# HIGHER INVARIANTS: TOPOLOGICAL INSULATORS

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# Main References

M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X. L. Qi, S. C. Zhang
*Science*, **318**, (2007), 766-770

D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava, M. Z. Hasan, *Nature*, **452**, (2008), 970-975

M. Z. Hazan, C. L. Kane, Topological Insulators, *Rev. Mod. Phys.*, **82**, (2010), 3045-3067

H. Schulz-Baldes, S. Teufel, *Comm. Math. Phys.*, **319**, (2013), 649-681

E. Prodan, B. Leung, J. Bellissard, "The non-commutative $n$th-Chern number ($n \geq 1$)", *(in preparation)*, (2013)

# Content

1. Topological Insulators
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3. The $\mathbb{Z}_2$-Invariant
4. Magneto-Electric Response

# I - TOPOLOGICAL INSULATORS

M. Z. Hazan, C. L. Kane, Topological Insulators, *Rev. Mod. Phys.*, **82**, (2010), 3045-3067

# Two Dimensional Compounds

M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X. L. Qi, S. C. Zhang
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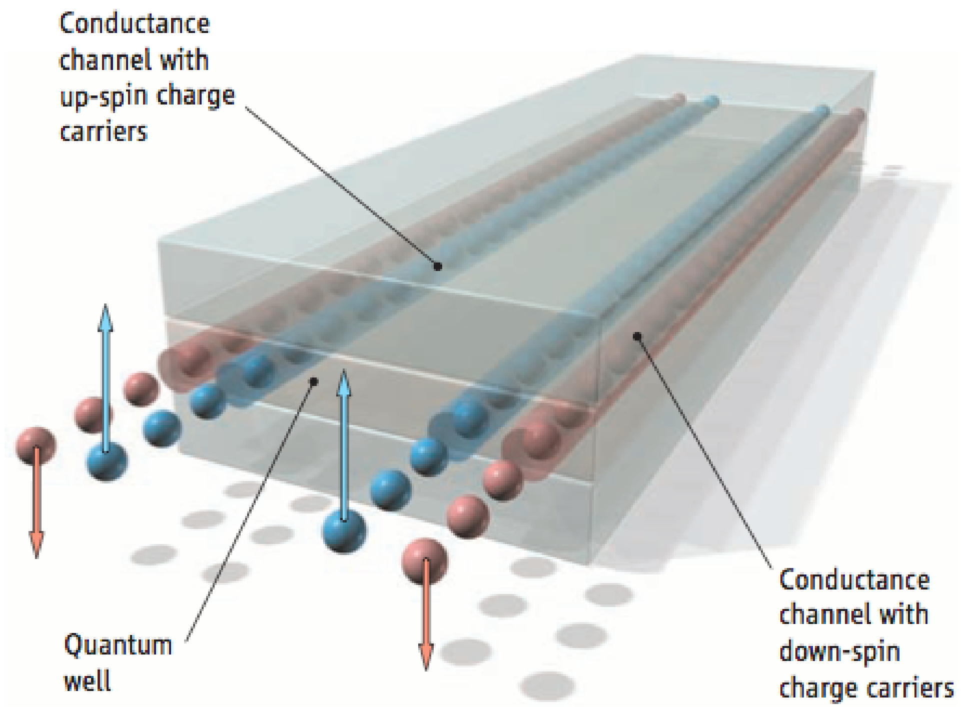


Schematic of the spin-polarized edge channels in a quantum spin Hall insulator.

2D-$HgTe$ semi-conductor with inverted band structure provide a way to create a spin polarized channel of electronic current, protected by topological invariant

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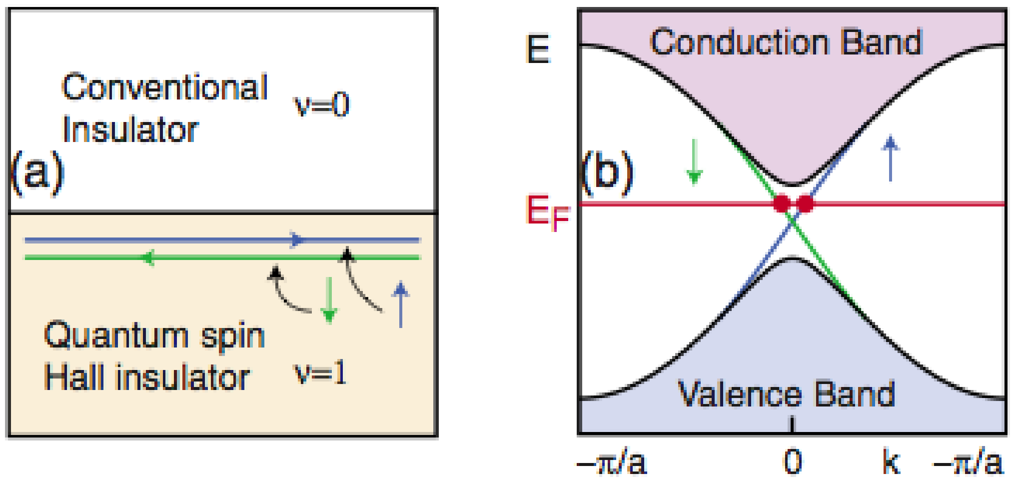


Edge states:
*Right* edge states interpolating between valence and conduction bands
Colors show the spin

*Slope =velocity*

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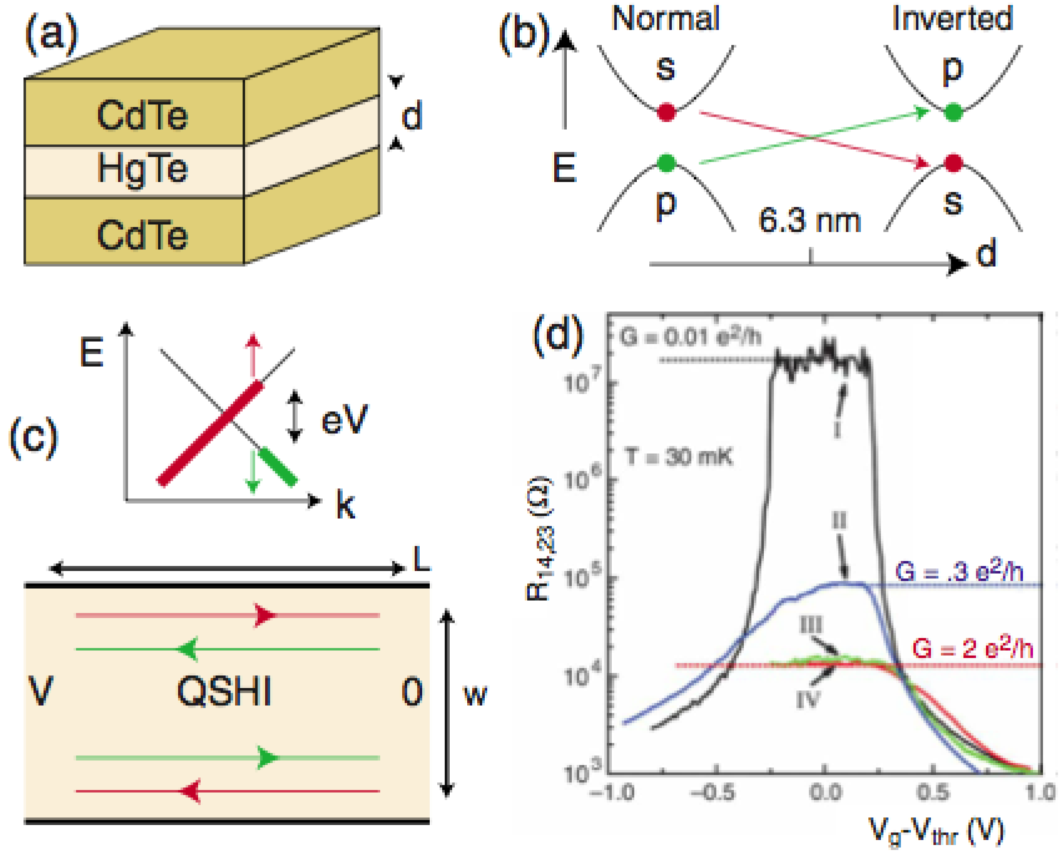


Edge states have quantized conductance

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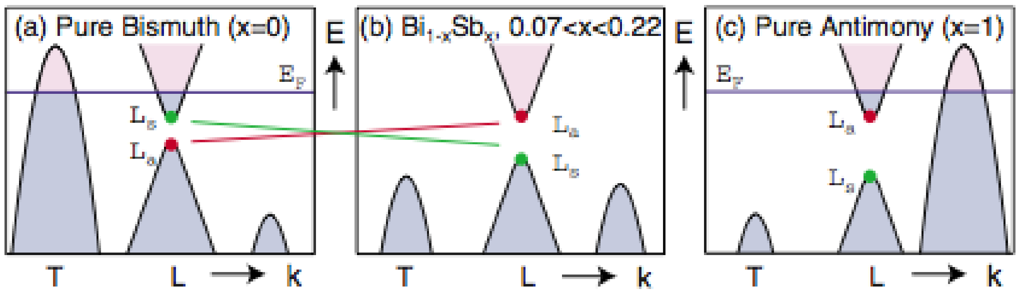


FIG. 8. (Color online) Schematic representation of the band structure of $Bi_{1-x}Sb_x$, which evolves from semimetallic behavior for $x<0.07$ to semiconducting behavior for $0.07<x<0.22$ and back to semimetallic behavior for $x>0.18$. The conduction and valence bands $L_{s,a}$ invert at $x\sim0.04$.

3D-$Bi_{0.9}Sb_{0.1}$
Inverted band structure

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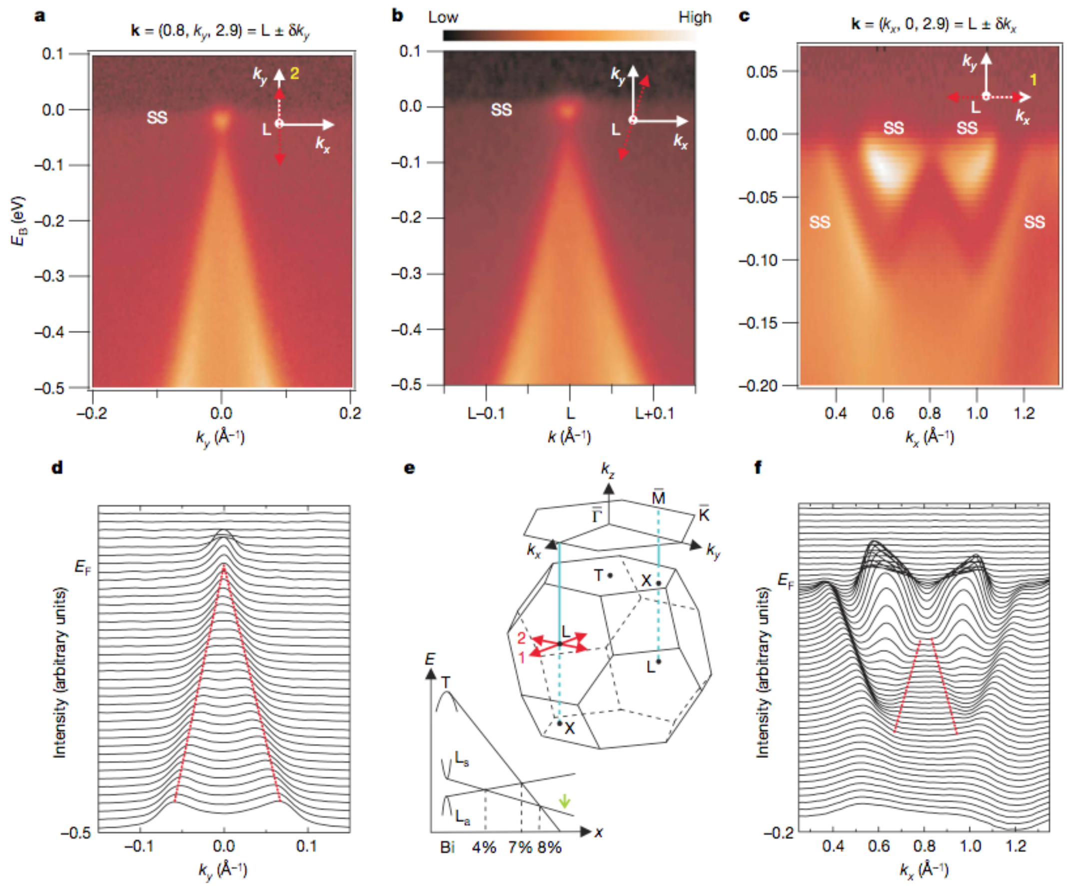


3D-$Bi_{0.9}Sb_{0.1}$
Dirac dispersion cone

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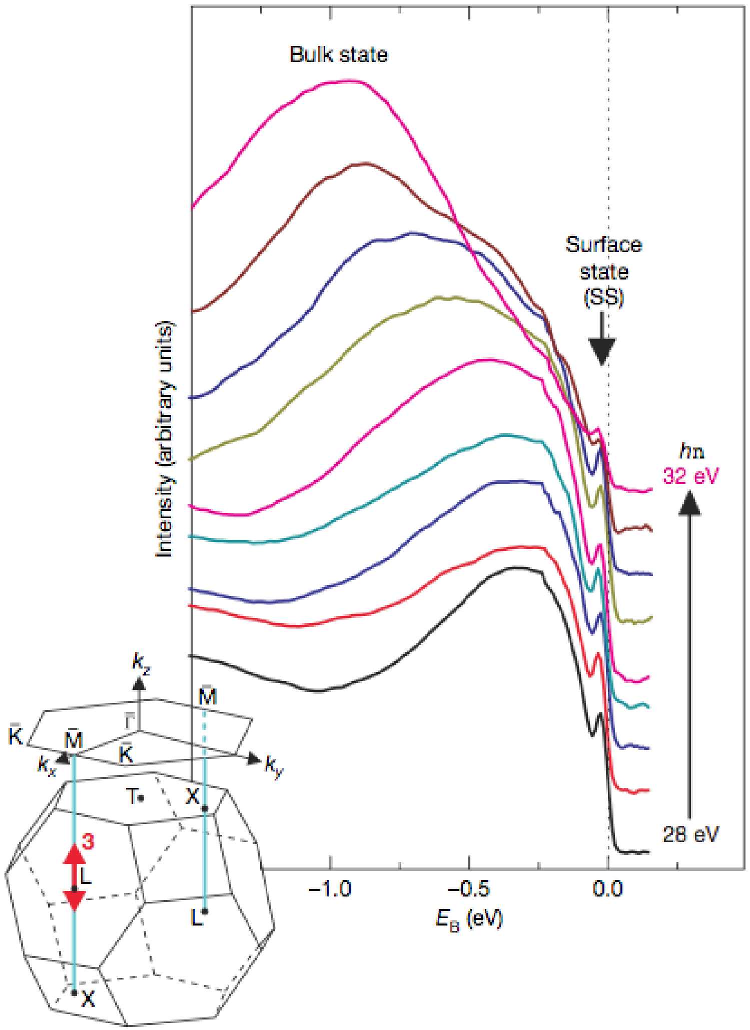
D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava & M. Z. Hasan,
*Nature*, **452**, (2008), 970-975



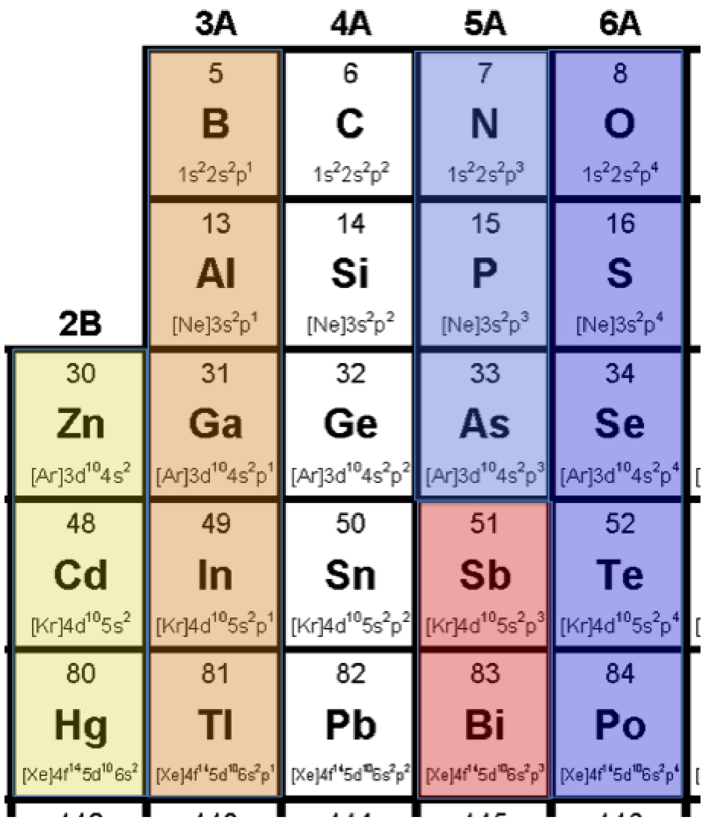

3D-$Bi_{0.9}Sb_{0.1}$
Surface states evidence

# II - Semiconductors

N. W. Ashcroft, N. D. Mermin, *Solid State Physics*, Holt, Rinehart and Winston Eds., (1976)

B. I. Shklovskii, A. L. Efros, *Electronic Properties of Doped Semiconductors*, Springer, (1984).

# The Columns II-VI



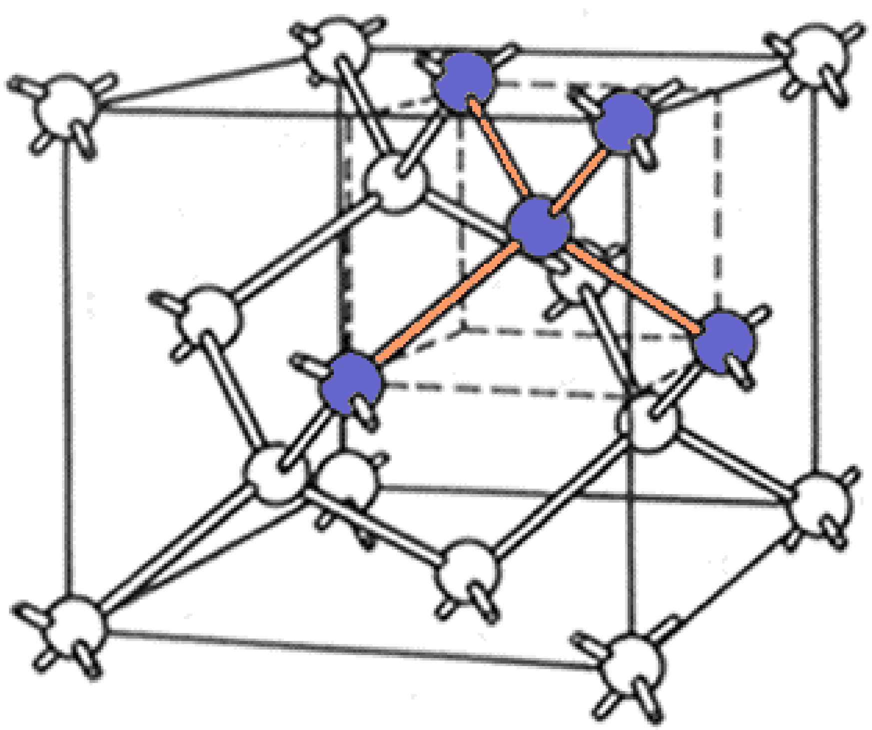

**Column IV:** *Si, Ge*
basic semiconductors,

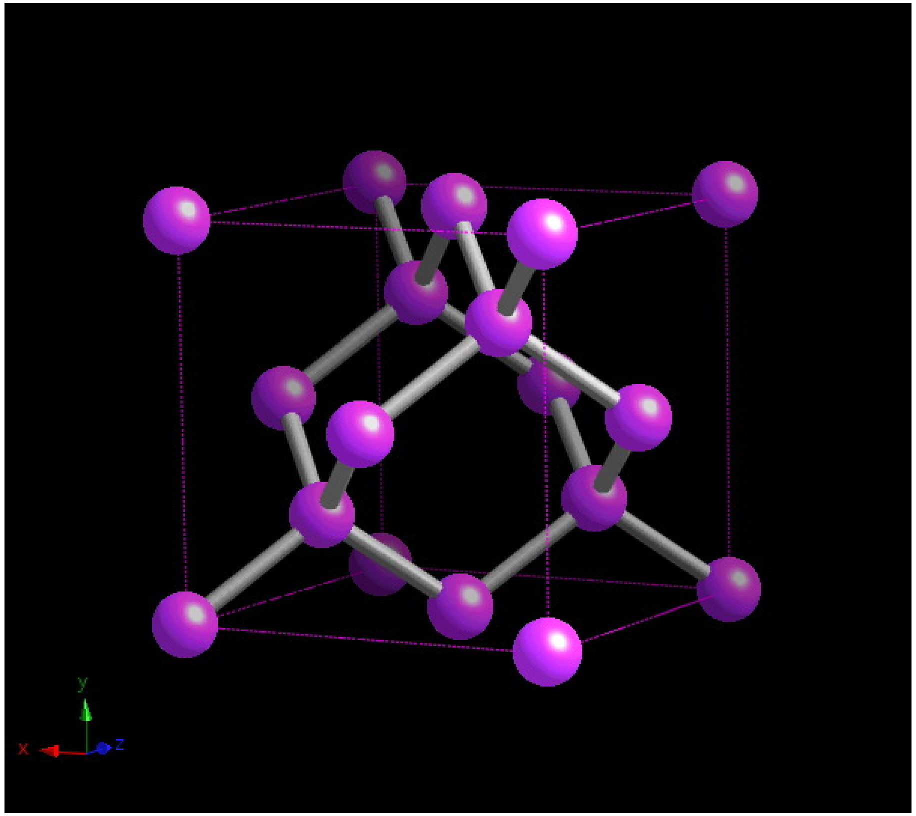
**III-V compound:**
like *Ga-As*

**II-VI compounds:**
like *Hg-Te, Cd-Te,*

**3D-compounds:**
$Bi_{1-x}Sb_x$

# The Diamond Lattice





# The Diamond Lattice

G. Leman, J. Friedel, *J. Appl. Phys.*, **33**, (1962), 281-285

- Projecting $\mathbb{Z}^4$ onto $\mathbb{R}^3$ perpendicular to $f = 1/2(1,1,1,1)$: each patch $\{m, m+e_1, m+e_2, m+e_3, m+e_4\}$ projects as a

*regular tetrahedron*

- If $i \in \{0,1,2,3\}$ then

$$\mathcal{E}_i = \left\{ m \in \mathbb{Z}^4 \,;\, \sum_{\alpha=1}^{4} m_\alpha = i \right\}$$

Then keep only the points in $\mathcal{E}_0 \cup \mathcal{E}_1$

- $m \in \mathcal{E}_0 \;\Leftrightarrow\; m + e_\alpha \in \mathcal{E}_1$ gives the *staggering* between tetrahedra.

# Chemical Bonds

G. Leman, J. Friedel, *J. Appl. Phys.*, **33**, (1962), 281-285

- Each atom has *4-valence electrons* in orbitals $s, p_x, p_y, p_z$ with same energy.
- Each such orbital is a *vector* in a Hilbert space $\Rightarrow \mathbb{C}^4$.
- Using the $\mathbb{Z}_4$ Fourier transform gives four linear combinations with the symmetry of the *tetrahedron*. The *electron density* points in space in the four directions of the tetrahedron.
- Each valence state creates a band in the lattice. The spins double their number, thus 8-*bands*
- Adding the $e-e$ *interaction* onsite leads to *splitting* of levels $\Rightarrow$ creates a gap between 4-*valence* and 4-*conduction* bands.

# Spin-Orbit Coupling

E. U. Condon, G. H. Shortley, *The Theory of Atomic Spectra*, Cambridge University Press (1935)

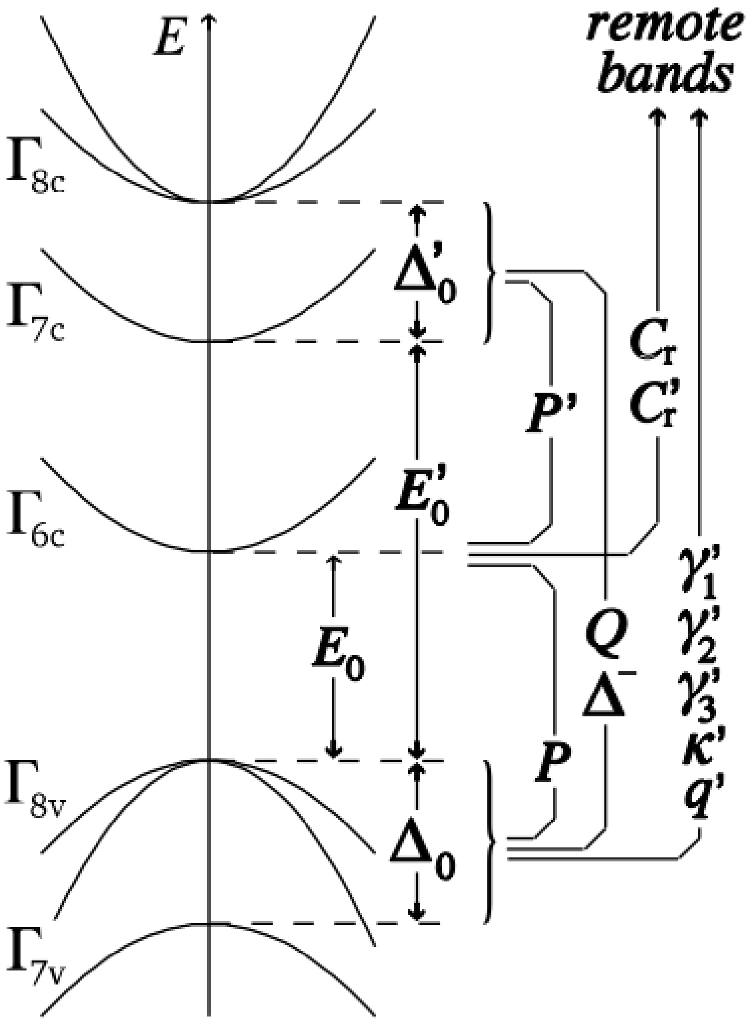
- The electron rotation around a nucleus creates a magnetic field which interact with its own spin (spin-orbit coupling)
- Relativistic corrections gives the spin-orbit energy

$$H_{SO} = \frac{\mu_B}{\hbar m_e e c^2} \frac{1}{r} \frac{\partial U(r)}{\partial r} \vec{L} \cdot \vec{S}$$

  - $\vec{L}$ is the *angular momentum*, $\vec{S}$ is the *spin*
  - $U(r)$ is the radial potential seen by the electron.
  - $\mu_B$=Bohr magneton, $m_e$=electron mass, $e$=electron charge, $c$=speed of light.

# Spin-Orbit Coupling

R. Winkler, *Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems*, Springer, (2003)




*If the diamond lattice is shared by* two atomic species*, the point symmetry between the two sublattices is broken. Then the spin-orbit interaction creates a* band splitting

# III - THE $\mathbb{Z}_2$-INVARIANT

M. Z. Hazan, C. L. Kane, Topological Insulators, *Rev. Mod. Phys.*, **82**, (2010), 3045-3067

M. Atiyah, I. M. Singer, Index Theory for Skew-Adjoint Fredholm Operators, *Inst. Hautes Études Sci. Publ. Math.*, **37**, (1969), 5-26

# Real Hilbert Spaces

- A Hilbert space can be seen as a *real Hilbert space* $\mathcal{H}$ equipped with a real linear operator $J$ such that

$$J^{-1} = J^T = -J \qquad\qquad \langle f|g\rangle_{\mathbb{C}} = \langle f|g\rangle_{\mathbb{R}} + \imath\langle Jf|g\rangle_{\mathbb{R}}$$

- Then $\mathbb{C}$ acts through $z = x + \imath y \mapsto x + Jy$
- A $\mathbb{C}$-linear operator $A$ is an $\mathbb{R}$-linear map such that $AJ = JA$.
- *Complex conjugacy* is given by an $\mathbb{R}$-linear map $C$ such that $C = C^{-1} = C^T$, $CJ + JC = 0$. Then any $f \in \mathcal{H}$ can be uniquely written as $f = f_0 + Jf_1$ with $Cf_i = f_i$

# Time Reversal Symmetry

- For the time dependent *Schrödinger equation* the time-reversal symmetry is given by $C$:

$$\imath\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi \quad\Rightarrow\quad -\imath\hbar\frac{\partial\overline{\psi}}{\partial t} = -\frac{\hbar^2}{2m}\Delta\overline{\psi} + V\overline{\psi}$$

- For the relativistic *Dirac equation* the time-reversal symmetry is given by an operator $\Theta$ such that $\Theta^2 = -1$. The same occurs for spin-orbit coupling.

- In the real version of Hilbert spaces this gives two $\mathbb{R}$-linear map $J, \Theta$ such that *(Clifford Algebra)*

$$J^{-1} = J^T = -J \qquad \Theta^{-1} = \Theta^T = -\Theta \qquad \Theta J + J\Theta = 0$$

# Kramers Degeneracy

- Let $H = H^*$ be a *time-reversal symmetric* selfadjoint operator. In the real version then $H$ is an $\mathbb{R}$-linear map on $\mathcal{H}$ commuting with both $J, \Theta$.

- If $f \in \mathcal{H}$ is an *eigenstate* of $H$, namely $Hf = Ef$, then $H\Theta f = E\Theta f$ is another one.

- However $\langle \Theta f | f \rangle_{\mathbb{C}} = 0$. Since $\|f\| = \|\Theta f\|$, it follows that every eigenvalue is *twice degenerate*.

# Momentum Space

- If the Hamiltonian is *periodic* on the diamond lattice, Bloch theory implies that it can be seen as a $k$-dependent $8 \times 8$-matrix with $k \in \mathbb{B} \simeq \mathbb{T}^3$. Matrix *indices* label the *8-orbitals* close to the Fermi level.
- *Time reversal* symmetry implies

$$\Theta H(k) \Theta^{-1} = H(-k)$$

- Let $\Lambda$ be the set of points in the Brillouin zone such that $k = -k$.
- At each point $k \in \Lambda$, the matrix $H(k)$ commutes with $\Theta$ and its eigenstates are *Kramers-degenerate*.

# The $\mathbb{Z}_2$-index

- Each *occupied band*, labelled by $m$, is given by a Bloch function $u_m(k)$ with values in the Hilbert space $\mathcal{H}$. Let

$$W_{m,n}(k) = \langle u_m(k) | \Theta u_n(-k) \rangle$$

- $W(k)$ is unitary and $W^T(k) = -W(-k)$. In particular it is *antisymmetric* at points of $\Lambda$.

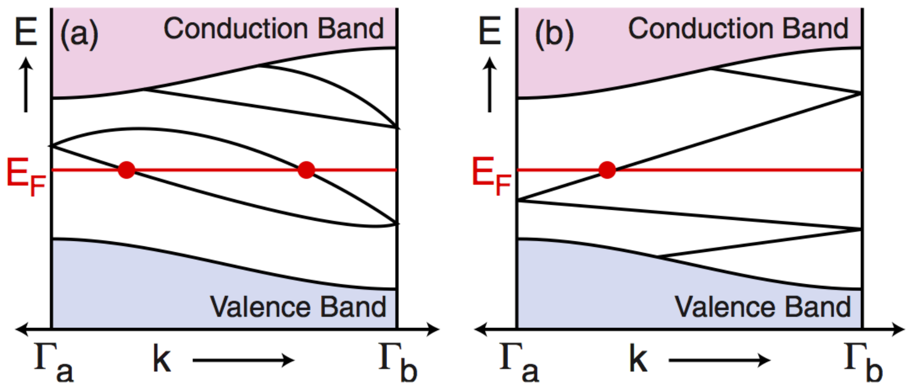
  *(Smoothness is required ! The $u_m(k)$ must be time-reversal "compatible" !)*

- Then the *$\mathbb{Z}_2$-index* $\nu \in \mathbb{Z}_2$ is defined by

$$(-1)^{\nu} \stackrel{def}{=} \prod_{k \in \Lambda} \frac{\mathrm{Pf}[W(k)]}{\sqrt{\det(W(k))}}$$

# Edge States

- In experiments, a *spin-polarized current* is protected on the *edges* of the quantum well. This edge is $1D$.
- Truncated space along the edge leads to new *eigenstates in the Fermi gap*. The corresponding eigenfunction are *localized* on the edges. If the edge is a straight line, the periodicity along the edge allows to use Bloch theory with $k \in \mathbb{T}$.




*Edge states are* doubly degenerate *on* $\Lambda$. *The* parity *of the number of states with energy* $E_F$ *is given by* $\nu$

# Disordered Case: Numerical Results

E. Prodan, B. Leung, *Phys. Rev. B*, **85**, 205136, (2012)

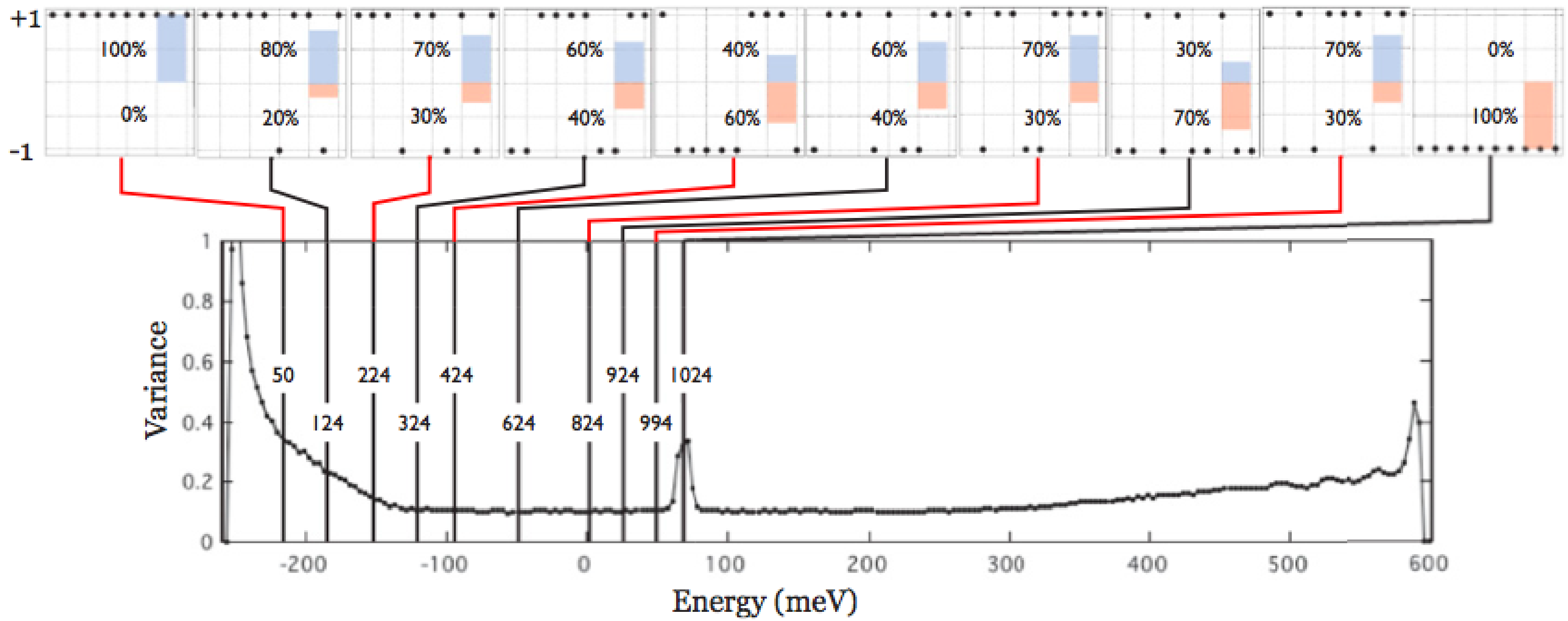



FIG. 5. (Color online) The upper panels show the $\mathbb{Z}_2$ invariant computed along the path (1) of Fig. 4 on an $8\times8\times8$ unit-cell lattice via twisted boundary conditions. The dimension of the occupied space was slowly reduced from 1024 to 124, as indicated in the figure. For each $\mathbb{Z}_2$, the calculation was repeated for 10 random disorder configurations and the output is shown by the full dots, exactly how it occurs in the actual calculation. The percentages of the $\mathbb{Z}_2 = \pm 1$ occurrences are displayed in each panel. The lower panel shows the variance of the level spacings for $W = 300$ meV, and the averaged Fermi levels (see the vertical lines) corresponding to each $\mathbb{Z}_2$ calculation.

## Open Problems

- Is the definition of $\nu$ amenable to an index theory valid also for *disordered systems* ?

- Atiyah-Singer developed a $\mathbb{Z}_2$-index theory for antisymmetric Fredholm operators. Is $\nu$ equal to such an index ?

# IV - MAGNETO-ELECTRIC RESPONSE

# Main References

## Periodic Case:


R. D. King-Smith, D. Vanderbilt, *Phys. Rev. B*, **47**, (1993), 1651-1654

X. L. Qi, T. L. Hughes, S. C. Zhang, *Phys. Rev. B*, **78**, (2008), 195424

A. M. Essin, J. E. Moore, D. Vanderbilt, *Phys. Rev. Lett.*, **102**, (2009), 146805

A. M. Essin, A. M. Turner, J. E. Moore, D. Vanderbilt, *Phys. Rev. B*, **81**, (2010), 205104

A. Malashevich, I. Souza, S. Coh, D. Vanderbilt, *New J. Phys.*, **12**, (2010), 053032


## Disordered Case:


B. Leung, E. Prodan, *J. Phys. A: Math. and Theor.*, **46**, (2013), 085205

H. Schulz-Baldes, S. Teufel, *Comm. Math. Phys.*, **319**, (2013), 649-681

E. Prodan, B. Leung, J. Bellissard, "The non-commutative $n$th-Chern number ($n \geq 1$)", *(in preparation)*, (2013)

# Magneto-Electric Response Coefficient

- The *magnetization* $\vec{M}$ induced by the electronic *orbital* motion induced by a small *electric field* $\vec{E}$ is given to lowest order by the response coefficient at zero magnetic field $\vec{B}$

$$\alpha_{ij} = \left.\frac{\partial M_j}{\partial E_i}\right|_{\vec{B}=0}$$

- Equivalently the electric *polarization* $\vec{P}$ of the orbital motion induced by a small *magnetic field* is also given by the same coefficient

$$\alpha_{ij} = \left.\frac{\partial P_i}{\partial B_j}\right|_{\vec{E}=0}$$

# Magneto-Electric Response Coefficient

- For a periodic $3D$-insulator, with Bloch functions $u_m(k)$ representing the *occupied bands* let $\mathcal{A}_j^{mn}$ be the *Berry connection* defined by

$$\mathcal{A}_j^{mn}(k) = \left\langle u_m(k) \left| \frac{\partial}{\partial k_j} \, u_n(k) \right. \right\rangle$$

- *Then the tracial part is given by* *(Qi, Hughes, Zhang '06)*

$$\theta \stackrel{def}{=} \frac{1}{3}\sum_{i=1}^{3} \alpha_{ii} = \frac{1}{2\pi} \int_{\mathbb{B}} d^3k \, \epsilon^{ijl} \, \mathrm{Tr}\left[\mathcal{A}_i \partial_j \mathcal{A}_l - \frac{2\imath}{3} \mathcal{A}_i \mathcal{A}_j \mathcal{A}_l\right]$$

- The *r.h.s.* is a topological invariant called the *Chern-Simons action*.

# Polarization

- There is a problem in *defining unambiguously* the electric polarization of a solid.
- However the *change* of the polarization under an adiabatic evolution can be defined through *perturbation theory* *(King-Smith & Vanderbilt '93)*. *(Ex.: piezoelectric, magnetoelectric response)*
- The *adiabatic* variation of the polarization is given by

$$\frac{\partial \vec{P}}{\partial \lambda} = \mathcal{T}_{\mathbb{P}}\left[\rho(\lambda)\, \vec{J}(\lambda)\right] \qquad \vec{J}(\lambda) = \imath\left[H(\lambda), \vec{X}\right]$$ **(charge current)**

where $\rho(\lambda)$ is the adiabatic evolution of the *density matrix* defining the quantum state of the system.

# Polarization

- Let $\lambda \in [0,1] \mapsto H(\lambda)$ be a *smooth* adiabatic evolution of the Hamiltonian. It will be assumed that a *spectral gap persists* along the way at the Fermi level and that $\rho(\lambda = 0) = P_F$.
- The adiabatic evolution is driven by

$$\imath\epsilon \frac{\partial \rho}{\partial \lambda} = [H(\lambda), \rho(\lambda)] \qquad\qquad \epsilon \downarrow 0$$

- Then *(King-Smith & Vanderbilt '83, Schulz-Baldes & Teufel '13)*

$$\Delta\vec{P} = \int_0^1 d\lambda \, \frac{\partial \vec{P}}{\partial \lambda} = \int_0^1 d\lambda \, \mathcal{T}_{\mathbb{P}}\Big(P_F(\lambda) \left[\partial_\lambda P_F(\lambda), \vec{\nabla} P_F(\lambda)\right]\Big) + O(\epsilon^\infty)$$

# Magnetization

- A similar formula can be established for the $3D$-magnetization $\vec{M}$ at zero temperature *(Schulz-Baldes & Teufel '13)*

$$M_i = \frac{\imath\, \epsilon^{ijk}}{2} \mathcal{T}_{\mathbb{P}} \Big( |E_F - H| \, \big[ \partial_j P_F, \partial_k P_F \big] \Big)$$

- The previous formula holds also if the *Fermi level* belongs to a *mobility gap*, namely if $P_F \in \mathcal{S}$ is Sobolev *(Schulz-Baldes & Teufel '13)*.

# Magneto-Electric Response Coefficient

- Differentiating the polarization *w.r.t.* to the magnetic field can be done using a *Itô derivative* $\delta_B$ acting on the observable algebra *(JB '88)*

- It gives *(Leung & Prodan '13)*

$$\theta = \frac{1}{2}\int_0^1 d\lambda\, \mathcal{T}_{\mathbb{P}}\left(P_F dP_F dP_F dP_F dP_F\right) + \frac{\imath}{3}\,\mathcal{T}_{\mathbb{P}}\left((1-2P_F)dP_F\delta_B P_F\right)\Big|_{\lambda=0}^{\lambda=1}$$

- Here $\lambda$ is introduced as a *fourth dimension* and then

$$df = \partial_\lambda f d\lambda + \sum_{i=1}^{3} \partial_i f dk_i$$

# Magneto-Electric Response Coefficient

- If $\gamma$ is *adiabatic smooth paths* in the the Hamiltonian space, let $\Theta\gamma$ be the path obtained in the Hamiltonian space by *time-reversal symmetry*. Then $\gamma - \Theta\gamma$ is a *loop* in the Hamiltonian space.
- The magneto-electric response is then given by *(Qi, Hughes, Zhang '06, Leung & Prodan '13)*

$$\Delta\theta(\gamma - \Theta\gamma) = \frac{1}{2}\oint_{\gamma-\Theta\gamma} d\lambda\, \mathcal{T}_{\mathbb{P}}\left(P_F dP_F dP_F dP_F dP_F\right) = \frac{1}{2}\mathbf{Ch}_2(P_F)$$

- This formula is still valid provided $P_F$ belongs to the Sobolev space $\mathcal{W}^{2,4}(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$ *(Leung, Prodan, JB '13)*

$$\mathcal{W}^{2,4}(\mathcal{A}, \mathcal{T}_{\mathbb{P}}) = \left\{ A \in \mathcal{A}\,;\, \mathcal{T}_{\mathbb{P}}(|A|^2) + \left(|\vec{\nabla} A|^4\right)^{1/2} < \infty \right\}$$

# Sobolev Norm & Localization

- The expression

$$\ell_4(E_F) = \left(|\vec{\nabla} P_F|^4\right)^{1/4}$$

has the dimension of a *length* and can be seen as a milder version of the *localization length* at the Fermi level.

- **Theorem** *In the case of strong enough independent disorder at each lattice site, the Aizenman-Molčanov technique apply to prove that* $\ell_4(E_F)$ *is finite so that* $P_F \in \mathcal{W}^{2,4}$

# Conclusion

- *the second Chern number* $\mathbf{Ch}_2(P_F)$ *is an integer.* (Connes '83)
- *The magneto-electric response* $\Delta\theta(\gamma - \Theta\gamma)$ *at zero magnetic field along an adiabatic loop of the Hamiltonian, is quantized and is given by half the second Chern number of the Fermi projection.*
- $\Delta\theta(\gamma - \Theta\gamma)$ *is either an integer or half an integer; both character survive in the limit of zero magnetic field, namely for topological insulators with non trivial* $\mathbb{Z}_2$ *invariant there are loops for which* $\Delta\theta(\gamma - \Theta\gamma)$ *is half an integer.*
- *This quantization survives if the solid is disordered whenever the Fermi level belongs to a mobility gap.*

*Thanks for listening !*