattice.

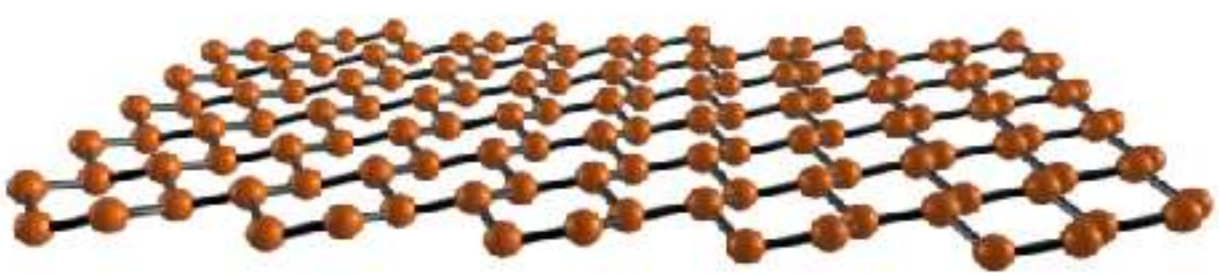
the story now is to find microscopic ways of breaking inversion

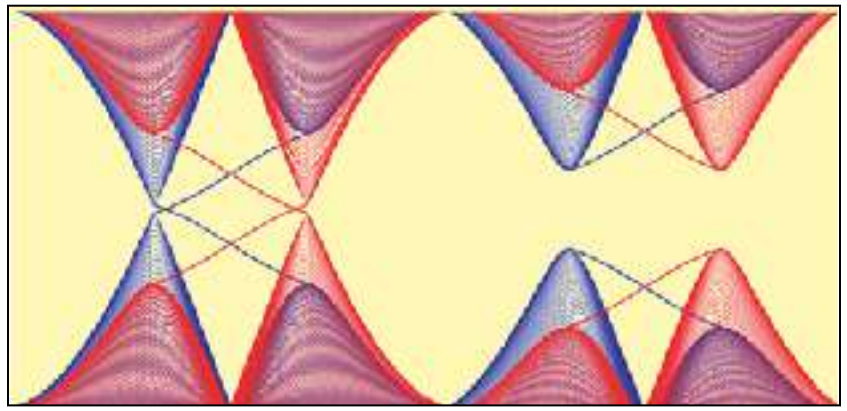


Stanene

breaks inversion: buckled structure

Germanene



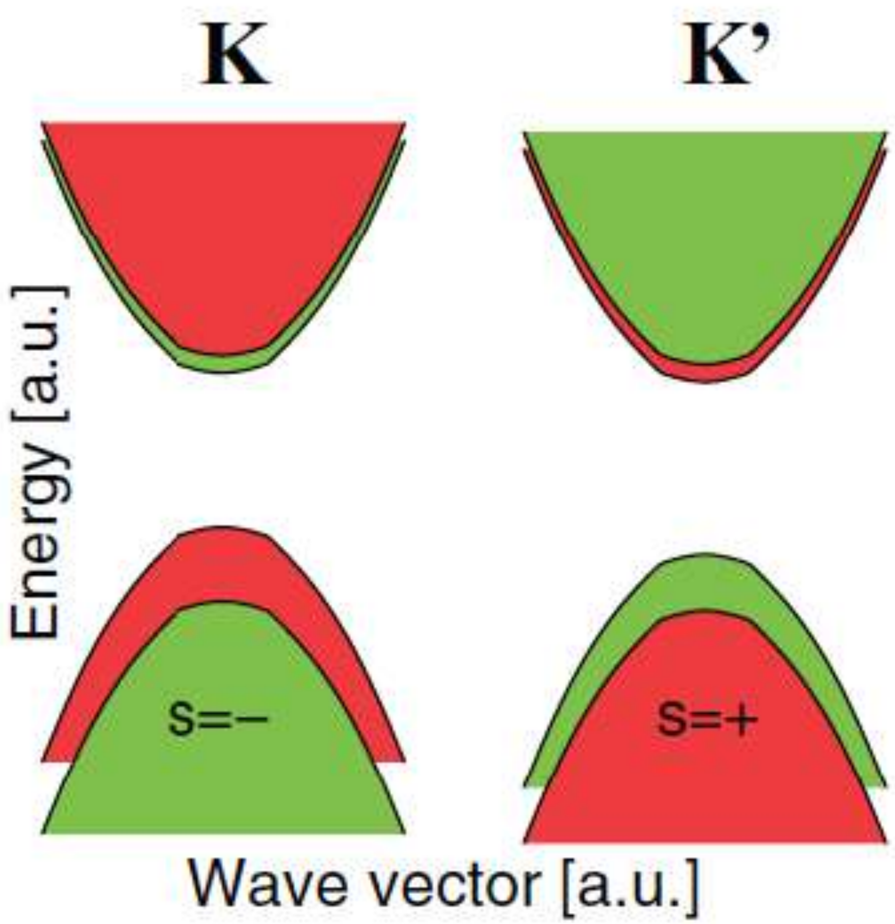


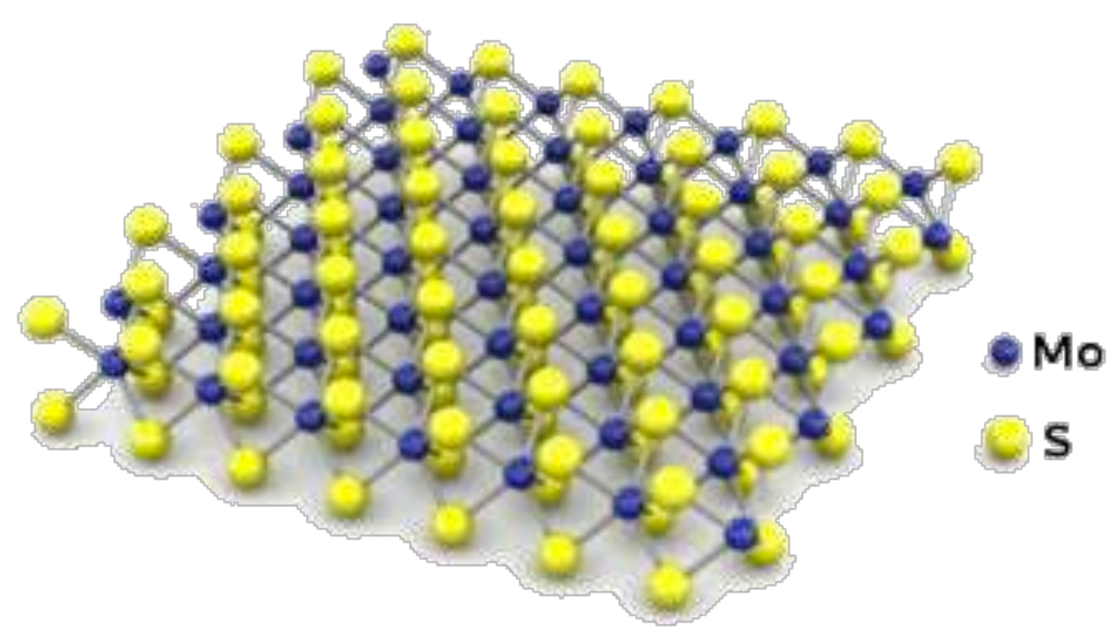
3. Dirac equation on a lattice.

Transition metal dichalcogenides:

$$|\psi\rangle = \begin{pmatrix} |J_3 = 0\rangle \\ |J_3 = \pm 2\rangle \end{pmatrix}$$

$$H(\boldsymbol{k}) = \tau\sigma_1 k_1 + \sigma_2 k_2 + \Delta\sigma_3 + \lambda\tau\frac{1}{2}(\sigma_3 - \sigma_0)s_3$$

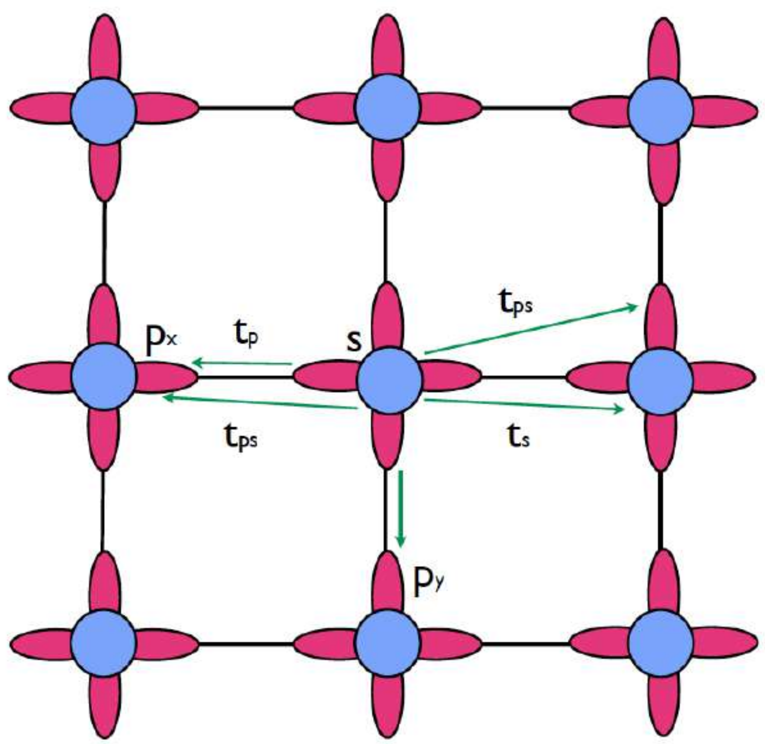




3. Dirac equation on a lattice.

BHZ model:

$$|\psi\rangle = a_0\,|l_3 = 0\rangle + a_1\,|l_3 = 1\rangle + a_{-1}\,|l_3 = -1\rangle$$



$$P = \tau_0$$

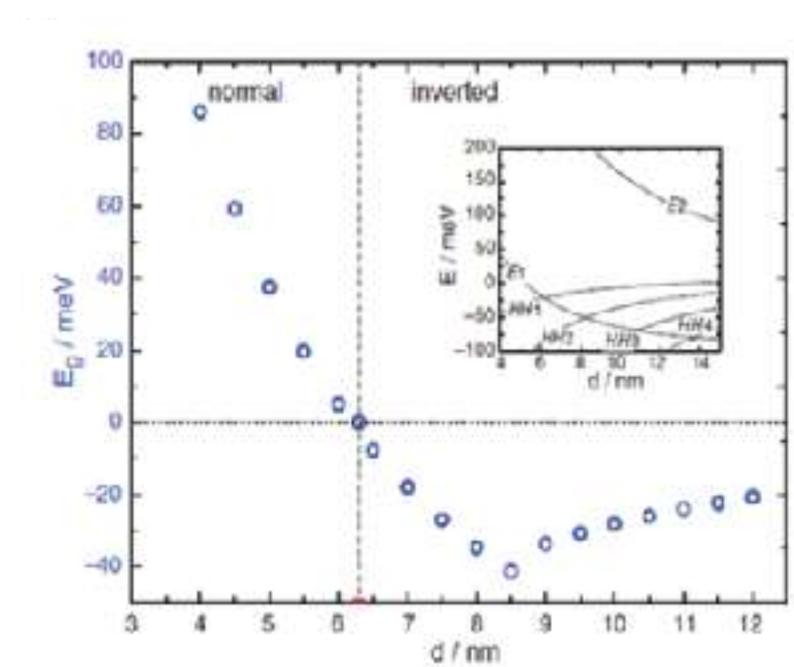
$$T = i s_2 \mathcal{K}$$

Spin-orbit breaks the l=1 degeneracy

But everything happens around the Γ point

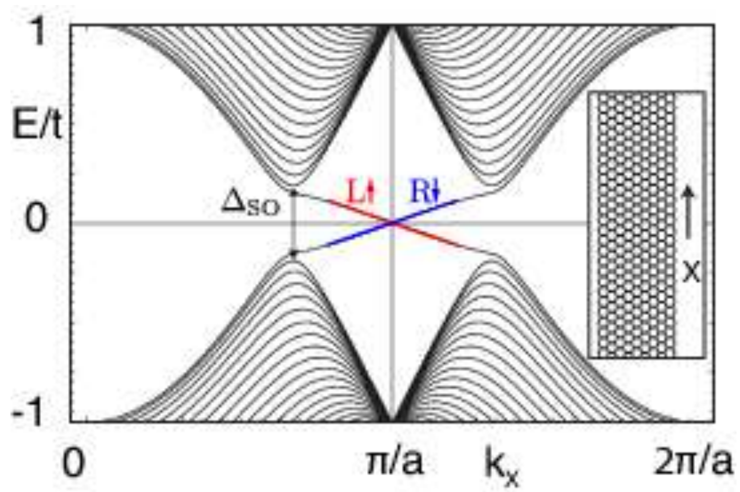
$$H(\boldsymbol{k}) = s\sigma_1 k_1 + \sigma_2 k_2 + m\sigma_3$$

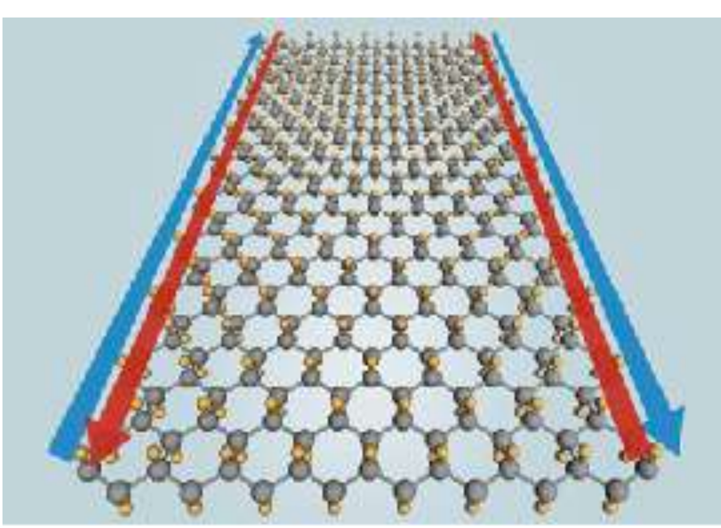
Low energy model for inverted HgTe/CdTe Quantum well structures

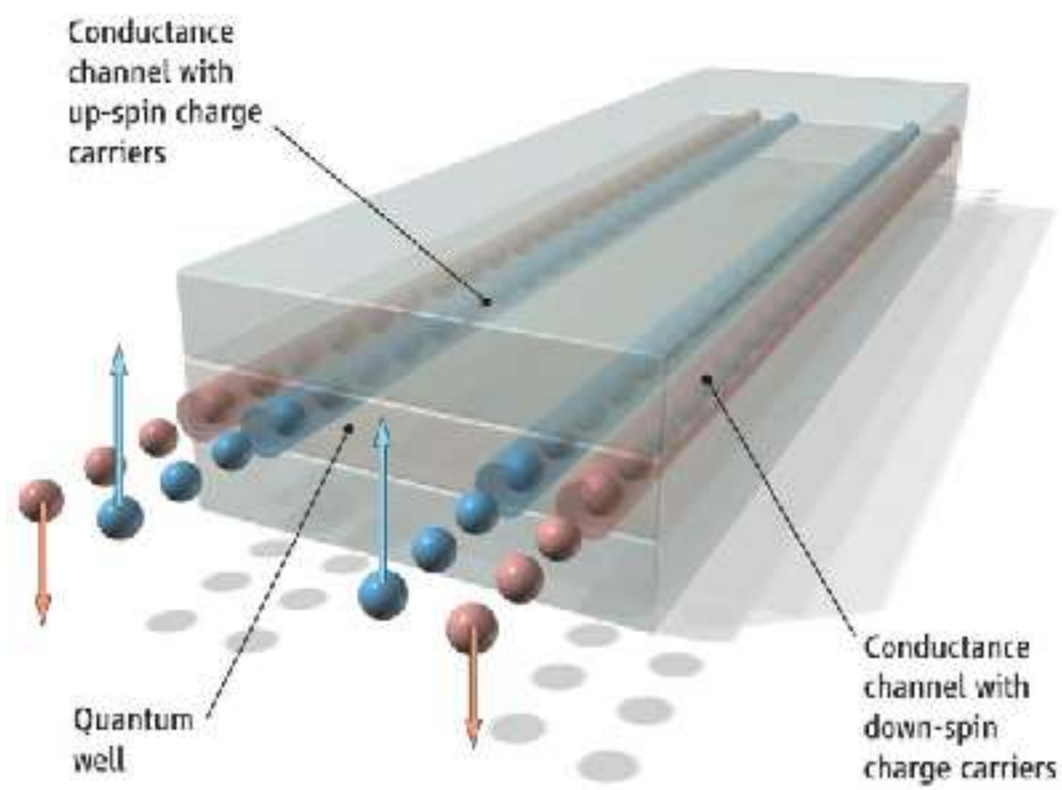


3. Dirac equation on a lattice.

giving a mass to massless Dirac fermions in graphene with spin orbit:

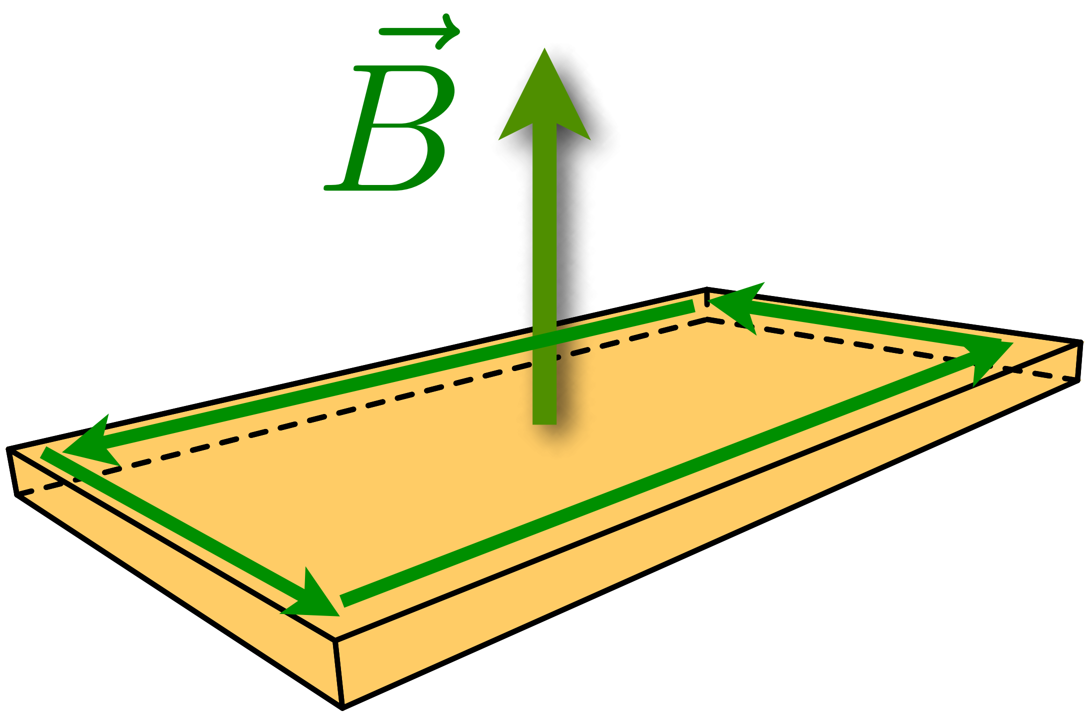






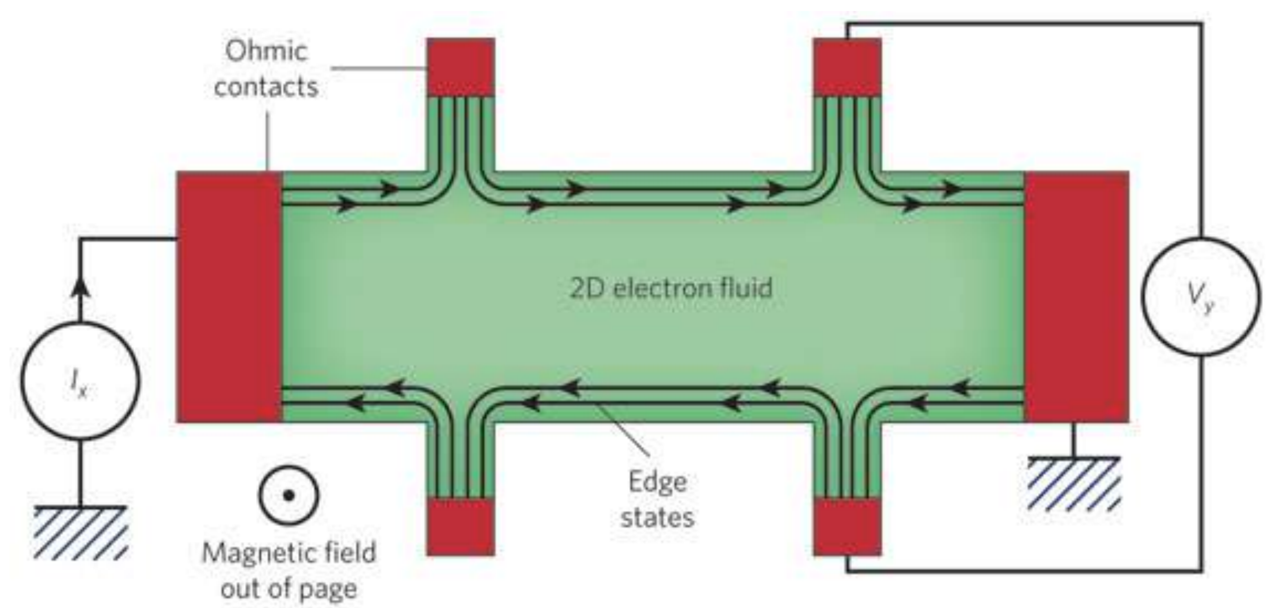
spin Hall insulator phase!

3. Dirac equation on a lattice.



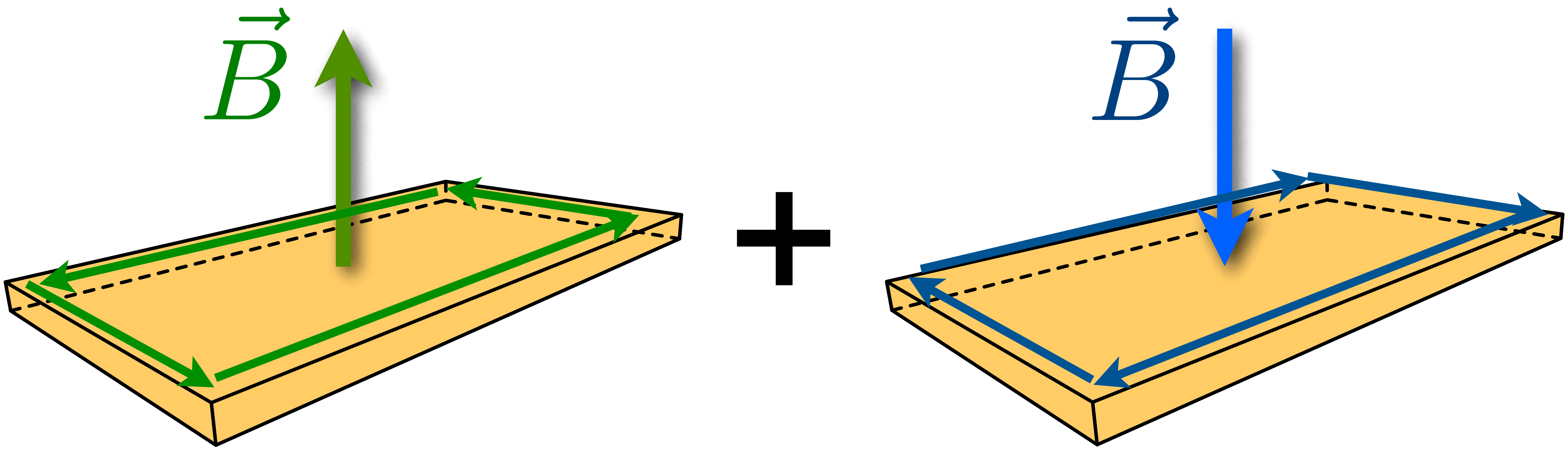
The presence of the magnetic field Induces the QHE phase: Finite (quantized) Hall conductivity and the presence of edge states

A magnetization is the same: Anomalous HE



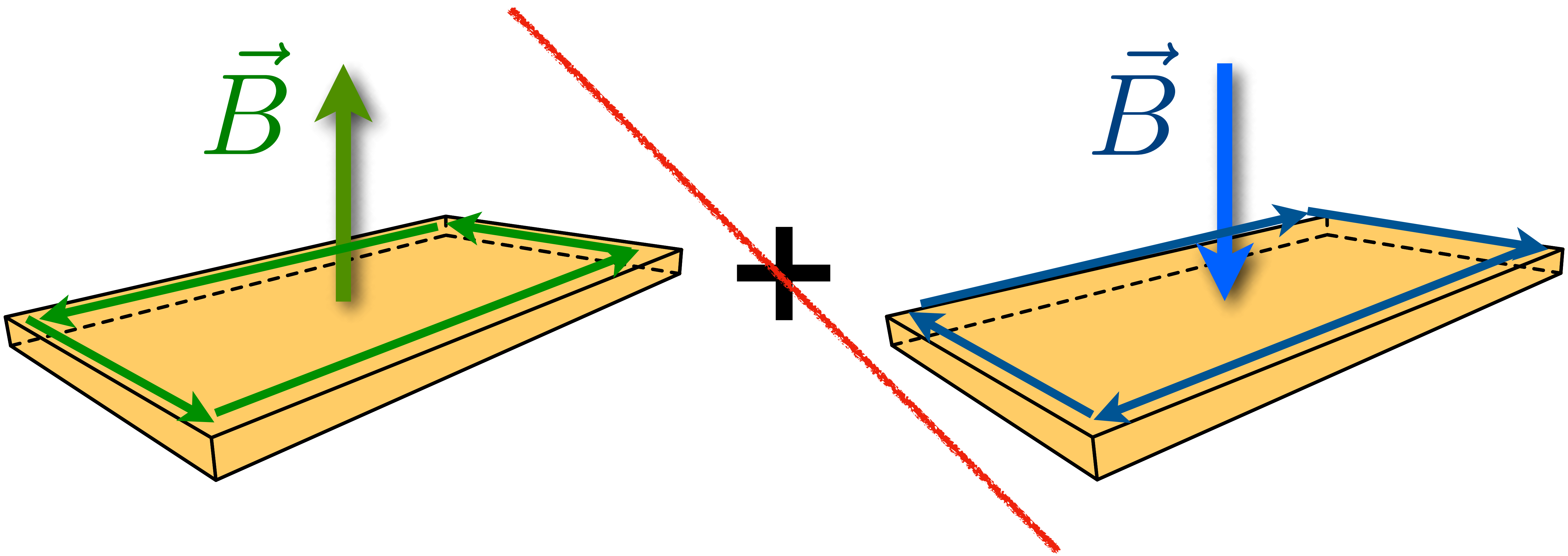
3. Dirac equation on a lattice.

$$t \to -t$$



3. Dirac equation on a lattice.

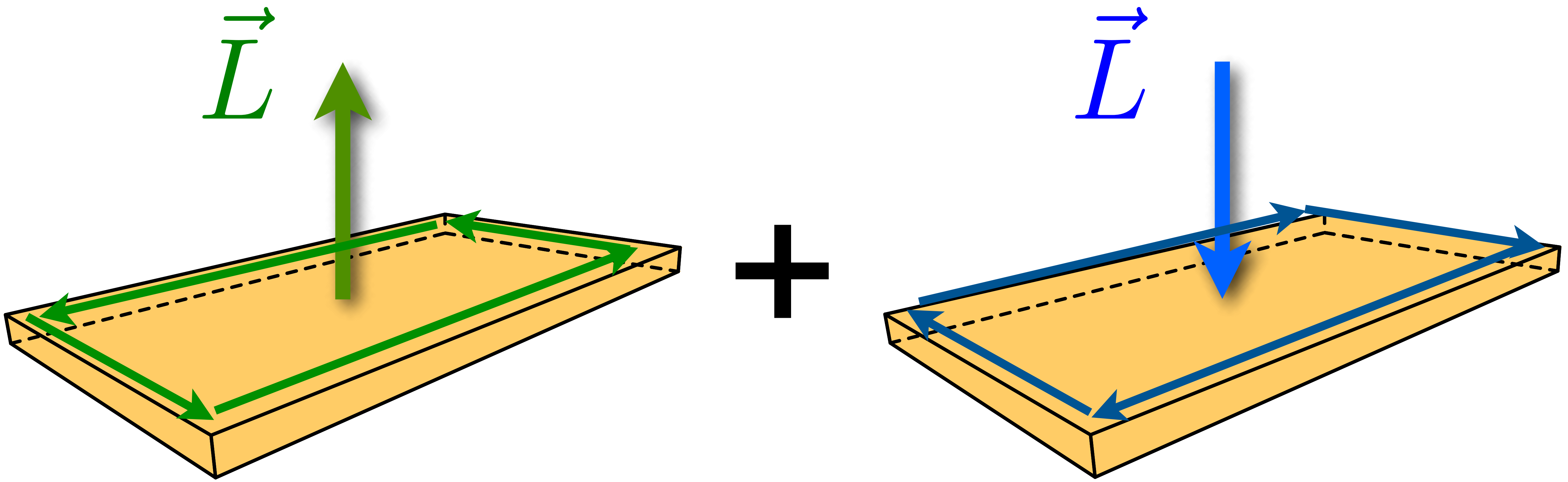
$$t \to -t$$



3. Dirac equation on a lattice.

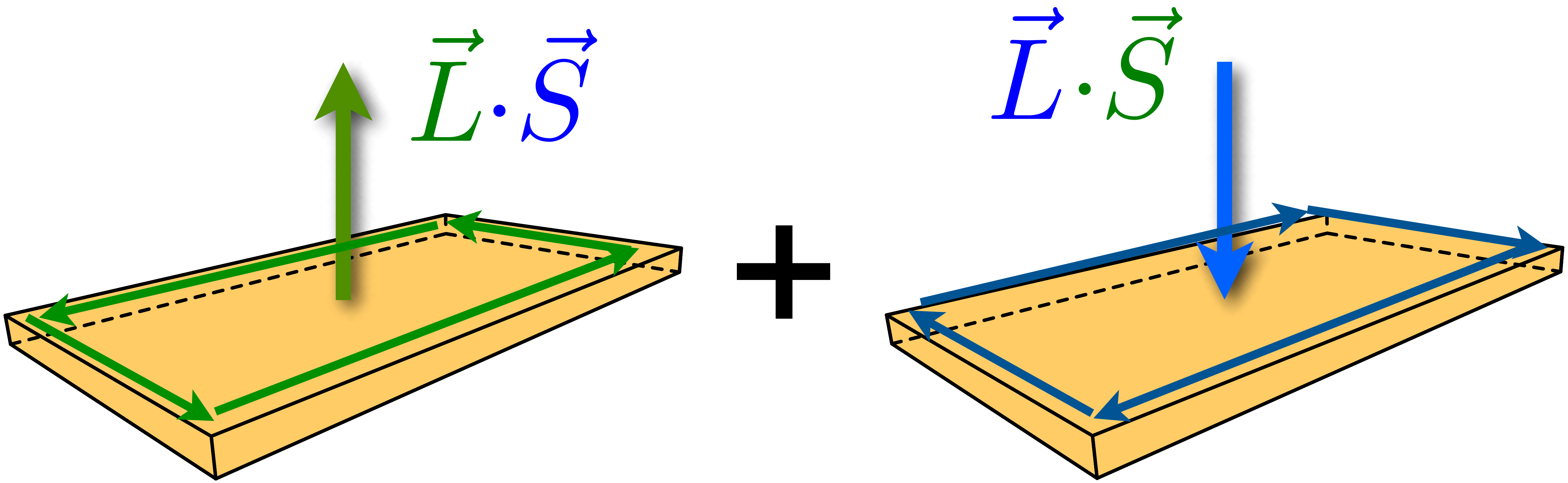
angular momentum plays the same role

$$t \rightarrow -t$$



3. Dirac equation on a lattice.

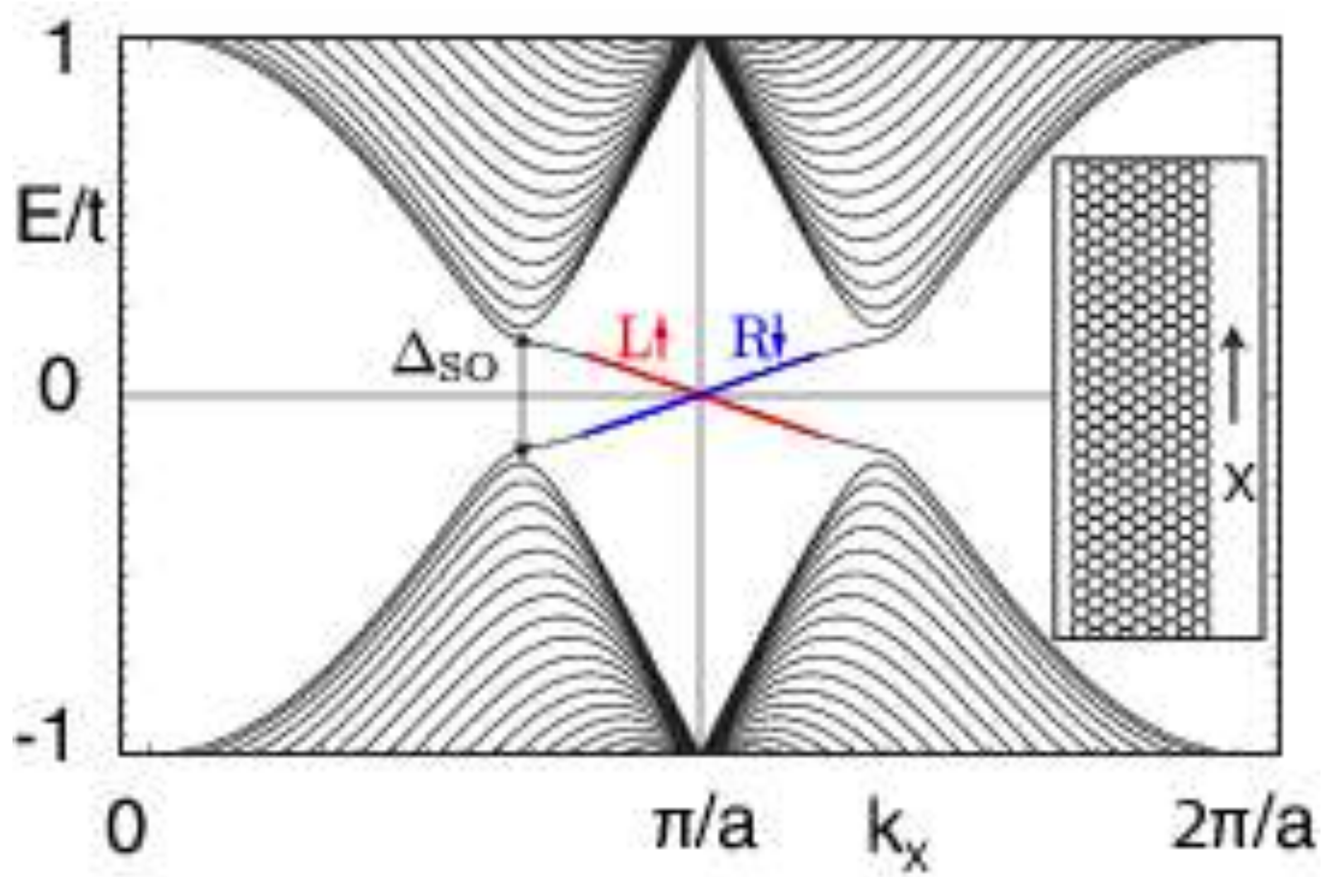
spin orbit term is time reversal invariant



Now Time reversal symmetric with the phenomenology
Of the Q(A)HE:
Quantum Spin Hall effect

3. Dirac equation on a lattice.

spin orbit term is time reversal invariant



Now Time reversal symmetric with the phenomenology
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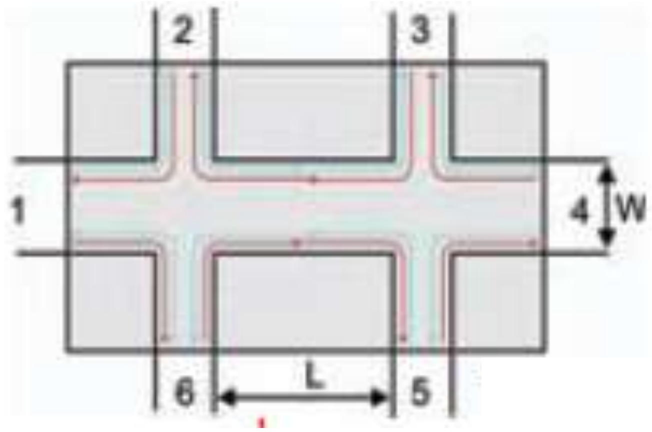
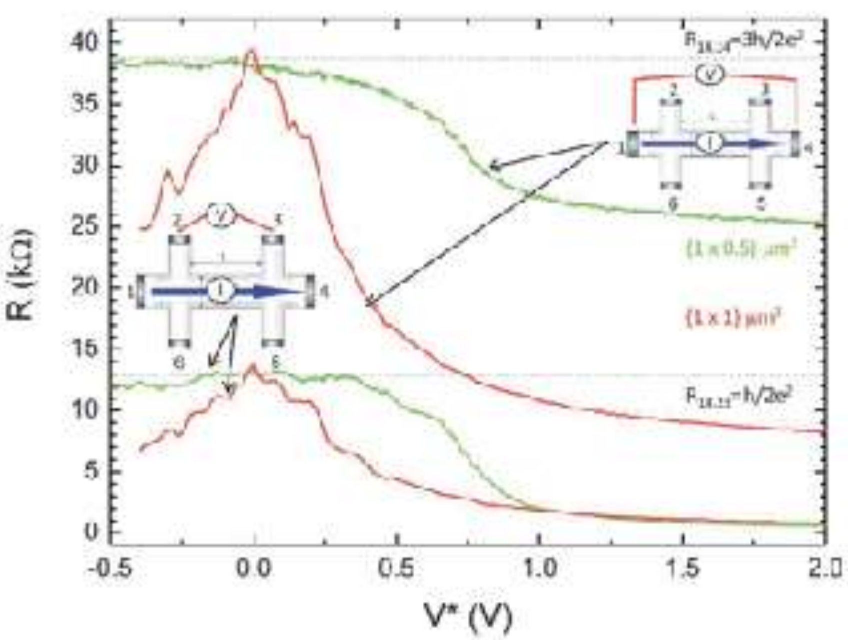
Quantum Spin Hall effect

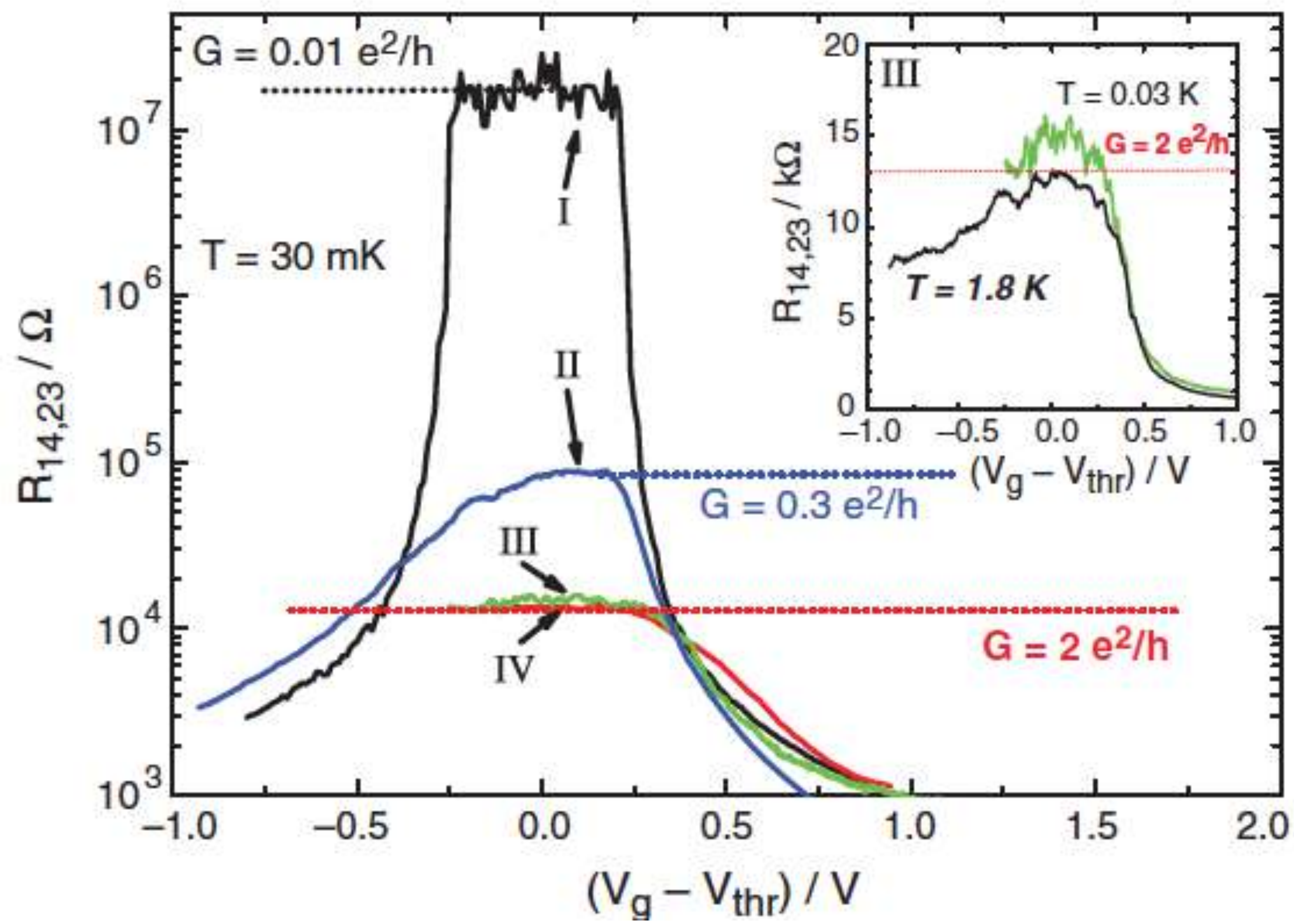
3. Physics of QHE with T: QSHE

L W Molenkamp (1956-)





A Roth et al. Science 325, 294 (2010)



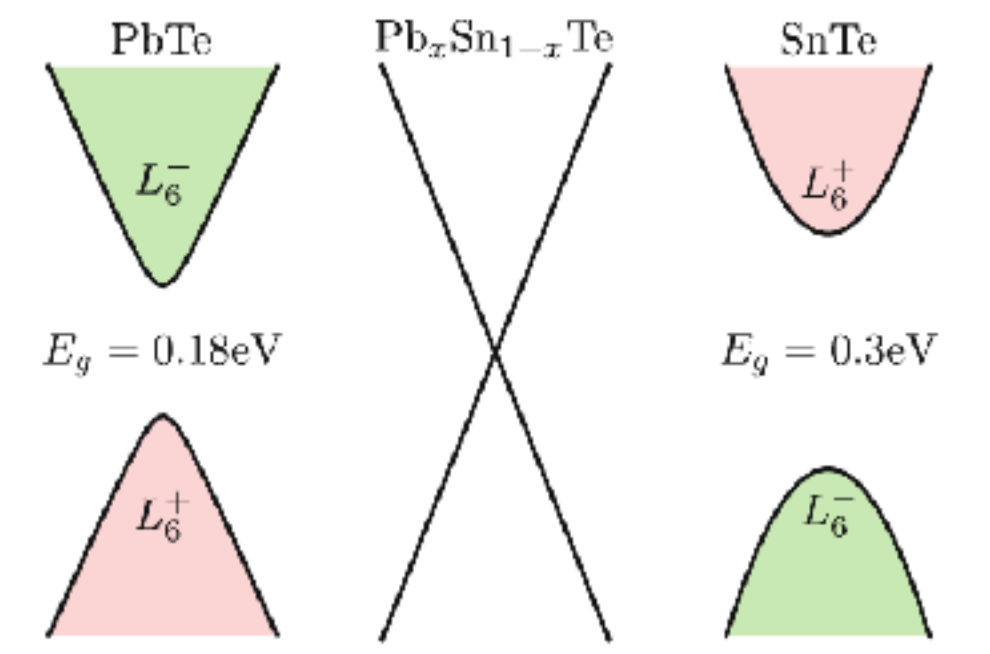
M Konig et al. Science 318, 766 (2007)

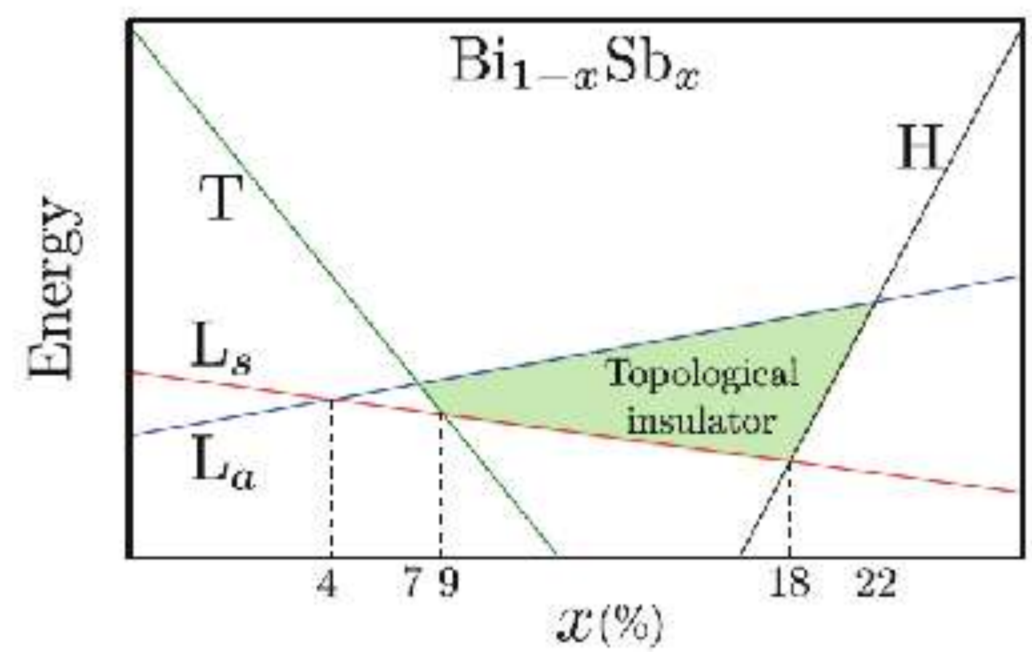
3. Dirac equation on a lattice: 3D

All we have discussed about symmetries applies to 3D as well

$$\begin{pmatrix} E - v\boldsymbol{\sigma}\cdot\boldsymbol{k} & m(\boldsymbol{k}) \\ m(\boldsymbol{k}) & E + v\boldsymbol{\sigma}\cdot\boldsymbol{k} \end{pmatrix} \begin{pmatrix} \phi_a \\ \phi_b \end{pmatrix} = 0$$

$$Pb_x Sn_{1-x} Te$$



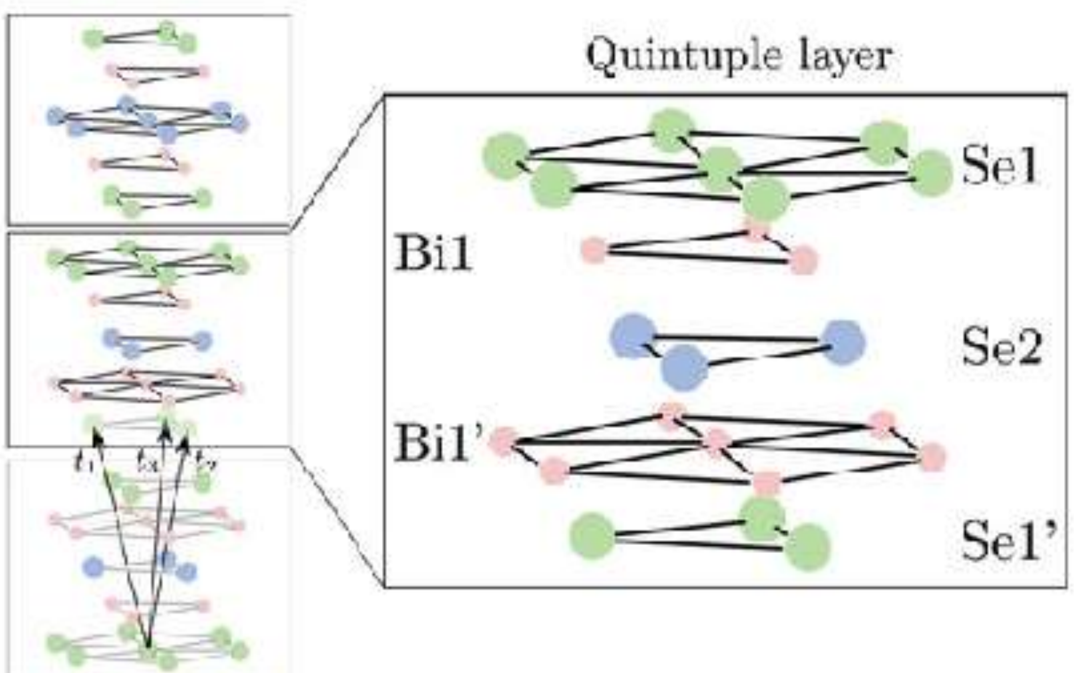


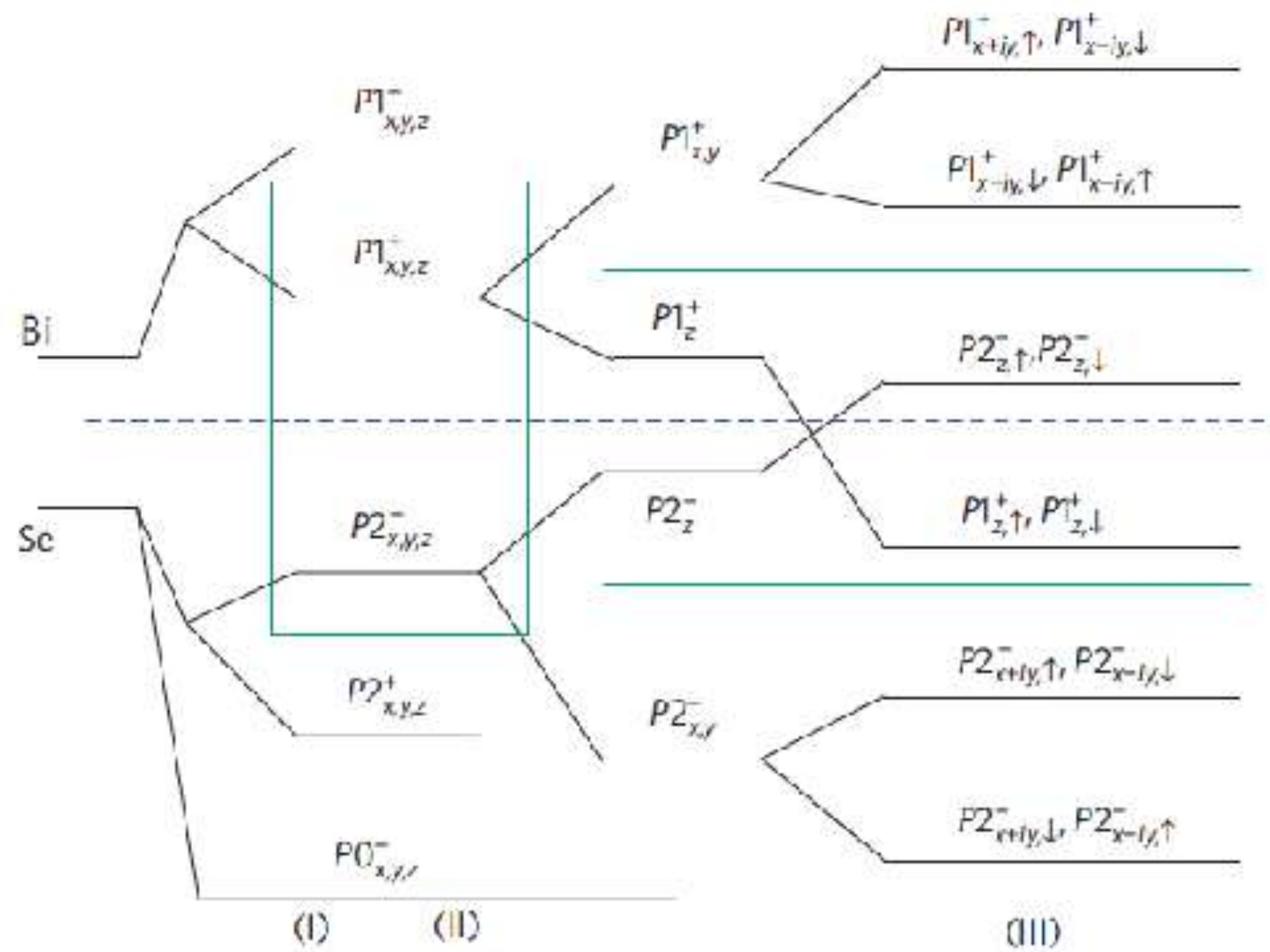
$$m(\boldsymbol{k}) = m_0 + \beta|\boldsymbol{k}|^2$$

3. Dirac equation on a lattice: 3D

All we have discussed about symmetries applies to 3D as well

$$\begin{pmatrix} E - v\boldsymbol{\sigma}\cdot\boldsymbol{k} & m(\boldsymbol{k}) \\ m(\boldsymbol{k}) & E + v\boldsymbol{\sigma}\cdot\boldsymbol{k} \end{pmatrix} \begin{pmatrix} \phi_a \\ \phi_b \end{pmatrix} = 0$$





$$m(\boldsymbol{k}) = m_0 + \beta|\boldsymbol{k}|^2$$

4. Conclusions

Dirac equation appears in the context of High Energy Physics to describe relativistic particles of semi-integer spin.

In Condensed Matter Physics, Bloch theorem together with time reversal and inversion symmetries allow for the same structure, both in 2D and in 3D, being the Dirac equation an emergent phenomenon.

The Dirac equation allows for the presence of edge states. The presence of these states is due to topological reasons linked to the bandstructure.

5. References.

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