# *Lecture course.*
# *Electronic structure of topological insulators and superconductors*

## *Part 1: Topological insulators*

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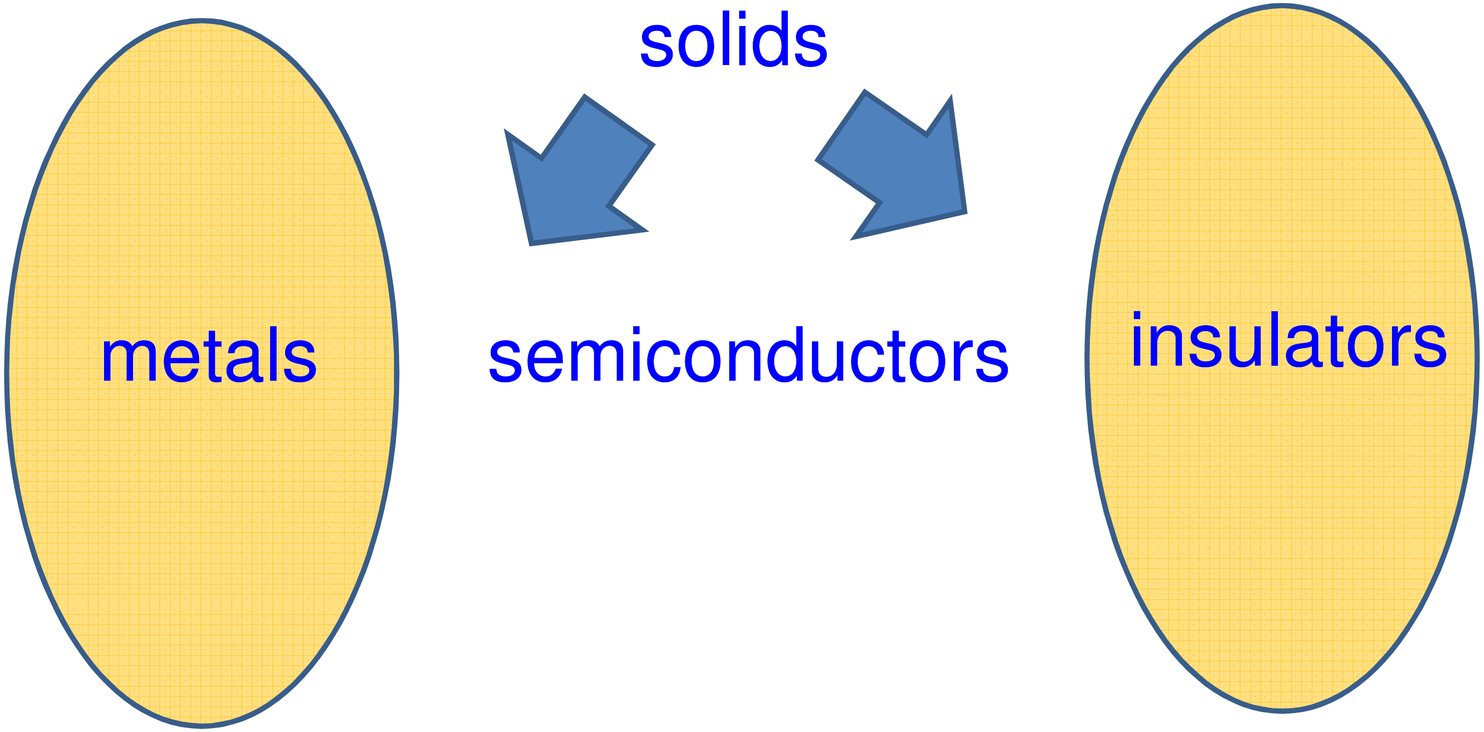
# *New state of matter*




Topological insulators are like insulators in the bulk and like metals at the surface

Neither fish nor meat….

# Outline

- **“Insulator”: What does it mean?**
  Band theory of solids.

- **“Topology”: What does it mean?** Some examples.

- **Are there states in the energy gaps of solids?**
  Tamm and Shockley states

- **Edge states and topology.**
  Quantum Hall effect.

- **Band inversion as an important mechanism of generation of topologically protected states. Volkov-Pankratov solution.**

- **2D topological insulators, HgTe/CdTe quantum wells.**

- **3D topological insulators.**

# Band theory of solids. Metals and insulators

$$\left(-\frac{\hbar^2\nabla^2}{2m}+U(\vec{r})\right)\psi=\varepsilon\psi$$

$$U(\vec{r})=U(\vec{r}+\vec{a})$$

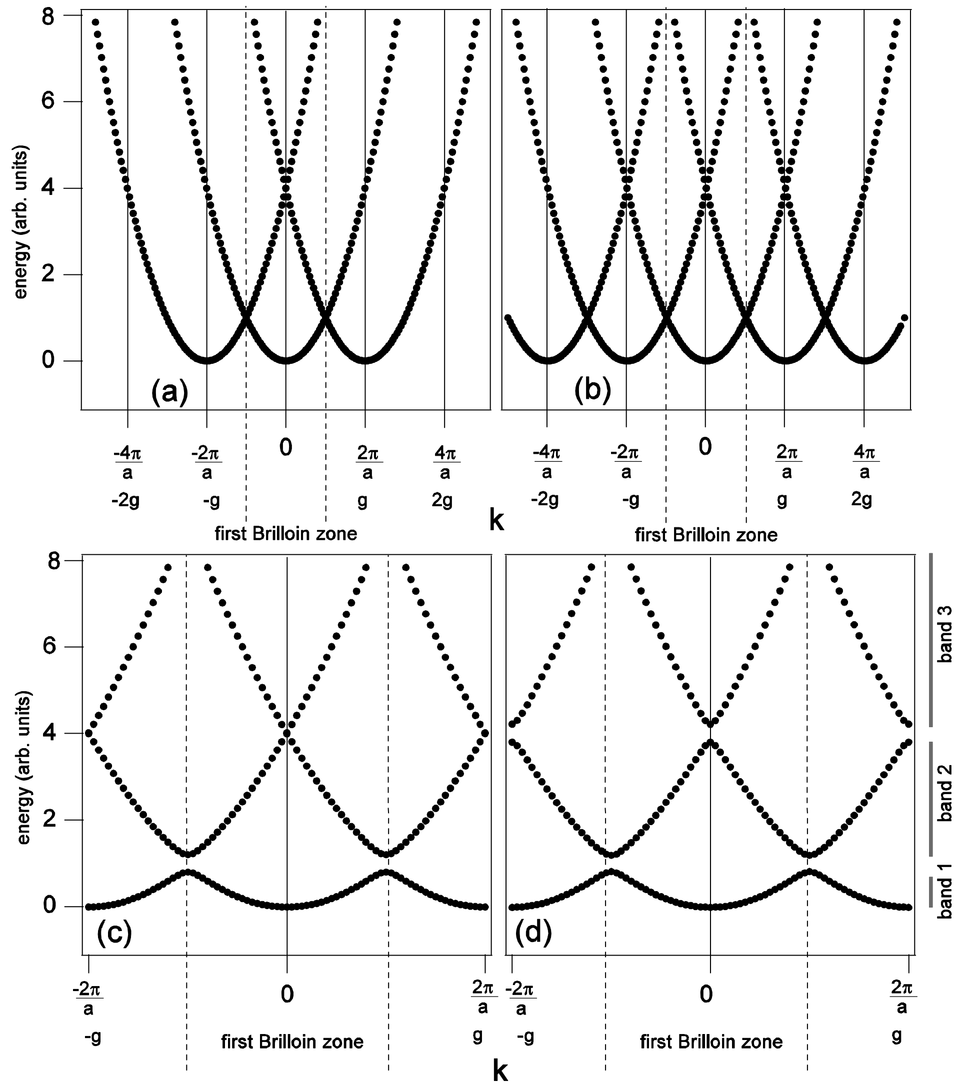
Bloch theorem

$$\psi_{s\vec{k}}=e^{i\vec{k}\vec{r}}u_{s\vec{k}}$$

$$u_{s\vec{k}}(\vec{r})=u_{s\vec{k}}(\vec{r}+\vec{a})$$

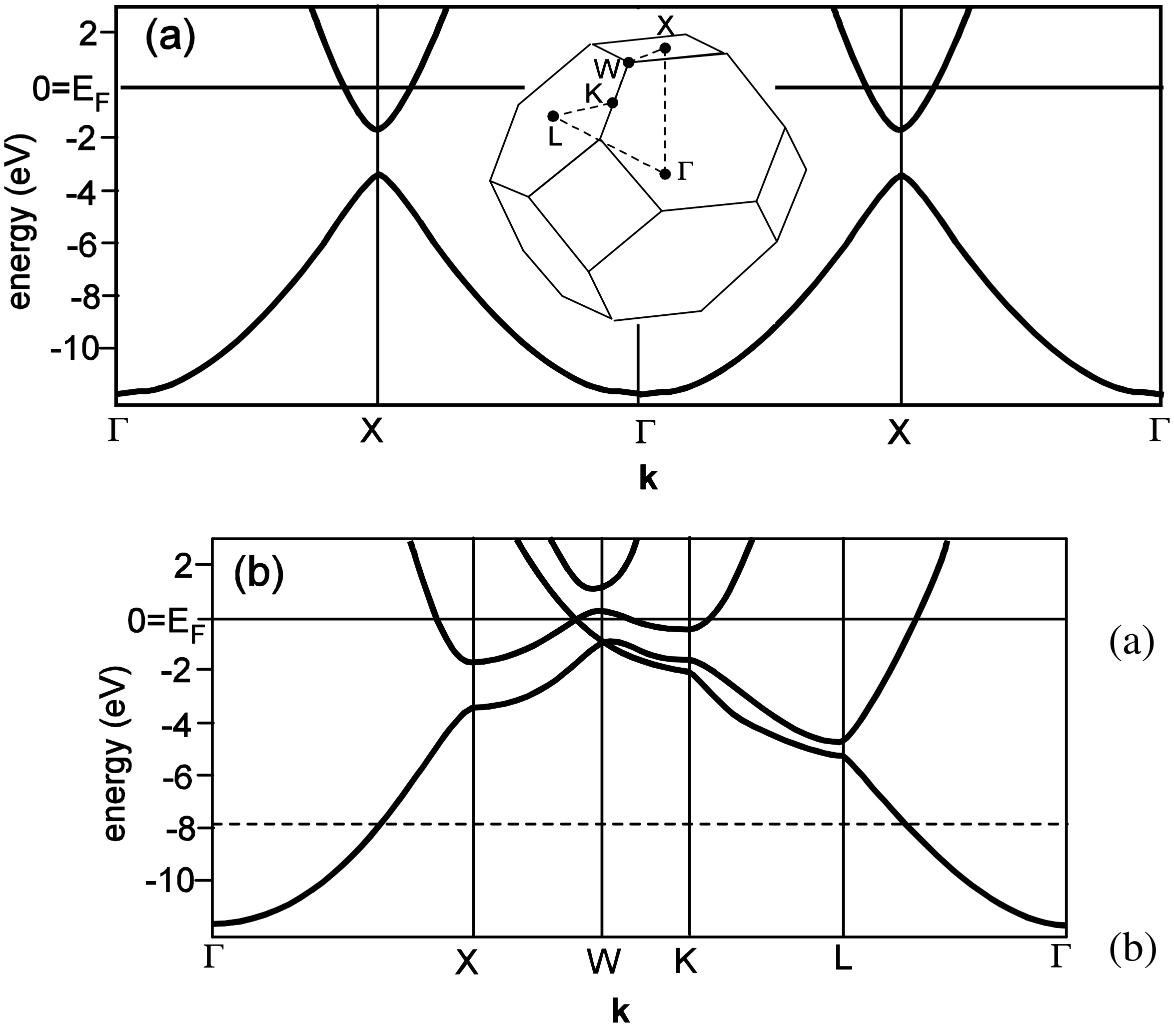
Energy vs quasimomentum

$$\varepsilon_s(\vec{k})=\varepsilon_s(\vec{k}+\vec{b})$$



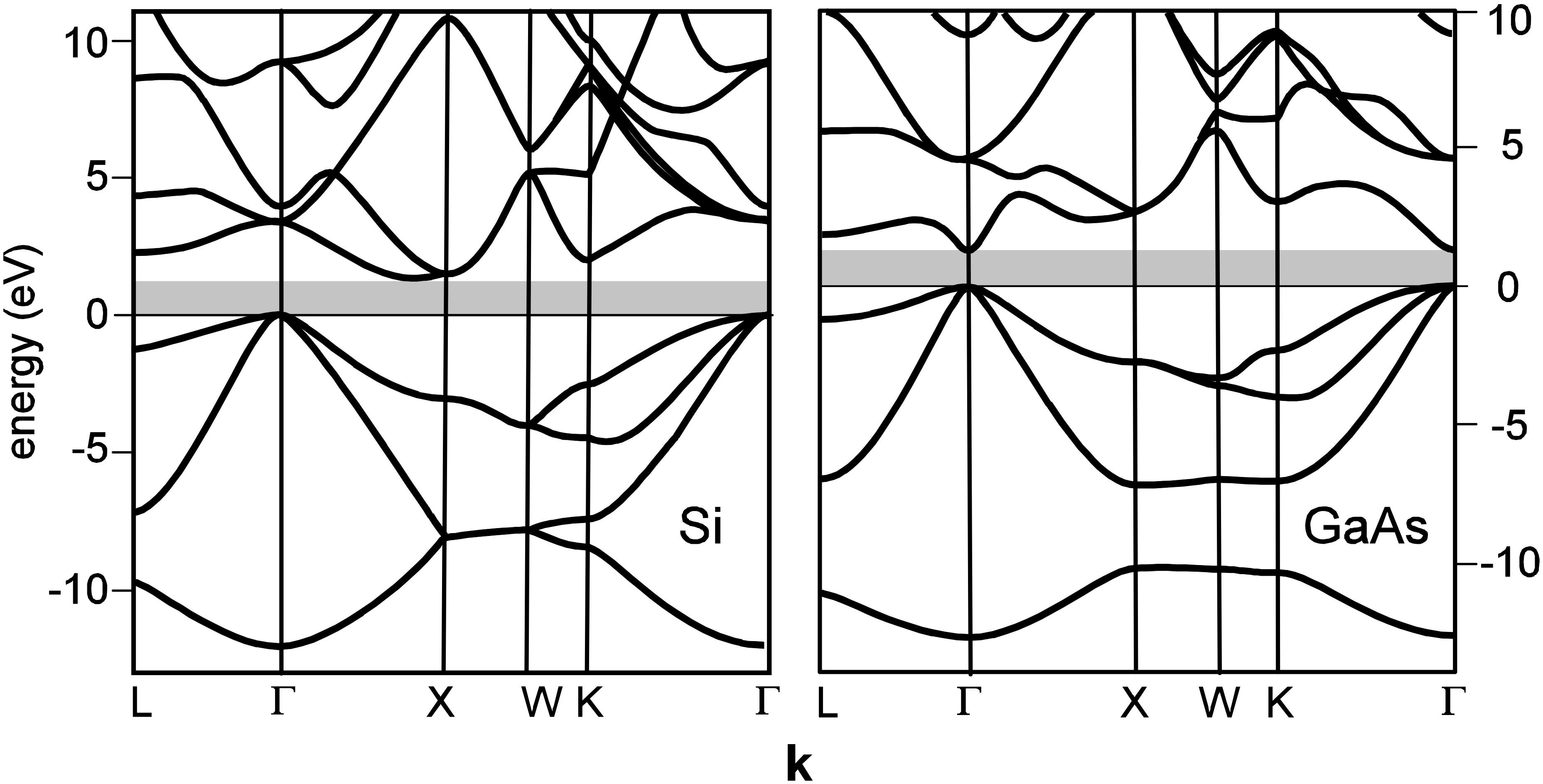
# FCC

(face centered cubic )




(a) Electronic energy bands in Al along the direction only. The inset shows the first Brillouin zone. (b) Energy bands in different directions given by the dashed path between high symmetry points of the Brillouin zone.

(b) The horizontal dashed line represents the fictitious Fermi level for aluminium with the same structure but only one valence electron instead of three. Band structure from H. .J. Levinson *et al.* , Phys. Rev. B **27**, 727 (1983).




Electronic energy bands for Si and GaAs. These materials have the same Brillouin zone as Al (see Fig. 1.6). The bands below the grey zone are completely filled and the bands above the grey zone are completely empty at zero temperature. The grey region represents an absolute band gap in the electronic structure. Band structures from M. Rohlfing *et al.* , Phys. Rev. B **48**, 17791 (1993).

# Band theory of solids. Metals and insulators

Spin projection as a quantum number

$$\sigma = \pm \frac{1}{2}$$

$$\vec{\sigma} = \left(\sigma_x, \sigma_y, \sigma_z\right)$$

Spin-orbit interaction and time – reversal symmetry

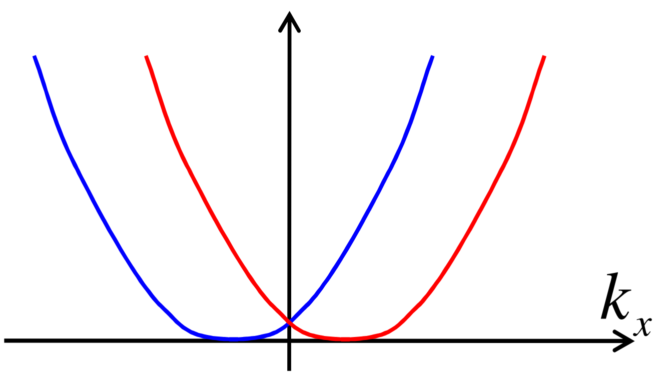
$$V_{so} = -\frac{e\hbar}{4m^2c^2}\vec{\sigma}\left[\vec{E}, \hat{\vec{p}}\right]$$

Kramers theorem and band spectrum

$$T\psi = i\sigma_y \psi^*$$

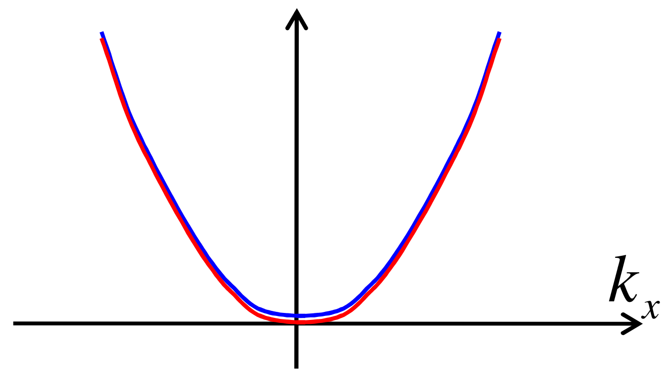
No inversion symmetry

$$\varepsilon_\sigma\left(\vec{k}\right) = \varepsilon_{\sigma'}\left(-\vec{k}\right)$$




Inversion symmetry

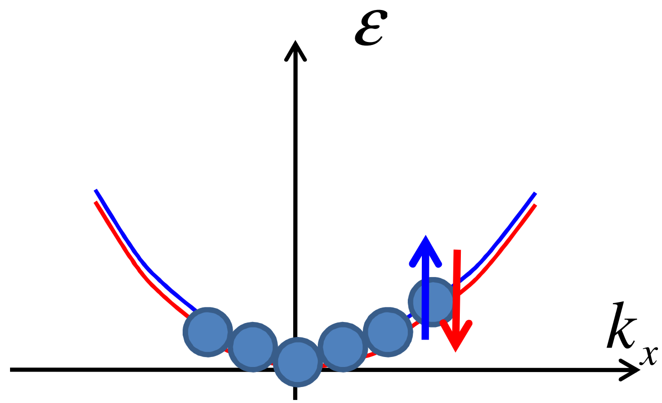
$$\varepsilon_\sigma\left(\vec{k}\right) = \varepsilon_\sigma\left(-\vec{k}\right)$$



# Band theory of solids. Metals and insulators

Q: How do we fill the bands by electrons?

A: by pairs with opposite spin
(if there are no spin-orbit effects)




N= number of k – states in each band
2N = number of states in the band accounting spin

Even or odd number of electrons in a primitive cell

# Band theory of solids. Metals and insulators

## Tight-binding approach

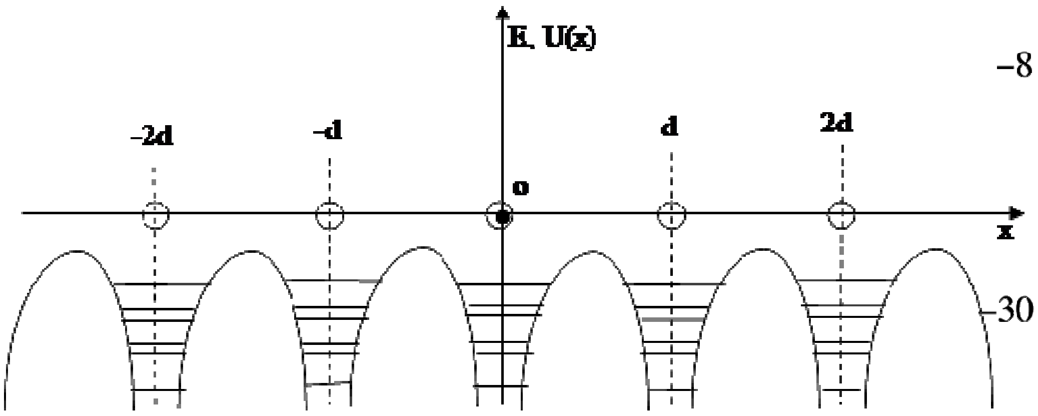
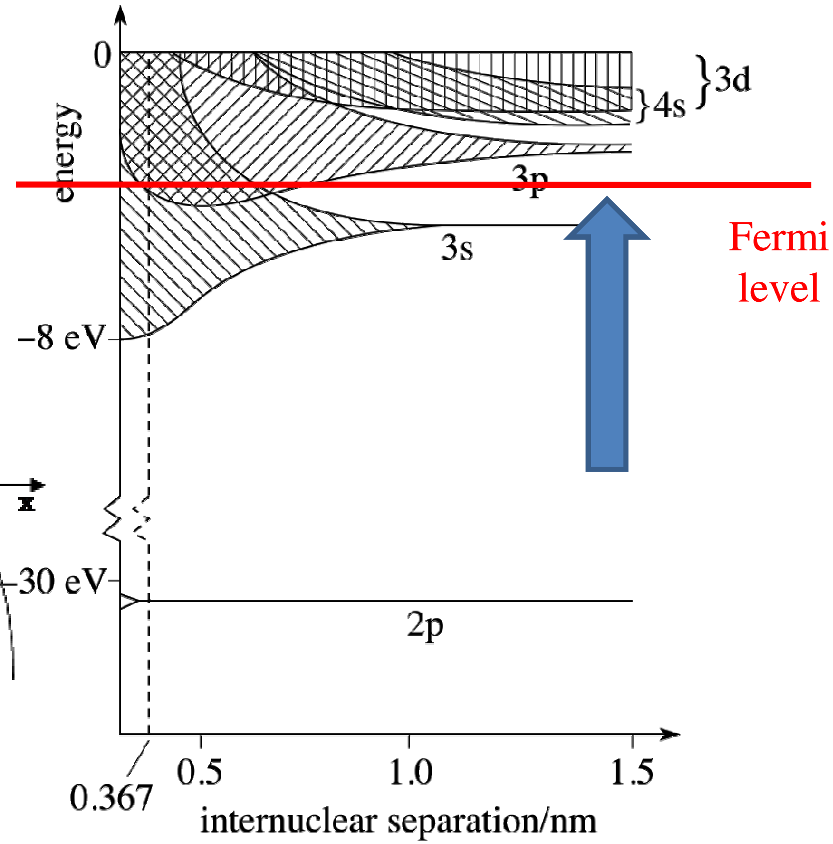



Рис. 5.1

## From insulator to metal. Overlapping of bands



# Band theory of solids. Metals and insulators

## Tight-binding approach

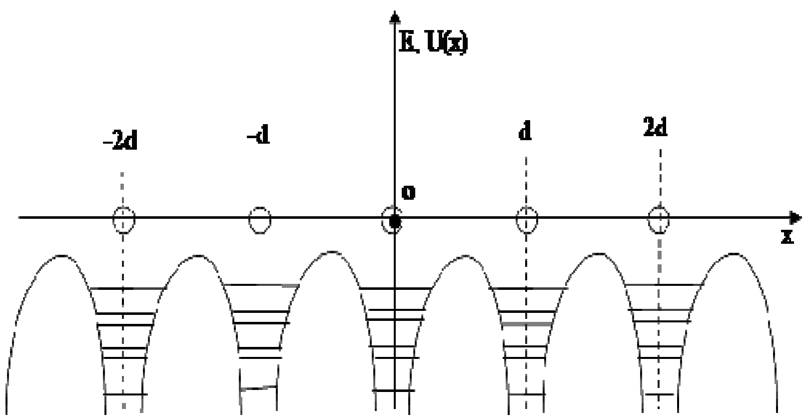
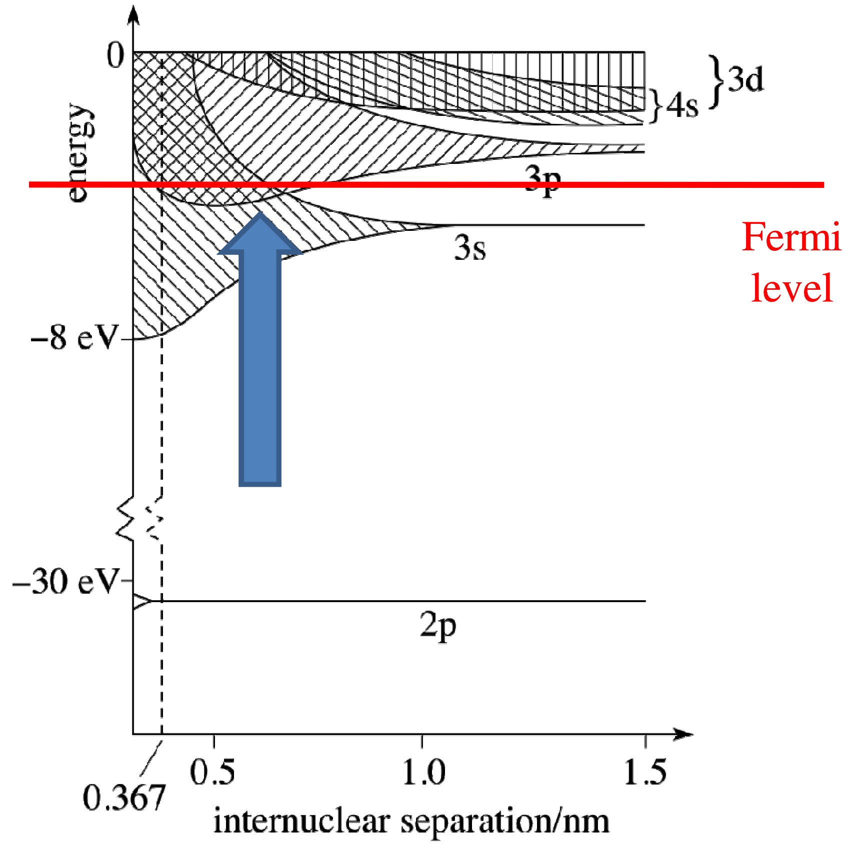
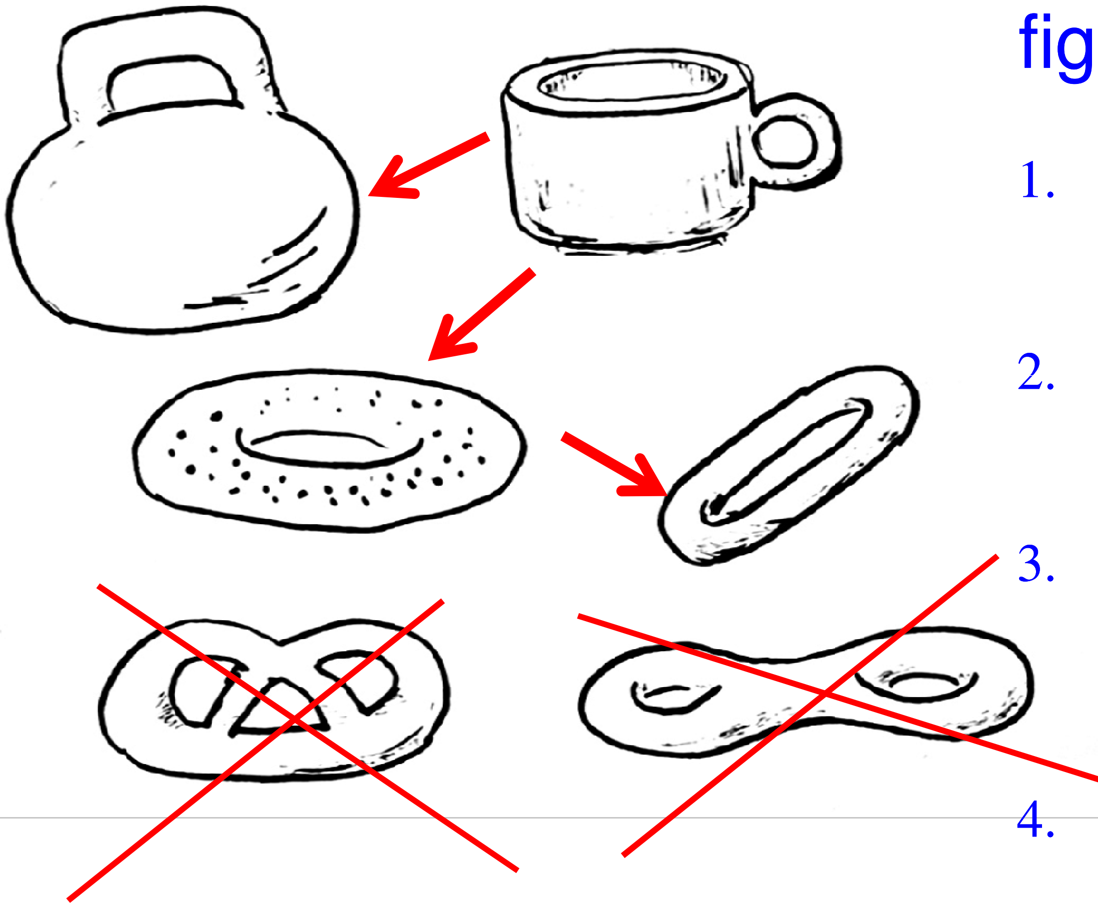



Рис. 5.1

## From insulator to metal. Overlapping of bands



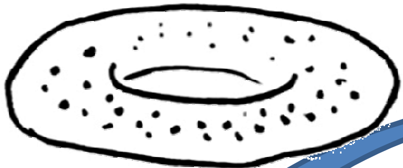
# *Topological arguments.*
# *The idea of "smooth" changes*



## How can we define that figures are "equal"?

1. We find some common property.
2. We find some number which characterizes this property.
3. This number must conserve under smooth transformations.
4. We call the number "topological invariant"

# Topological arguments.
# Why do we need them in physics?



"smooth" transformations

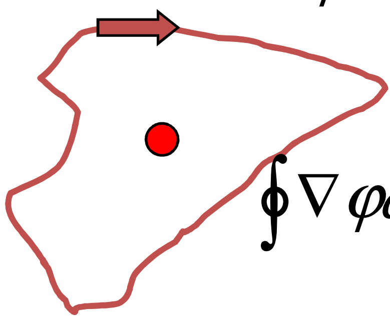
$$\hat{H}_1\psi = \varepsilon_1\psi \qquad \hat{H}_2\psi = \varepsilon_2\psi$$

1. Because we are lazy and like to establish some correspondence between the solutions!
2. Transitions between the states with different topology bring new physics and cost much energy.

# Some examples.
# Vortices in superfluids.

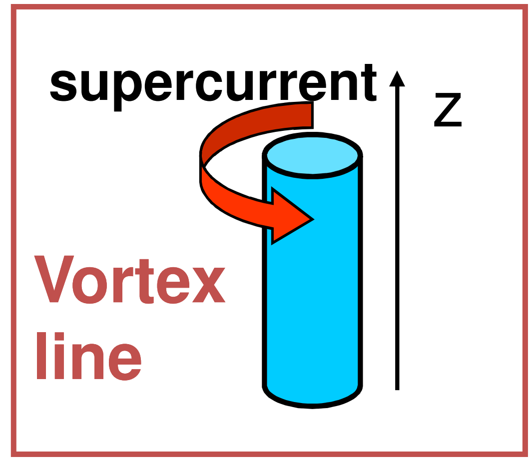
$$rot\nabla\varphi = 2\pi\delta(\vec{r})\vec{z}_0$$

$$rot\nabla\varphi \neq 0$$



$$\oint \nabla\varphi dl = 2\pi n$$

$$n = 0,1,2...$$




1. Increase in n =vortex creation which costs energy
2. Vortex can appear either at the boundary or with the antivortex partner.
3. Vortex line can not end in the bulk.
4. All types of vortices (Abrikosov, Josephson) are similar.

# *Insulators, semiconductors. Are there any states in the gaps?*

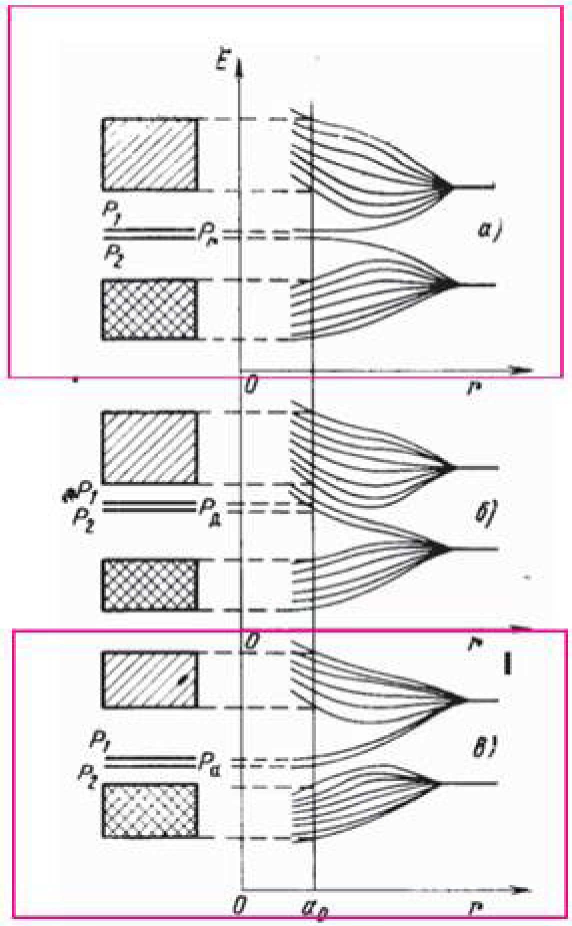
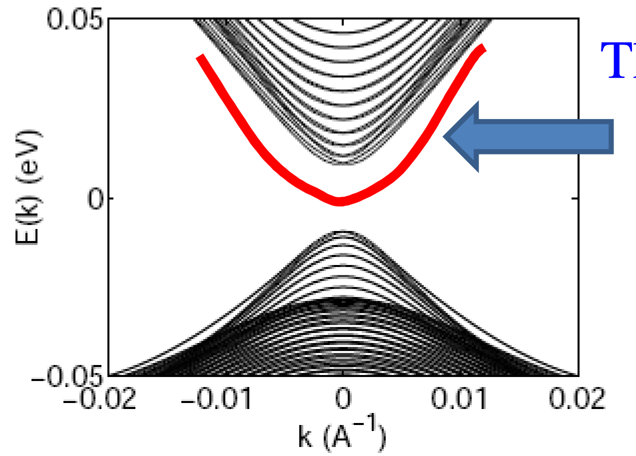



Рис. 9.2. Образование поверхностных уровней $P_1$ и $P_2$:
$P_r$ — рекомбинационные уровни; $P_д$ — донорные уровни; $P_а$ — акцепторные уровни.



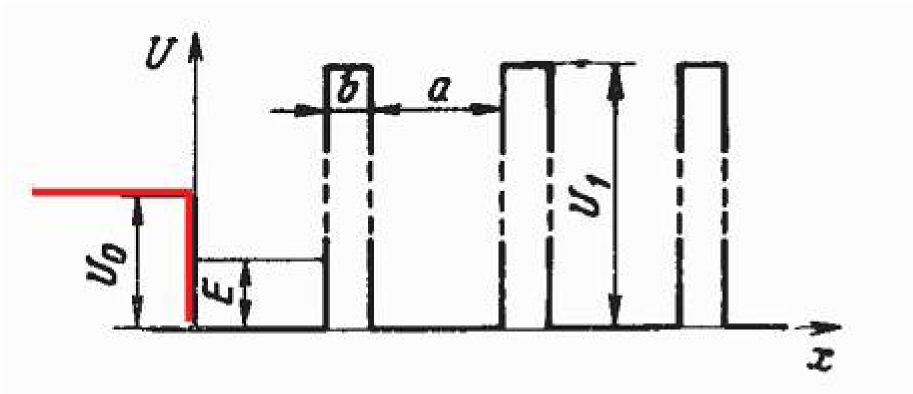

These states are easy to kill

Why it is interesting?

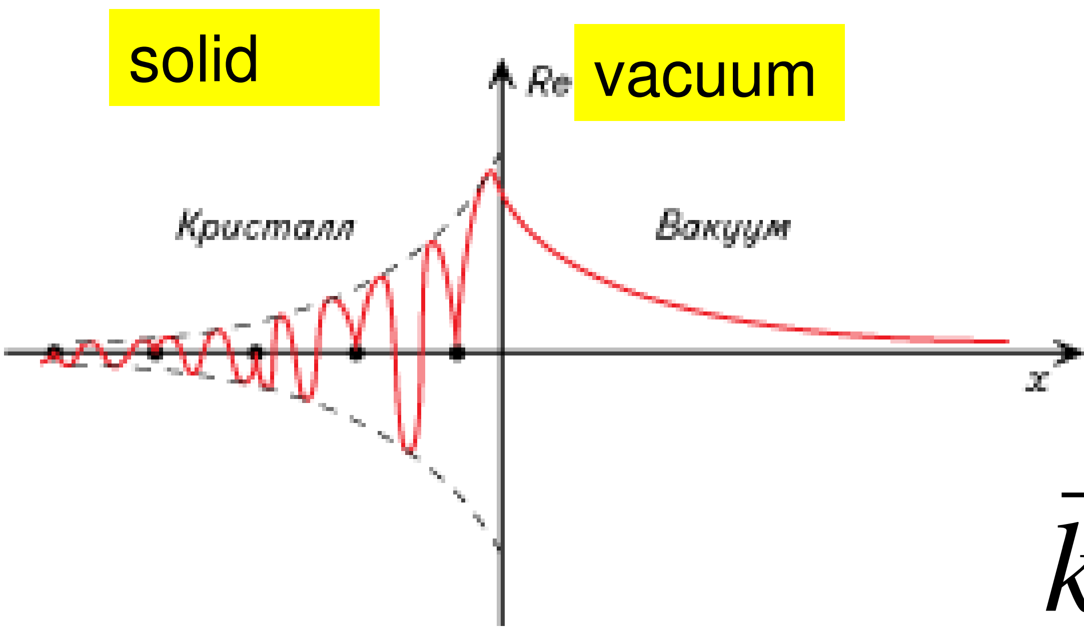
1. Subgap states affect the operation of all semiconducting devices.

2. We can get low-dimensional conductors in a simple way

# *The idea of Tamm states (1932)*




I.E.Tamm




$$\psi_{s\vec{k}} = e^{i\vec{k}\vec{r}} u_{s\vec{k}}$$

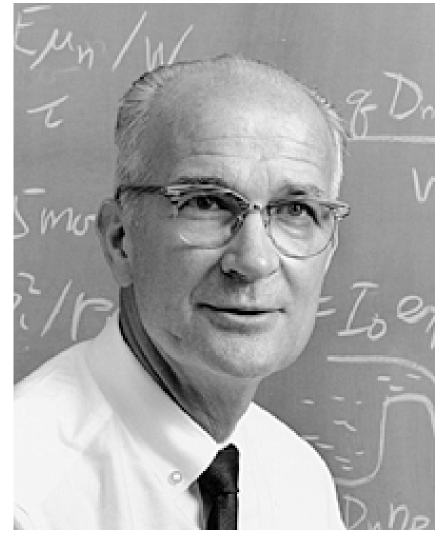
$\vec{k}$ ***- Complex valued***

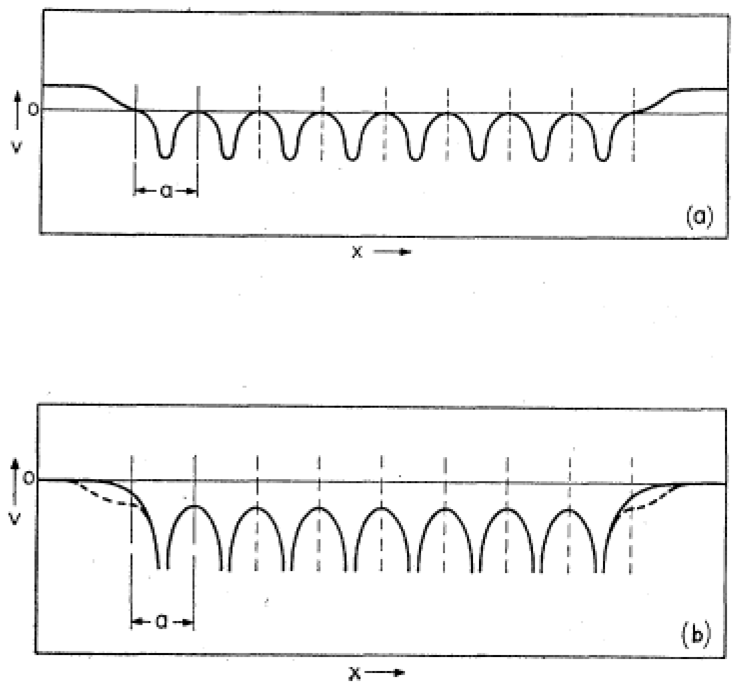
# Shockley states

AUGUST 15, 1939 PHYSICAL REVIEW VOLUME 56

## On the Surface States Associated with a Periodic Potential

WILLIAM SHOCKLEY
*Bell Telephone Laboratories, New York, New York*





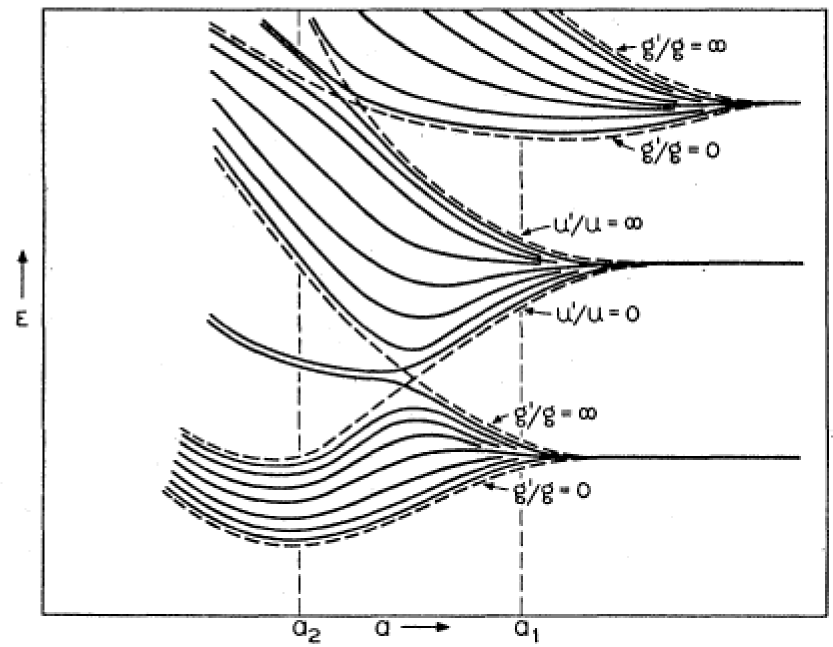
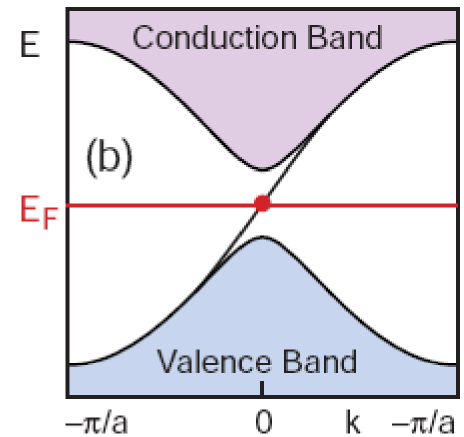




FIG. 2. Energy spectrum for a one-dimensional lattice with eight atoms.

# *Can we create the states in the gap which are robust to perturbations? Idea of bulk-boundary correspondence*

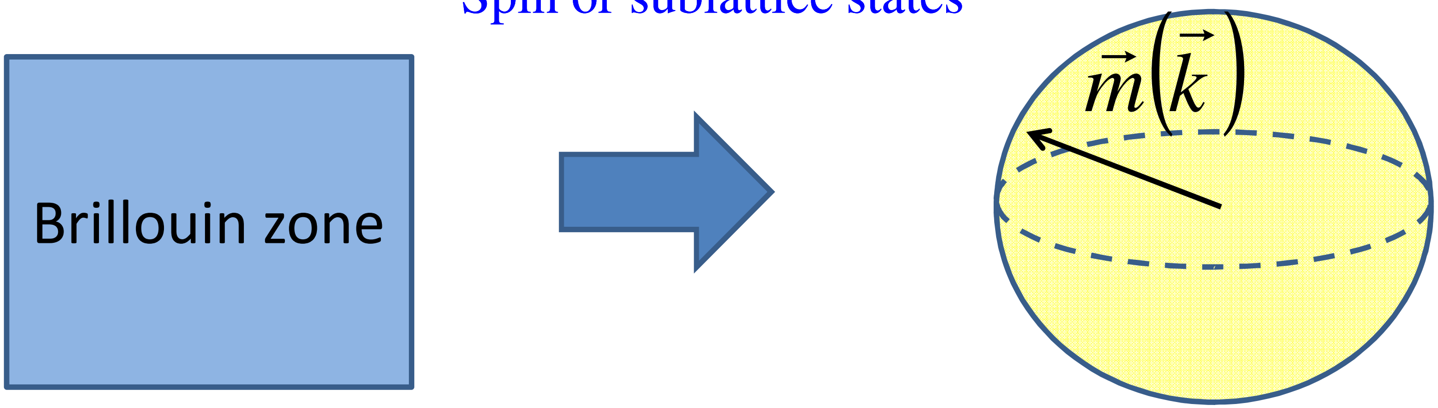
In 80s:
Quasiparticle states in He-3.
Superfluid order parameter in the bulk can generate localized states at the surface (G.E.Volovik)




Effective Hamiltonian

$$\hat{H}_{eff} = \vec{\sigma}\,\vec{m}(\vec{k})$$

Spin or sublattice states



# Topological invariants in systems with broken time-reversal symmetry. Berry phase

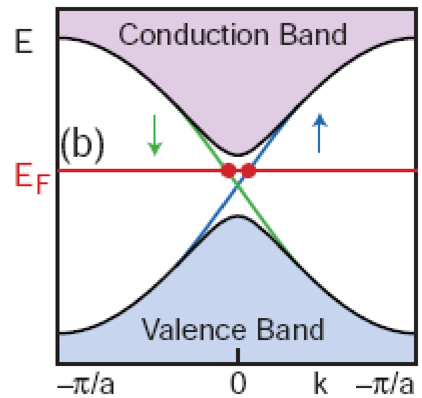
$$n = \frac{1}{2\pi}\sum_s \iint rot_{\vec{k}} \vec{A}_{eff}\, dk_x dk_y$$

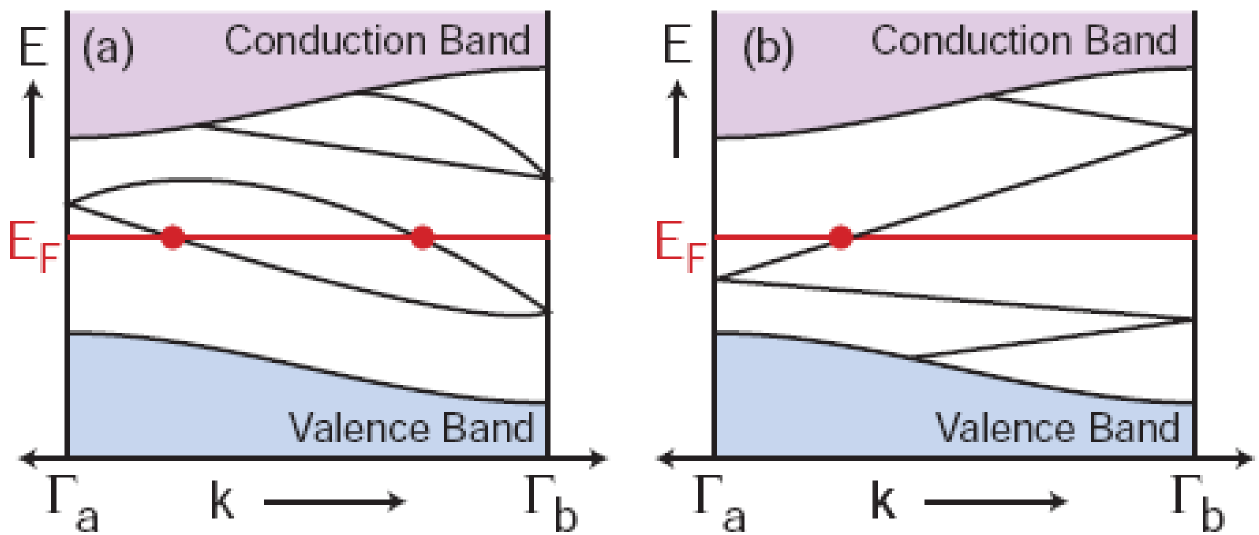
$$\vec{A}_{eff} = i\left\langle s\vec{k} \,|\, \nabla_{\vec{k}} \,|\, s\vec{k} \right\rangle$$

$$\hat{h}\left(\vec{k}\right) = \frac{\vec{m}\left(\vec{k}\right)}{\left|\vec{m}\left(\vec{k}\right)\right|}$$

$$n = \frac{1}{4\pi}\int d^2\mathbf{k}(\partial_{k_x}\hat{h} \times \partial_{k_y}\hat{h}) \cdot \hat{h}.$$

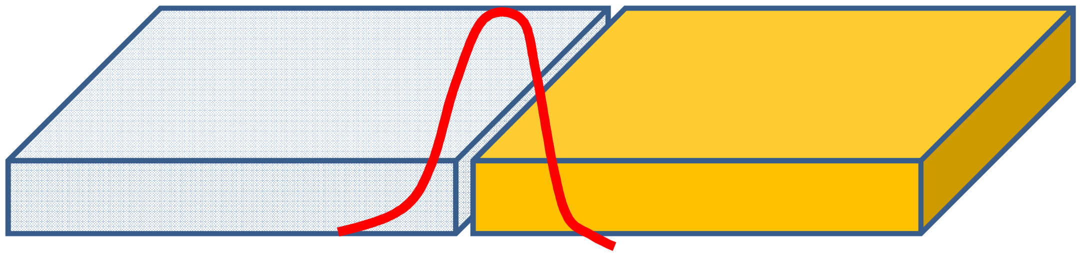
# *Topological invariants in systems with time-reversal symmetry.*
# *$Z_2$ invariant*



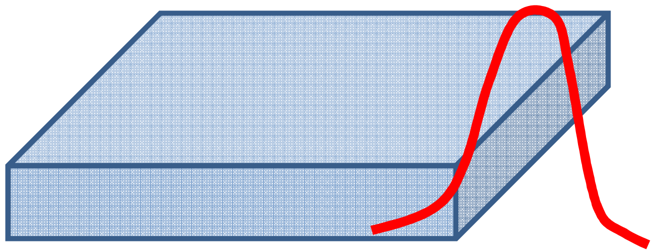



# General recipe: Interface between two media with different topology characteristics generates bound states

$$n_1 \neq n_2$$



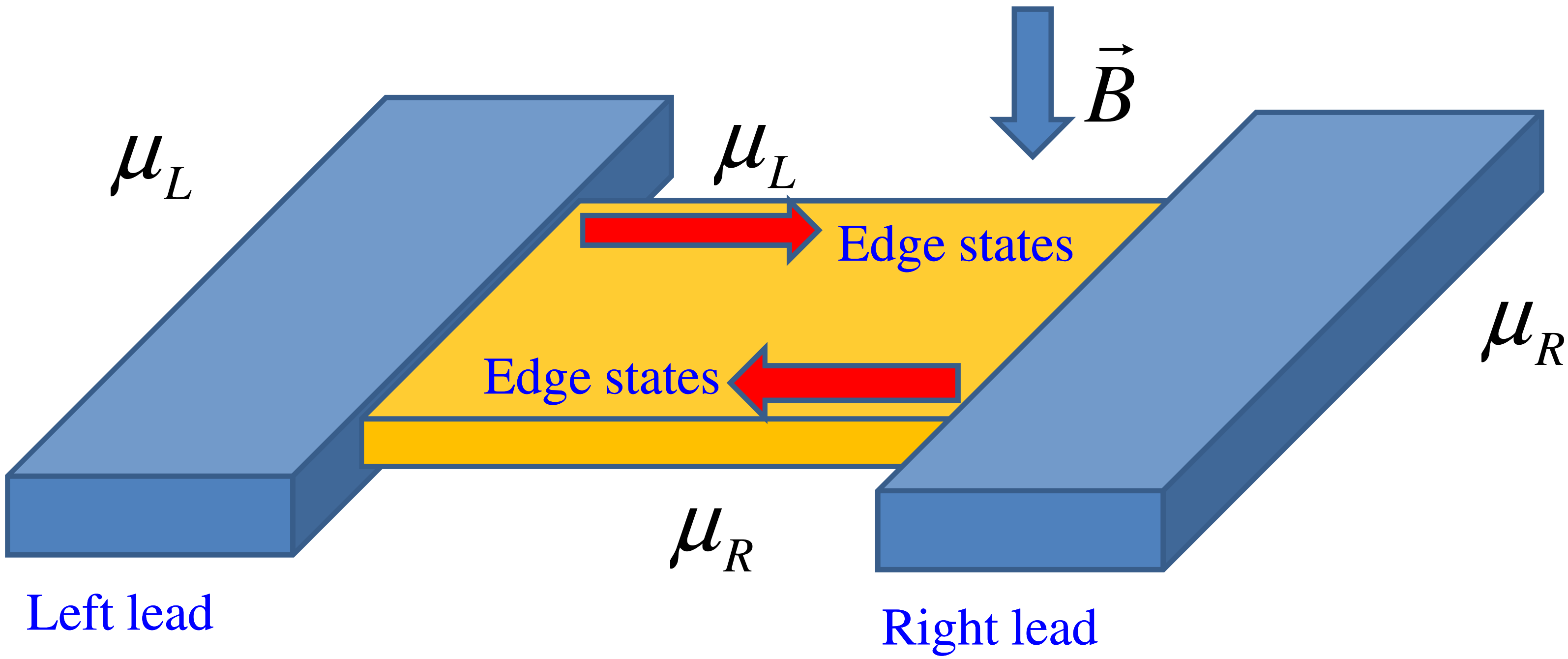
Gapless edge state



vacuum

Reason: we can not go “smoothly“ from the left medium to the right one

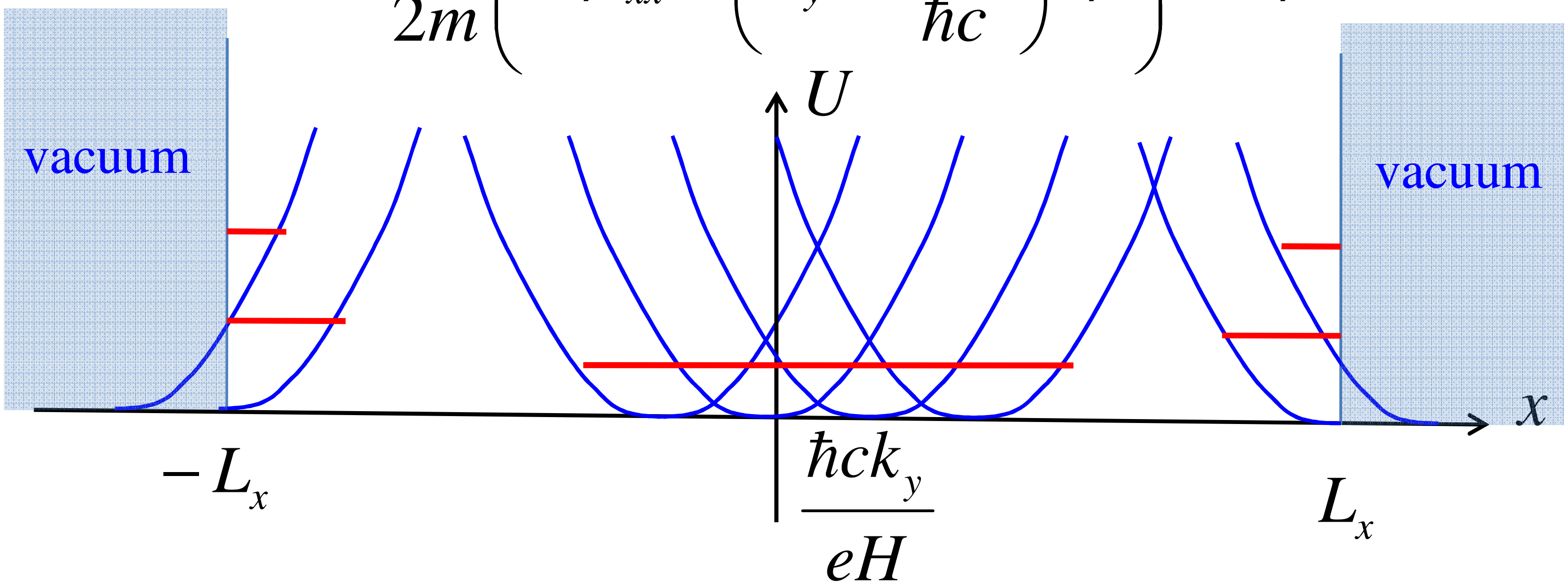
# Quantum Hall effect. Edge states.



# Quantum Hall effect. Edge states.

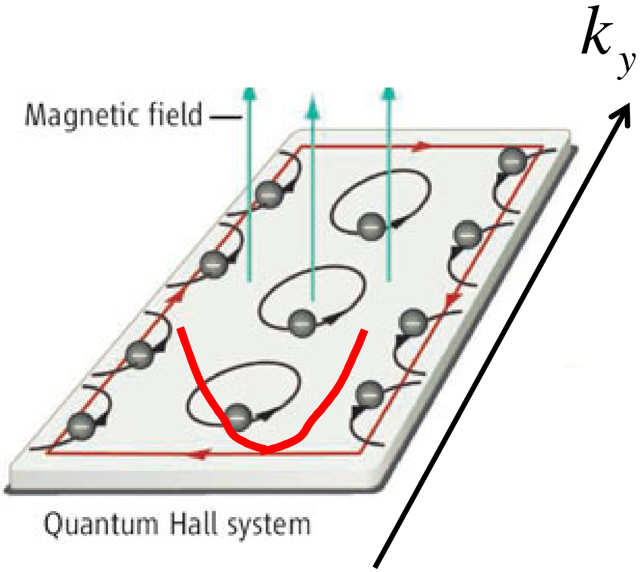
$$\Psi(x, y) = e^{ik_y y}\psi(x) \qquad A_y = Hx$$

$$\frac{\hbar^2}{2m}\left(-\psi''_{xx} + \left(k_y - \frac{eHx}{\hbar c}\right)^2 \psi\right) = \varepsilon\psi$$




$$\varepsilon = \hbar\omega_H \left(n + \frac{1}{2} + \sigma\right)$$

# Quantum Hall effect. Edge states.

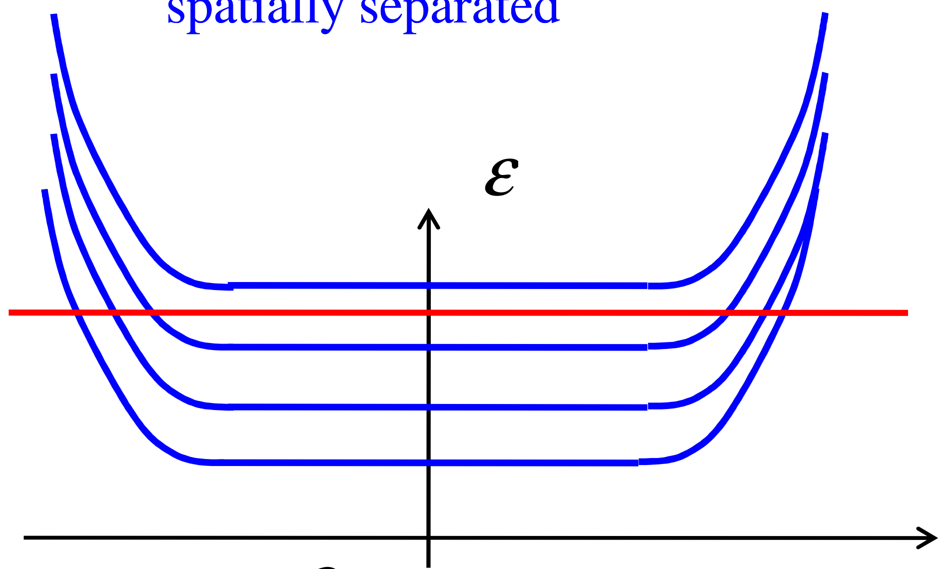



1. States in the bulk are localized

2. Edge states carry the current

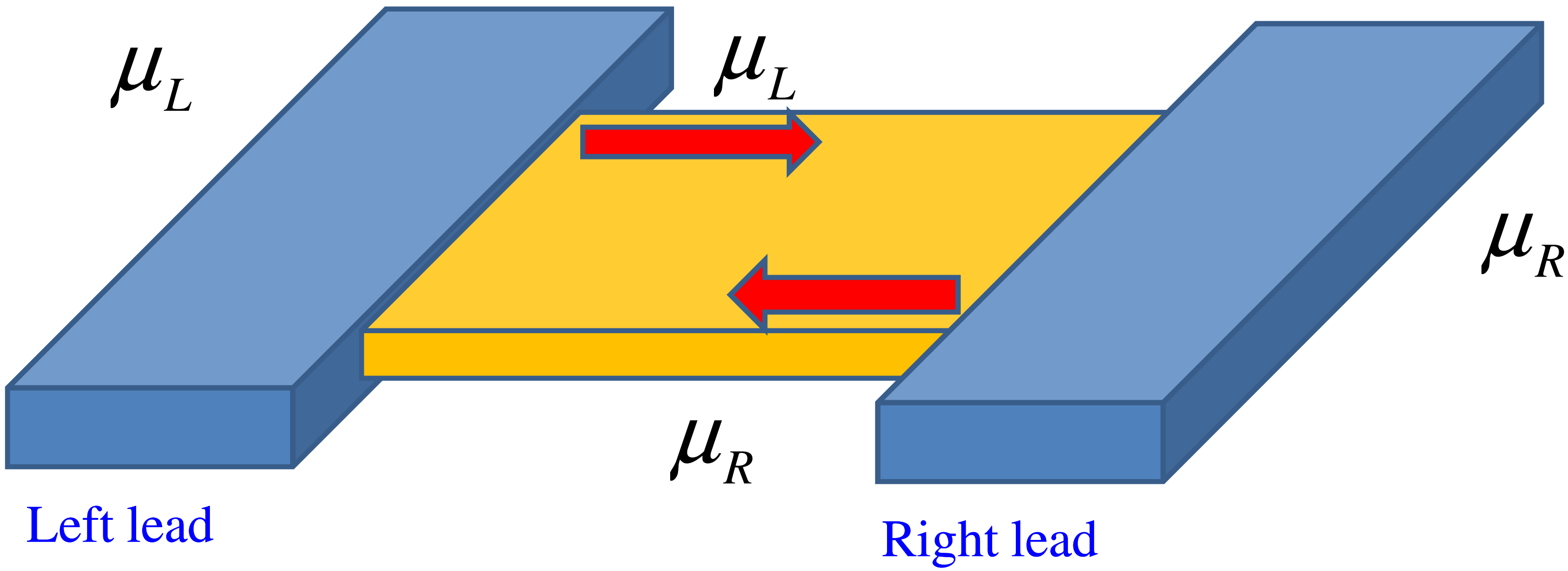
3. Scattering is weak!

Since the states with opposite momenta are spatially separated




$$V_g = \frac{\partial \varepsilon}{\hbar \partial k_y}$$

# Let us use the Landauer approach!

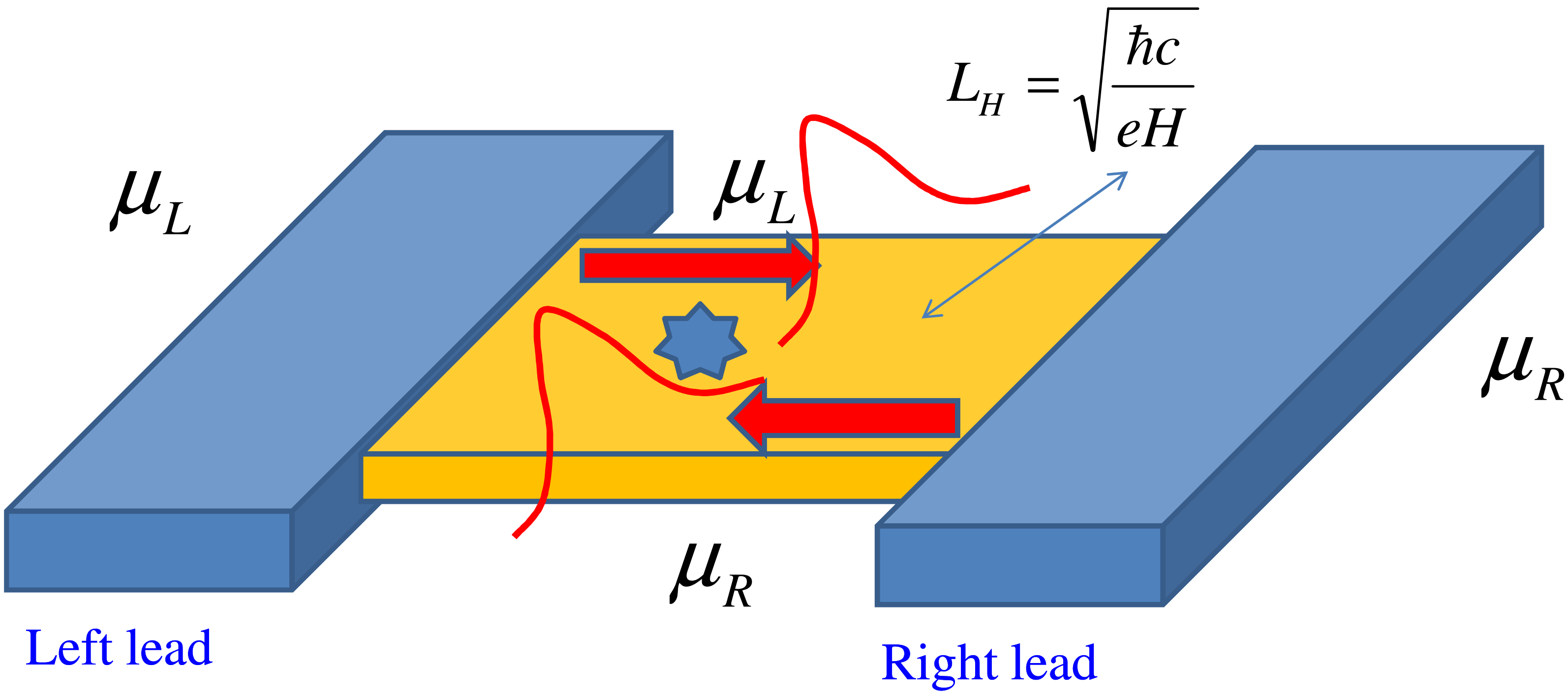



1. Left electrons carry the distribution function from the left reservoir

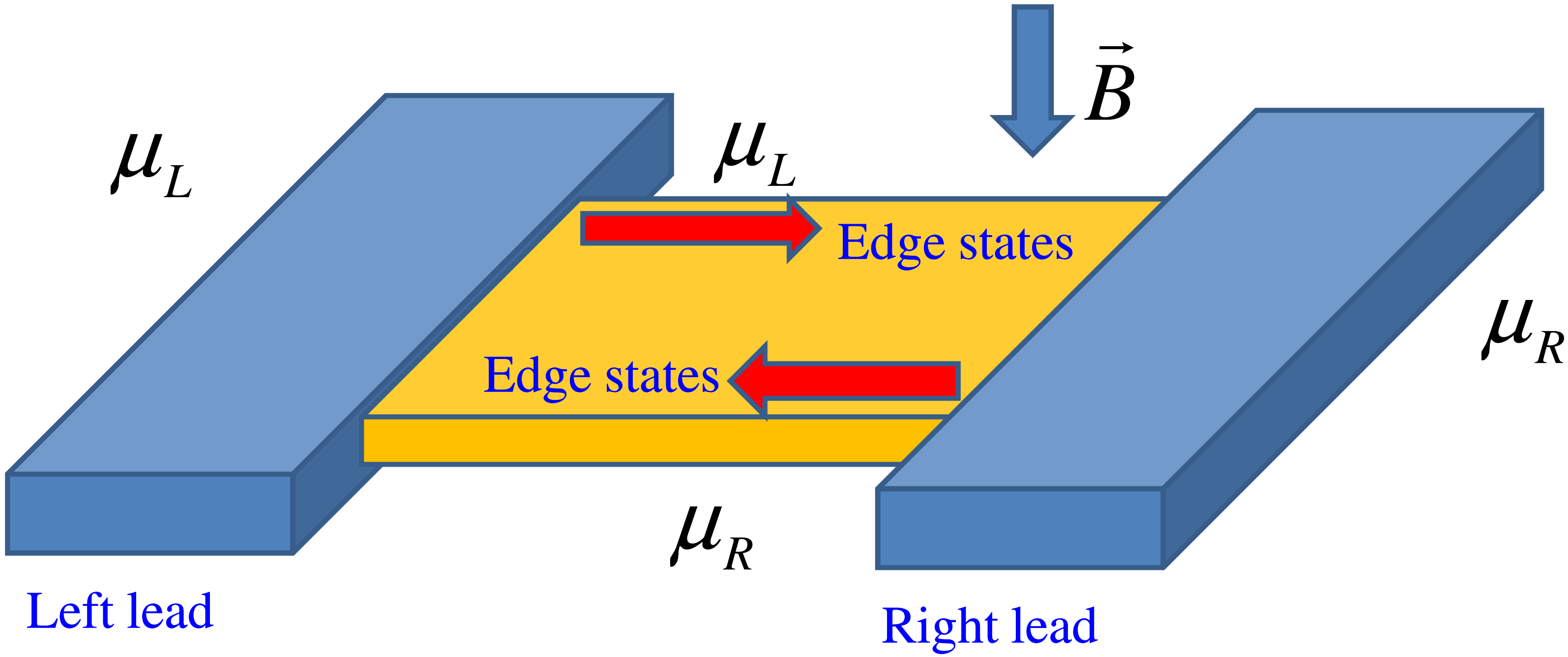
2. Right electrons carry the distribution function from the left reservoir

2. Relaxation of the distribution function occurs at large length scales

# Very small backscattering



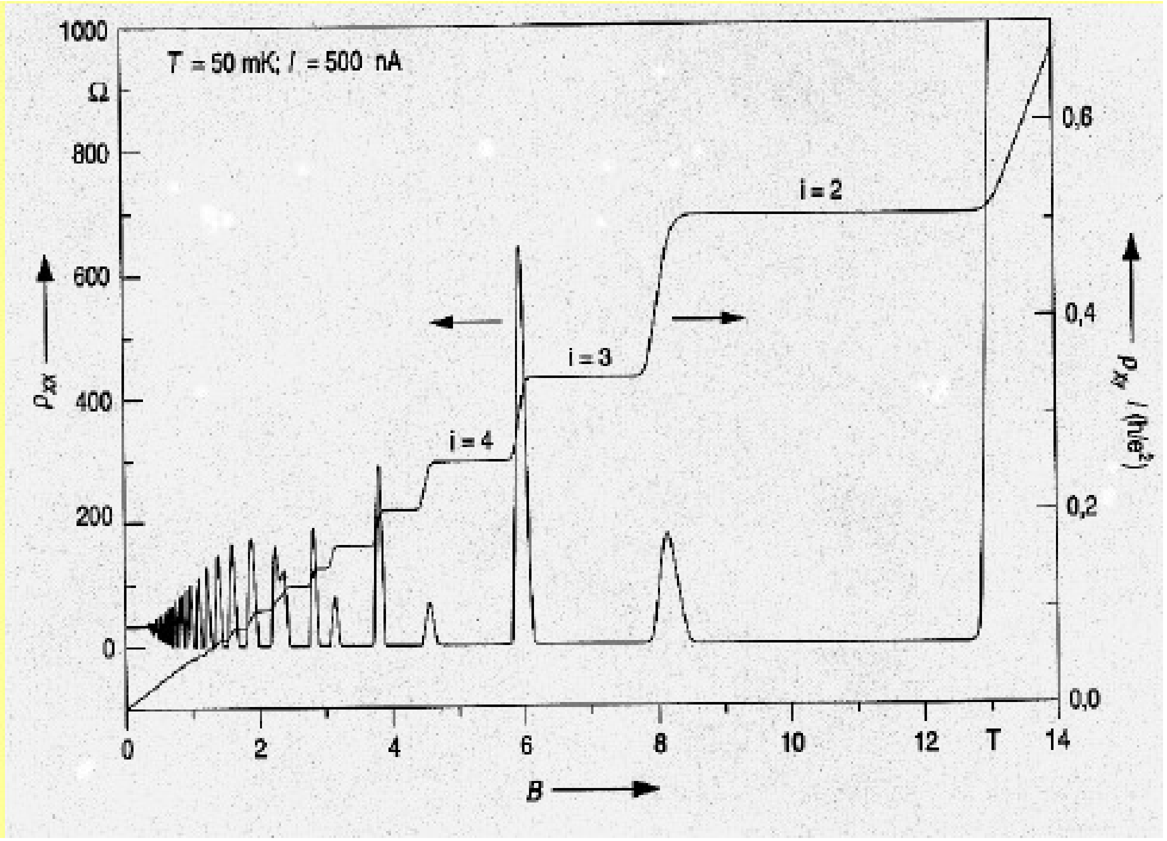
# Quantum Hall effect. Edge states.



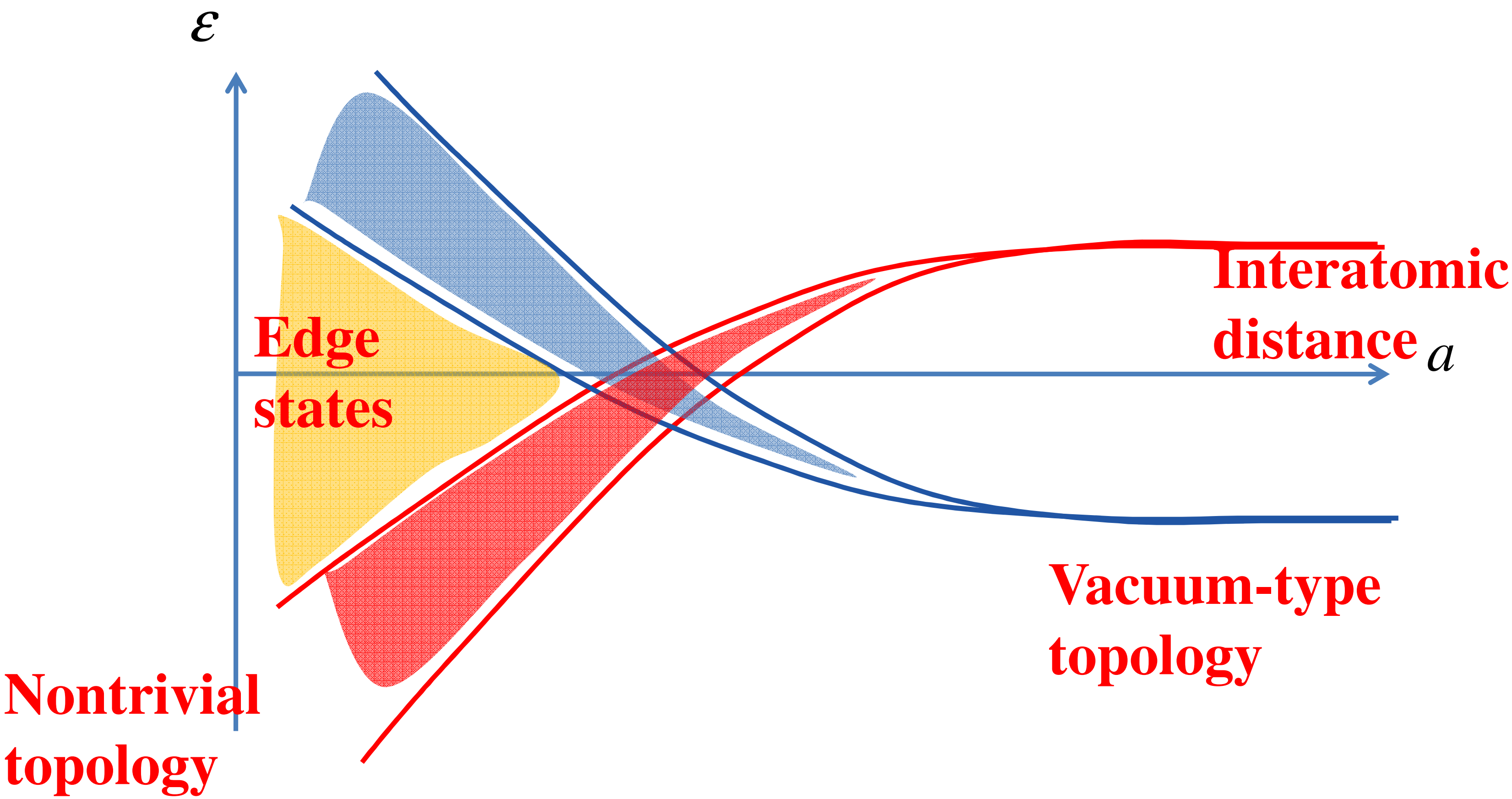

$$I_{R\to L} = \frac{e}{2\pi\hbar}\sum_n \int_{\varepsilon_n}^{\infty} f_R(\varepsilon)d\varepsilon \qquad \sigma_H = \frac{e^2}{2\pi\hbar}n$$

$$I_{L\to R} = \frac{e}{2\pi\hbar}\sum_n \int_{\varepsilon_n}^{\infty} f_L(\varepsilon)d\varepsilon \qquad n = \left[\frac{\mu}{\hbar\omega_H}\right]$$

# Quantum Hall effect. Edge states.



**Band inversion as an important mechanism of generation of topologically protected states.**

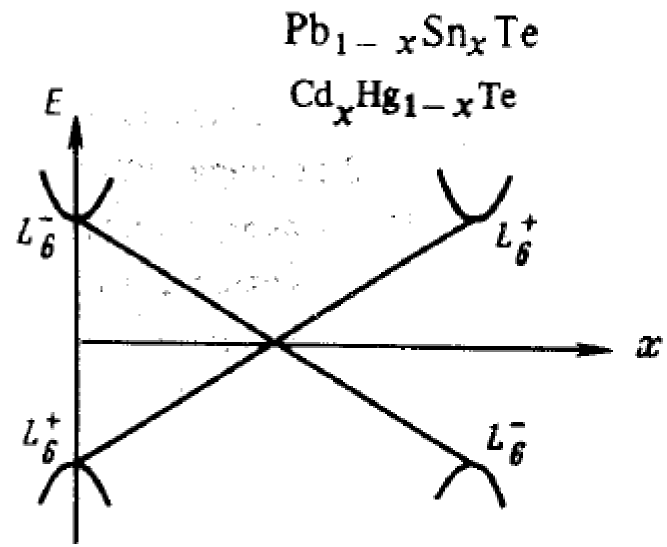


# Volkov-Pankratov solution for the interface with the band inversion

**Two-dimensional massless electrons in an inverted contact**

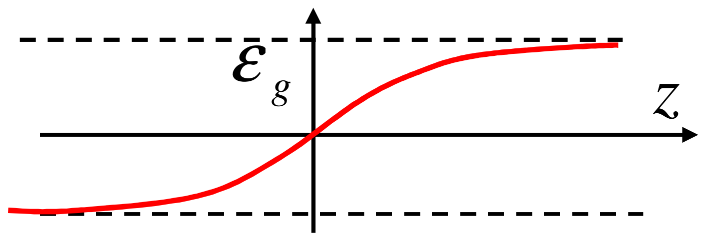
B. A. Volkov and O. A. Pankratov
*P. N. Lebedev Physics Institute, Academy of Sciences of the USSR*

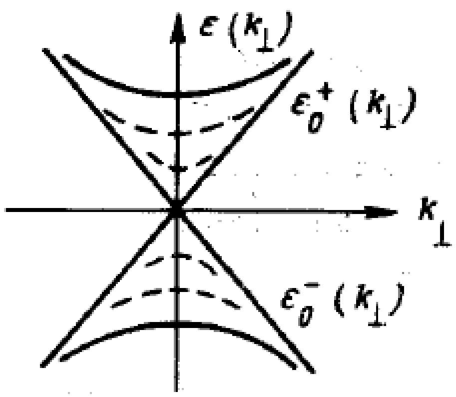
(Submitted 20 June 1985)
Pis'ma Zh. Eksp. Teor. Fiz. **42**, No. 4, 145–148 (25 August 1985)




$$\begin{pmatrix} -\epsilon & i\epsilon_g/2 + \vec{\sigma}\mathbf{p} \\ -i\epsilon_g/2 + \vec{\sigma}\mathbf{p} & -\epsilon \end{pmatrix} \begin{pmatrix} \chi_- \\ \chi_+ \end{pmatrix} = 0,$$

$$\epsilon_0^{\pm}(\mathbf{k}_\perp) = \pm \hbar v_\perp k_\perp$$

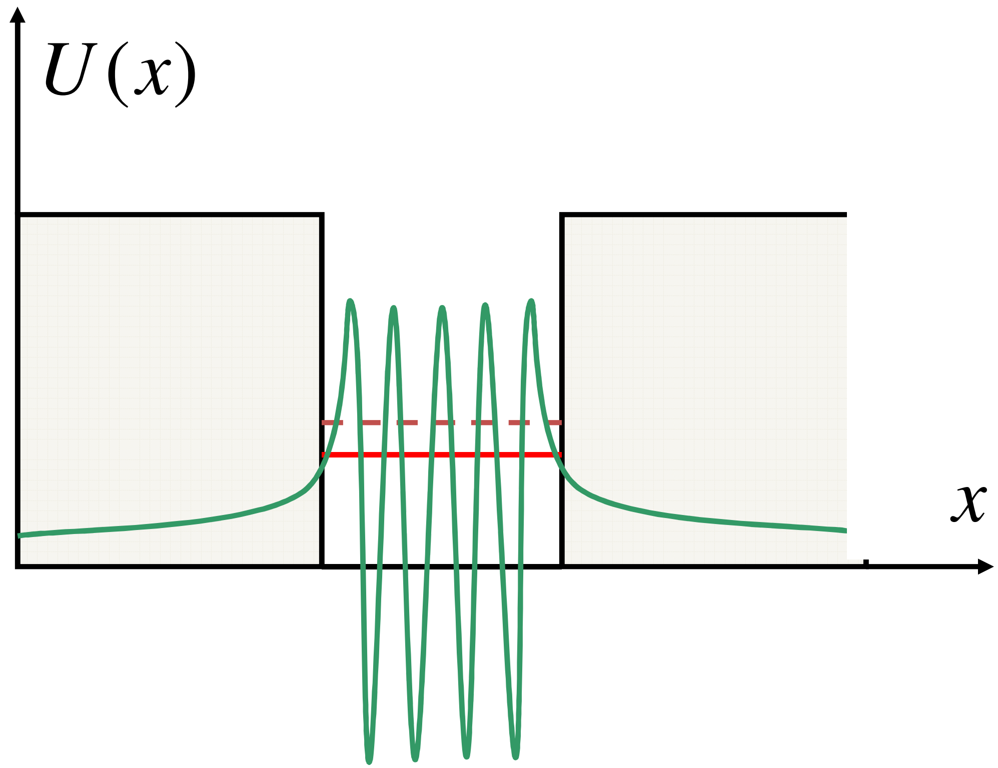



$$\Psi_{\pm} = A \begin{pmatrix} \pm\exp(-i\theta/2) \\ 0 \\ 0 \\ \exp(i\theta/2) \end{pmatrix} \exp\left\{ -\frac{1}{2\hbar v_{\parallel}} \int_0^z \epsilon_g(z)dz + i\mathbf{k}_\perp \mathbf{r} \right\}$$

$$\exp(i\theta) = (k_x + ik_y)/k_\perp$$

# Electron confinement in a well: standard quantum mechanics

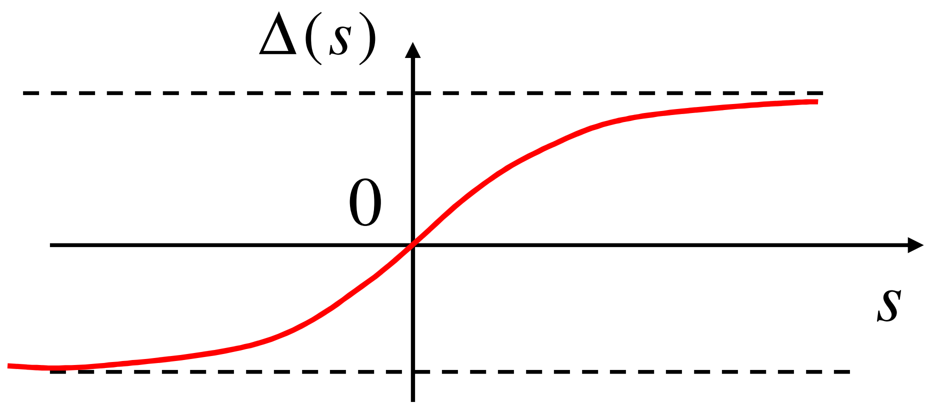


# Volkov-Pankratov solution for the interface with the band inversion.

## An alternative way to trap an electron comparing to the Shroedinger potential well

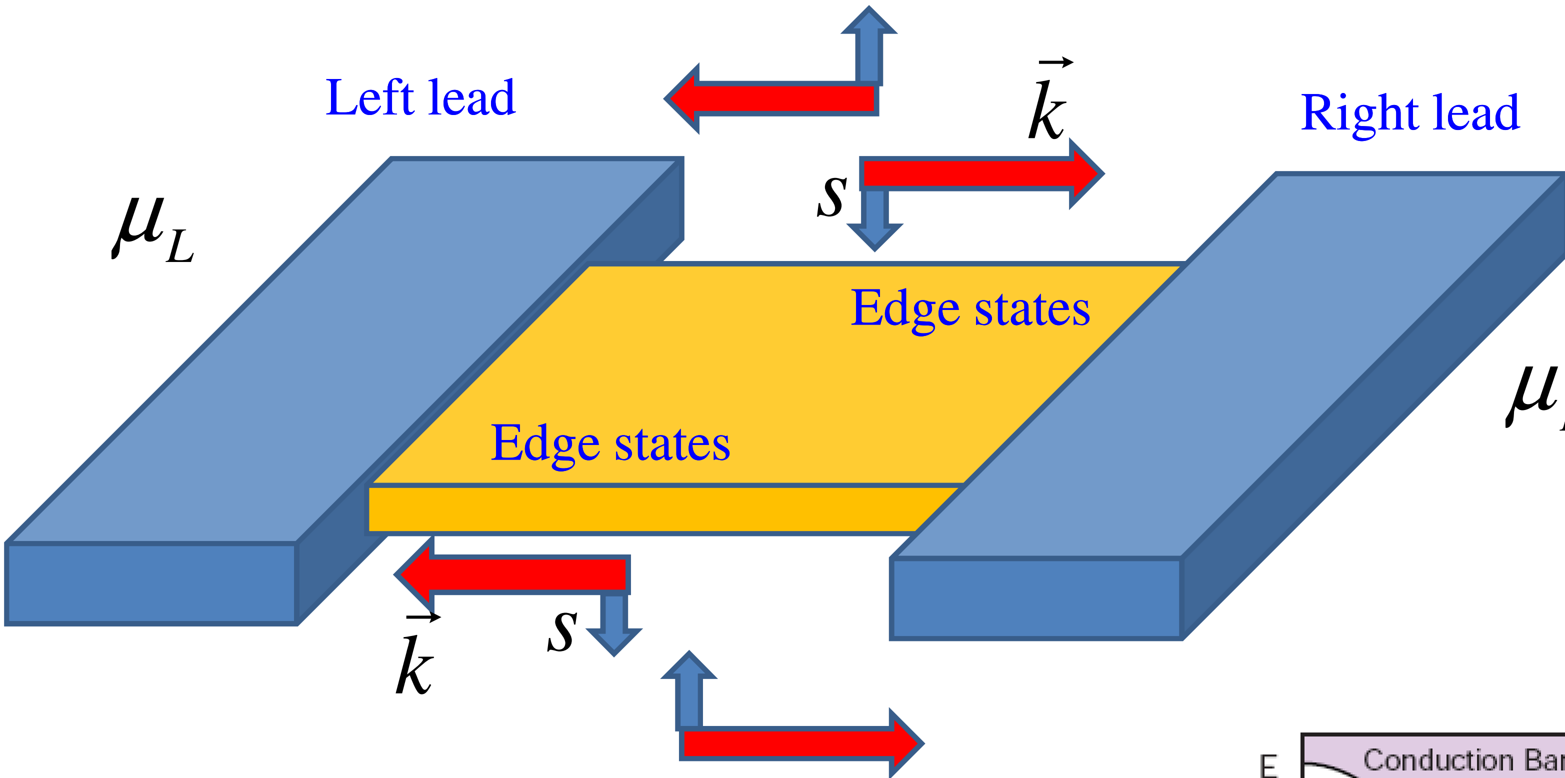
$$\hat{H} = -i\hbar V_{\perp}\hat{\sigma}_z \frac{\partial}{\partial s} + \hat{\sigma}_x \Delta(s)$$

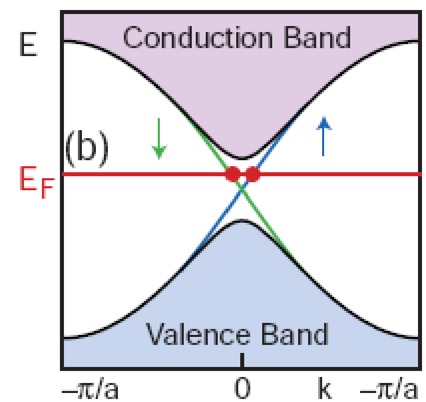
$$\hat{\Psi}_0 = \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1 \\ -i \end{pmatrix} \exp\left( -\frac{1}{\hbar V_{\perp}} \int_0^s \mathrm{Re}\,\Delta(t)\,dt \right)$$




**energy=0**

# *Zero magnetic field.*
# *Quantum spin Hall insulator*



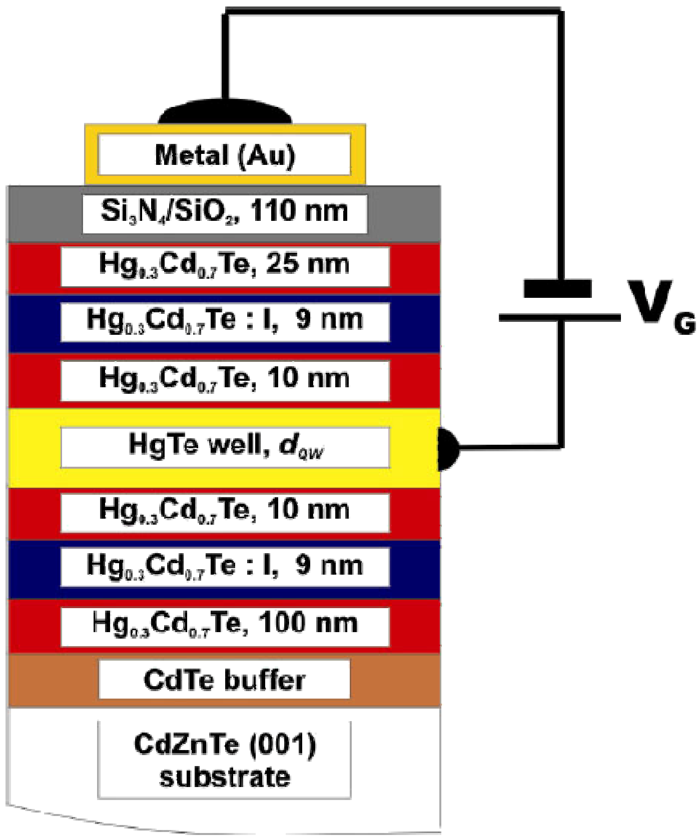




No backscattering without spin change

The Hall potential difference depends on the spin state

Nonzero spin current

# 2D topological insulators, HgTe/CdTe quantum wells.



# The band inversion effect and conductance through 2 half-channels

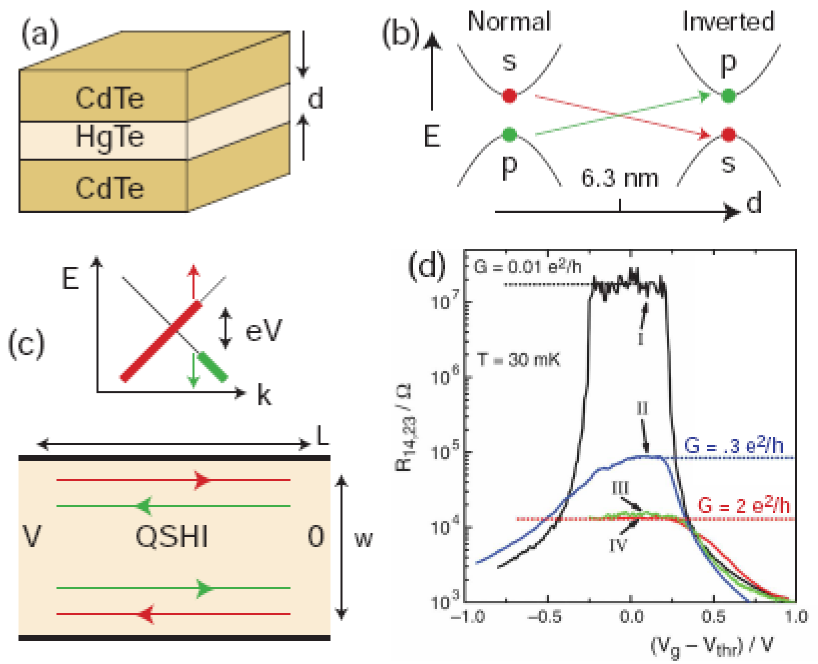



FIG. 6 (a) A HgCdTe quantum well structure. (b) As a function of layer thickness $d$ the 2D quantum well states cross at a band inversion transition. The inverted state is the QSHI state, which has helical edge states (c) that will have a non equilibrium population determined by the leads. (d) shows experimental two terminal conductance as a function of a gate voltage that tunes $E_F$ through the bulk gap (König, *et al.*, 2007). Sample I, with $d < d_c$ shows insulating behavior, while samples III and IV show quantized transport associated with edge states.

# 2D topological insulators, HgTe/CdTe quantum wells.

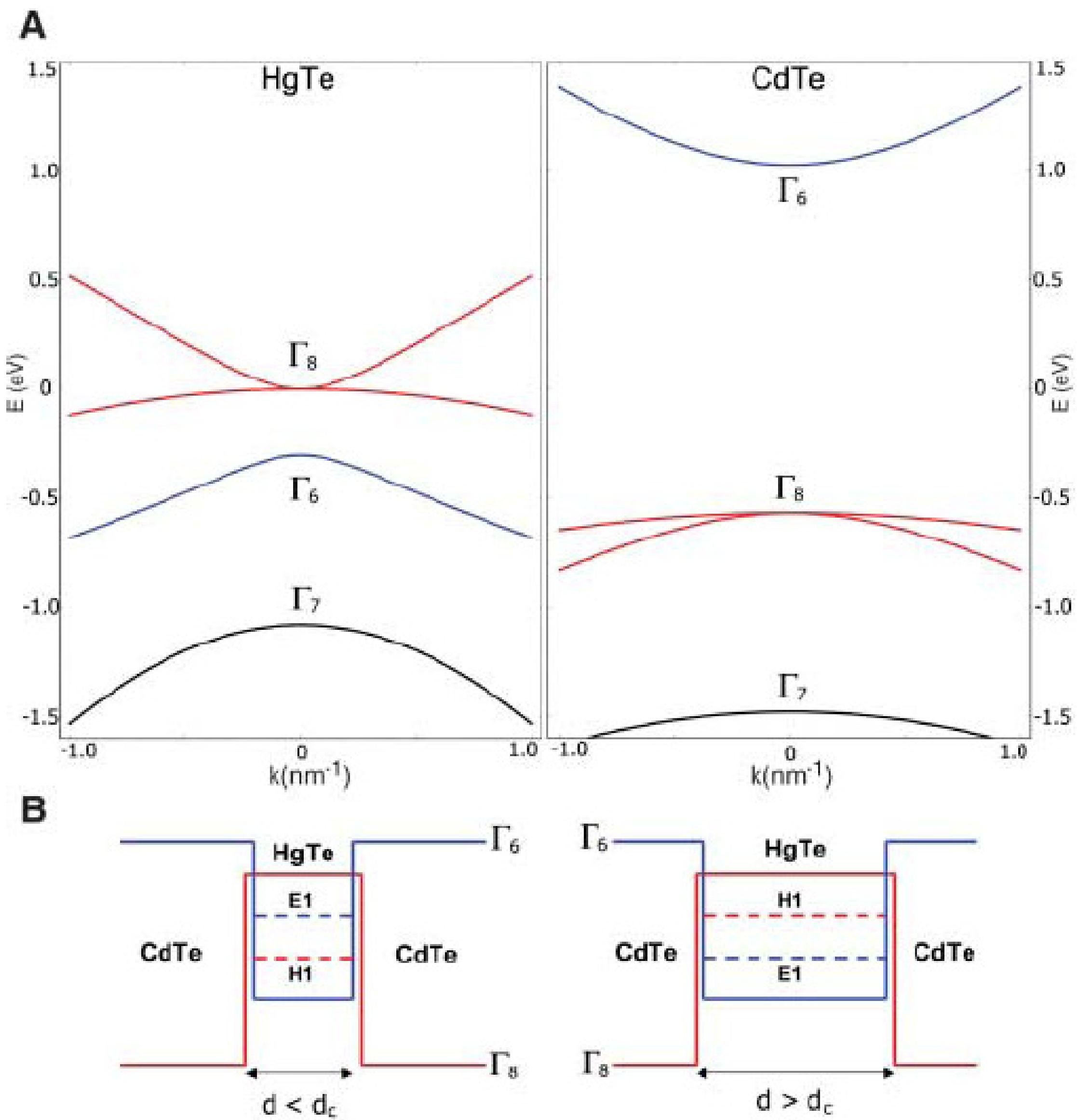



**Fig. 1.** (**A**) Bulk energy bands of HgTe and CdTe near the Γ point. (**B**) The CdTe-HgTe-CdTe quantum well in the normal regime $E1 > H1$ with $d < d_c$ and in the inverted regime $H1 > E1$ with $d > d_c$. In this and other figures, $\Gamma_8/H1$ symmetry is indicated in red and $\Gamma_6/E1$ symmetry is indicated in blue.

# 2D topological insulators, HgTe/CdTe quantum wells.

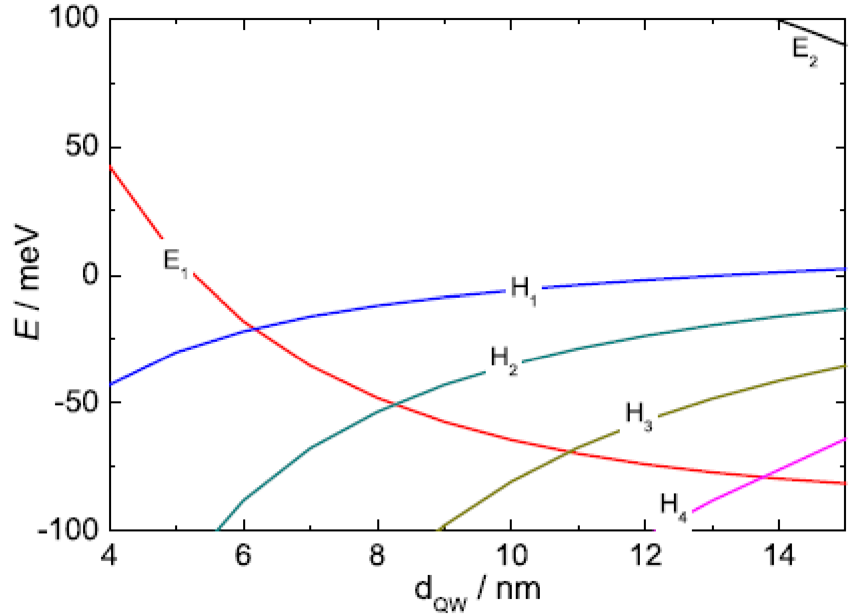
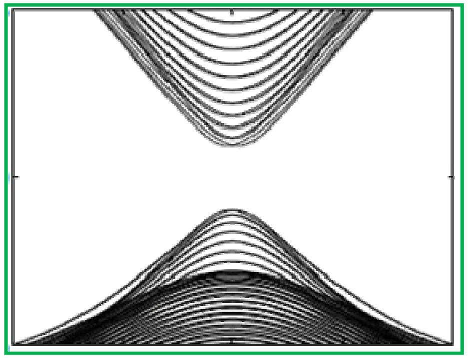
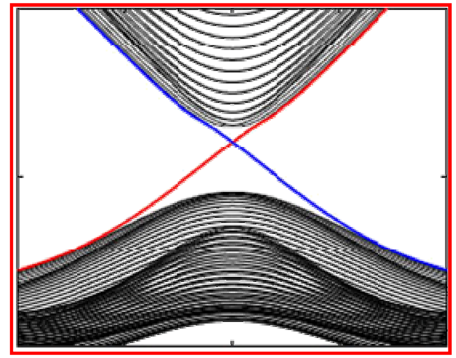
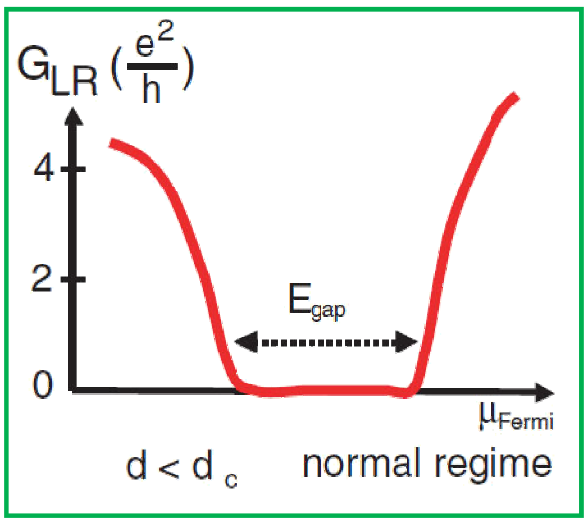


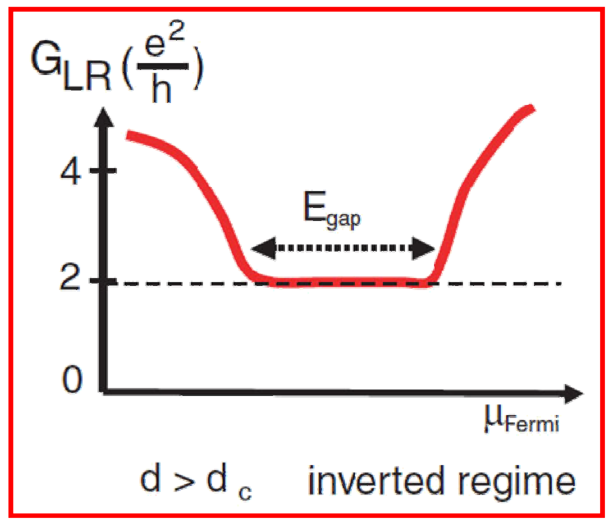

FIG. 3 Energy levels of the QW as a function of QW width. From König *et al.*, 2008.

# 2D topological insulators, HgTe/CdTe quantum wells.



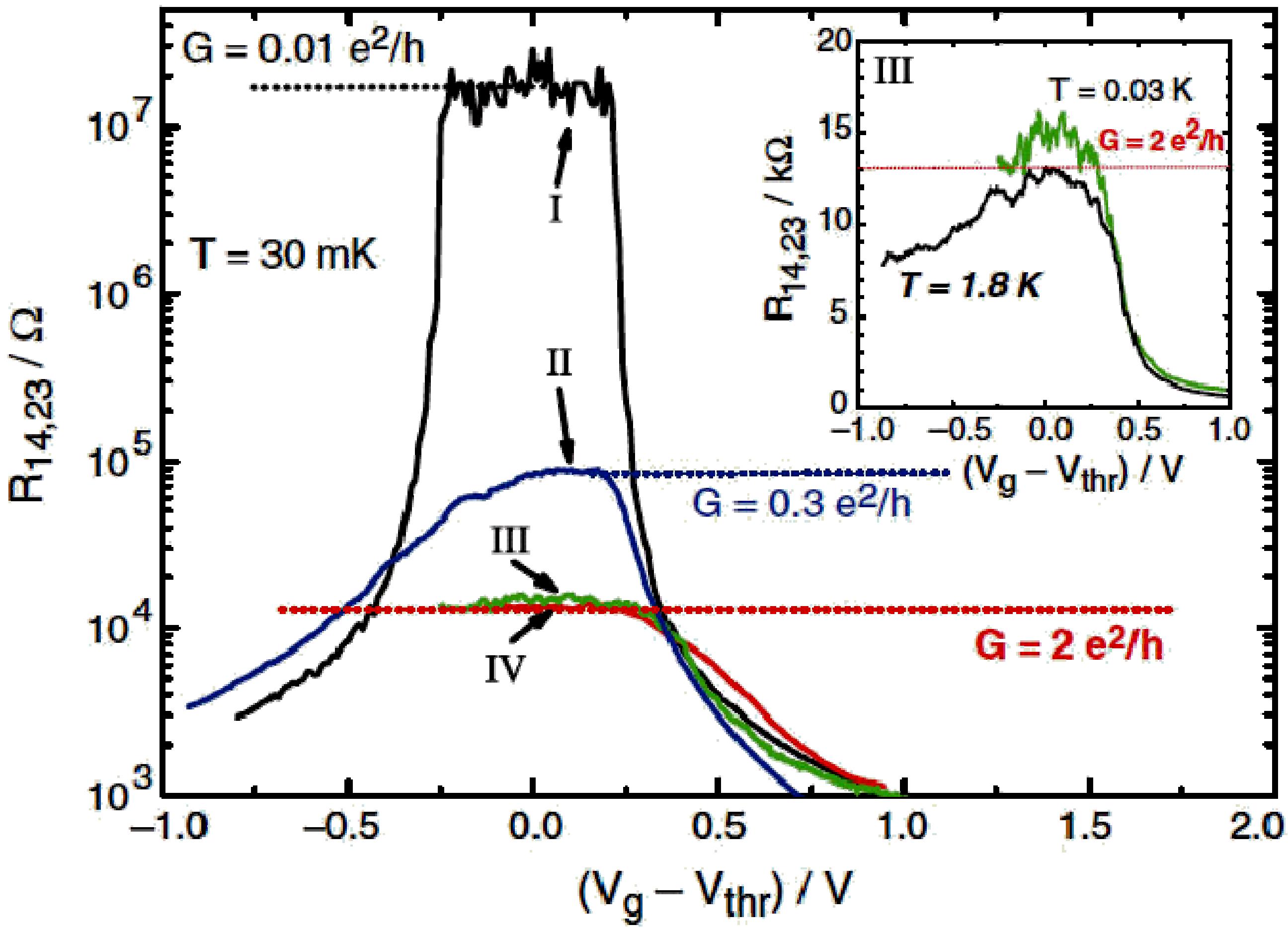




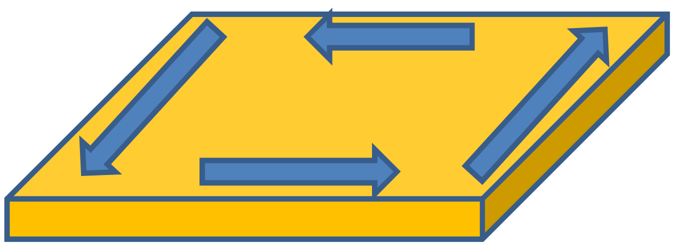
# 2D topological insulators, HgTe/CdTe quantum wells.

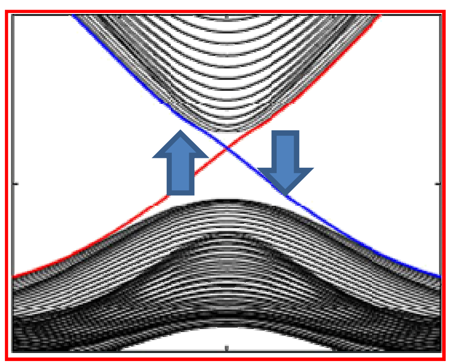
**Fig. 4.** The longitudinal four-terminal resistance, $R_{14,23}$, of various normal ($d$ = 5.5 nm) (I) and inverted ($d$ = 7.3 nm) (II, III, and IV) QW structures as a function of the gate voltage measured for $B$ = 0 T at $T$ = 30 mK. The device sizes are (20.0 × 13.3) μm$^2$ for devices I and II, (1.0 × 1.0) μm$^2$ for device III, and (1.0 × 0.5) μm$^2$ for device IV. The inset shows $R_{14,23}(V_g)$ of two samples from the same wafer, having the same device size (III) at 30 mK (green) and 1.8 K (black) on a linear scale.



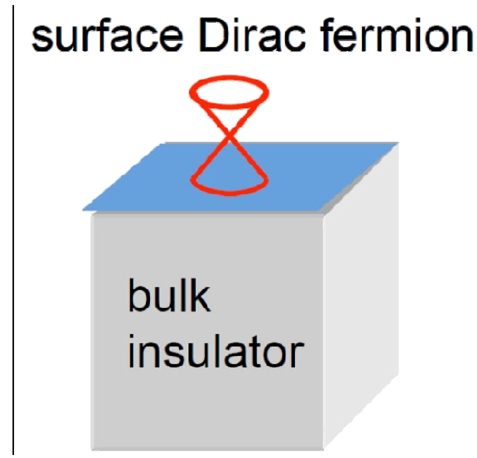
# From 2D to 3D topological insulators

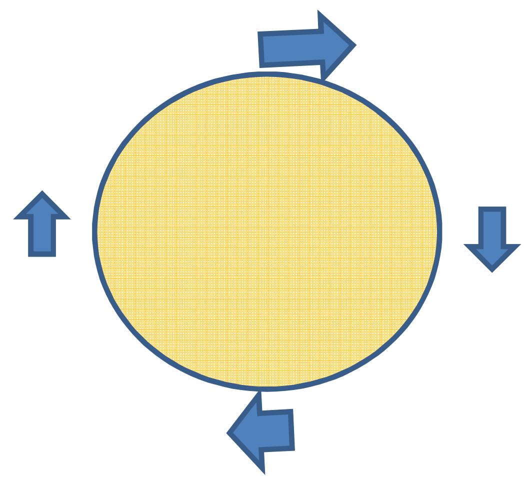
Edge states





Surface states



# 3D topological insulators

## Weak TI

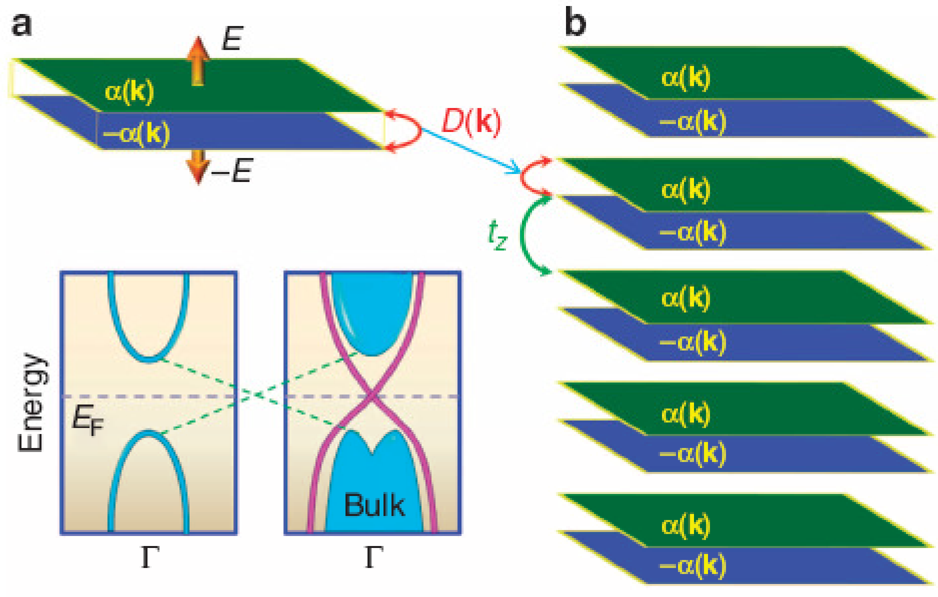
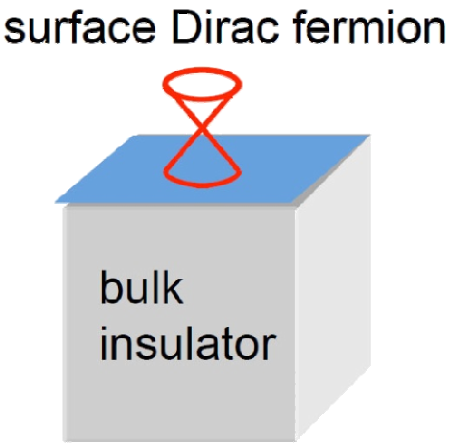



**Figure 1 | Rashba bilayer of 2DFGs and its heterostructure setup.** (**a**) A bilayer combination of opposite Rashba-type spin-orbit coupling 2DFGs, denoted by $\alpha(\mathbf{k})$, $-\alpha(\mathbf{k})$, representing $h_R^+$ and $h_R^-$, respectively in the Hamiltonian in Equation 1. $D(\mathbf{k})$ gives the interlayer electron tunneling between them. (**b**) As grown Rashba bilayers with finite inter-bilayer coupling, $t_z$. (**c**, **d**) Illustration of band dispersions for a bilayer 2DFG, and its heterostructure version, respectively. The emergence of an inverted band curvature in the valence bulk band marks the topological phase transition, as also demonstrated in first-principle bandstructure calculations[26], and ARPES data[14].

# 3D topological insulators




$$\mathcal{H}_{\rm surface} = -i\hbar v_F \vec{\sigma}\cdot\vec{\nabla},$$

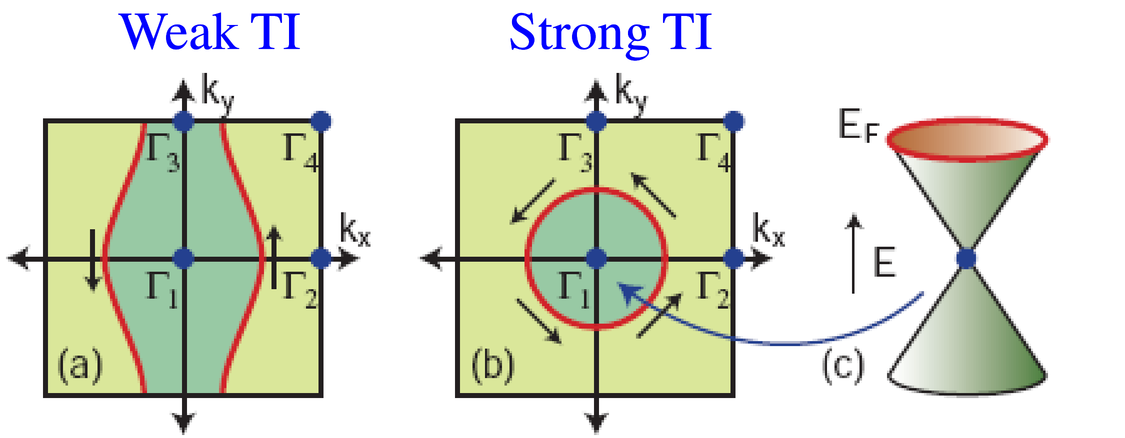
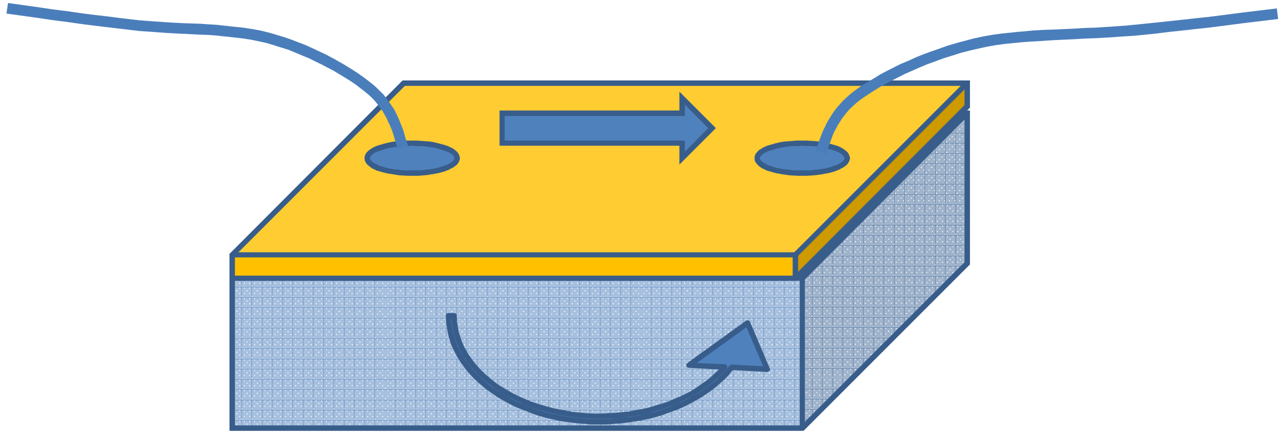



FIG. 7 Fermi circles in the surface Brillouin zone for (a) a weak topological insulator and (b) a strong topological insulator. In the simplest strong topological insulator the Fermi circle encloses a single Dirac point (c).

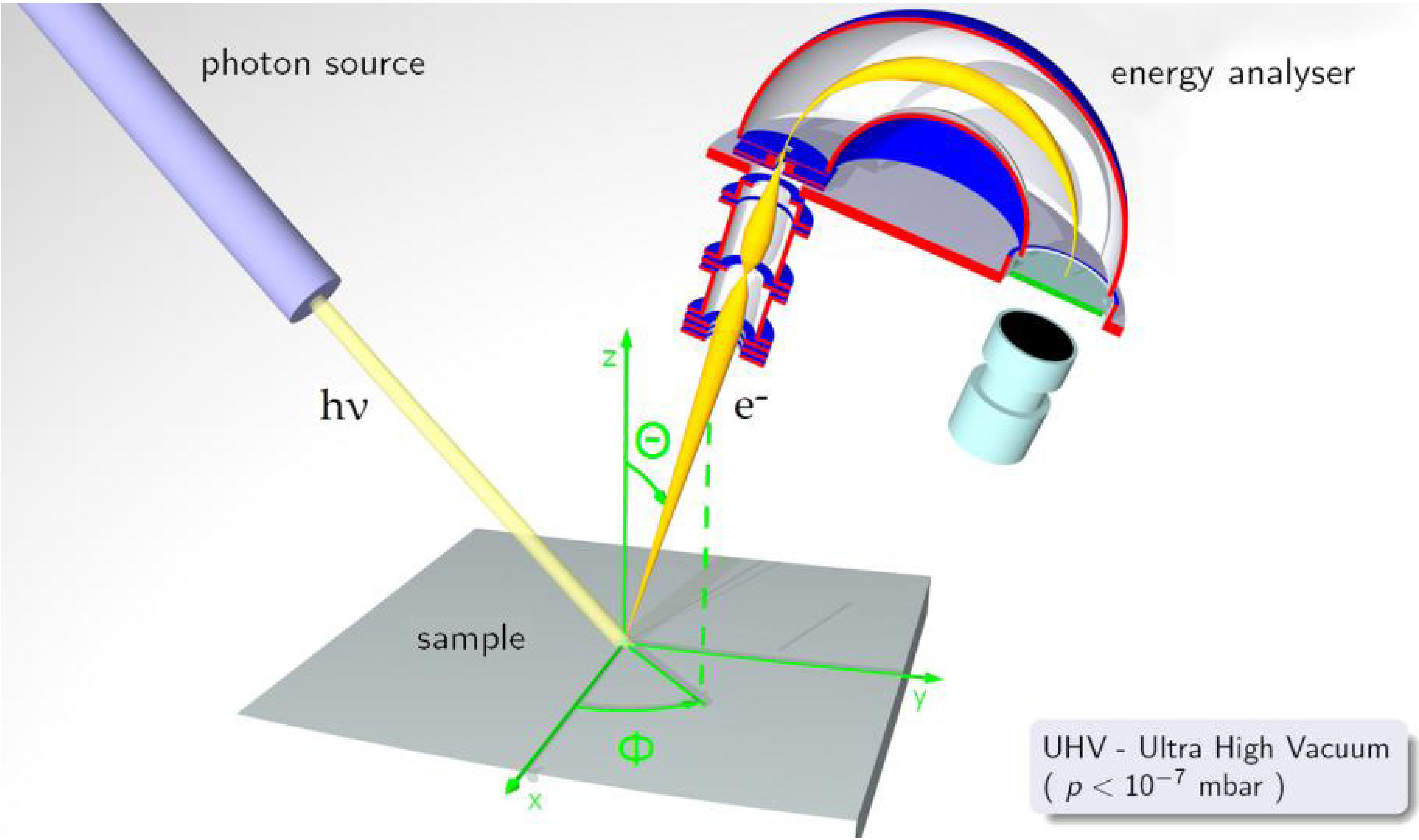
# 3D topological insulators.

## *Problem of measurements of surface states: finite conductivity of the bulk*



***Very clean materials are needed (no doping)***

# 3D topological insulators. ARPES data



# 3D topological insulators. ARPES data

First compound: bismuth antimony $Bi_{1-x}Sb_x$

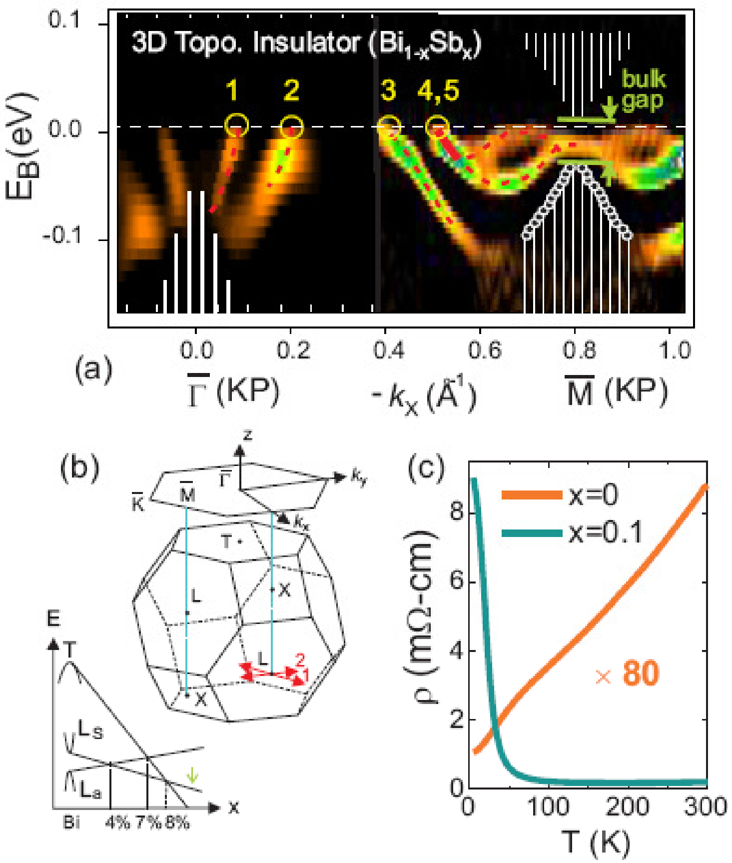



FIG. 9 Topological surface states in $Bi_{1-x}Sb_x$: (a) ARPES data on the 111 surface of $Bi_{0.9}Sb_{0.1}$ which probes the occupied surface states as a function of momentum on the line connecting the time reversal invariant points $\bar{\Gamma}$ and $\bar{M}$ in the surface Brillouin zone. Only the surface bands cross the Fermi energy 5 times. This, along with further detailed ARPES results (Hsieh, *et al.*, 2008) establish that the semiconducting alloy $Bi_{1-x}Sb_x$ is a strong topological insulator in the (1;111) class. (b) shows a schematic of the 3D Brillouin zone and its (111) surface projection. (c) contrasts the resistivity of semimetallic pure Bi with the semiconducting alloy.

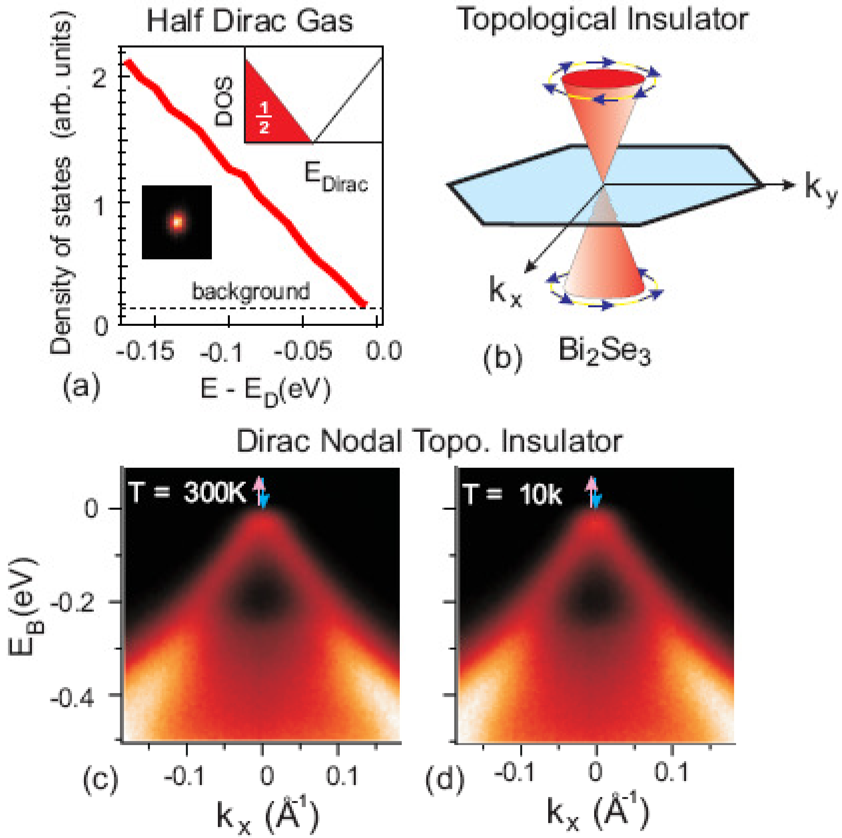



FIG. 13 Room temperature topological order in $Bi_2Se_3$: Topological order can be observed up to room temperature in the second generation topological insulators. (a) Crystal momentum integrated ARPES data near Fermi level exhibit linear fall-off of density of states, which combined with the spin-resolved nature of the states suggest that a half Fermi gas is realized on the topological surfaces. (b) Spin-texture map based on spin-ARPES data suggest that the spin-chirality changes sign across the Dirac point. (c) The Dirac node remains well defined up a temperature of 300K suggesting the stability of topological effects up to the room temperature (Hsieh, *et al.*, 2009b).

# 3D topological insulators. Bi2Se3. Spin resolved ARPES data

# 3D topological insulators. Spin resolved ARPES data

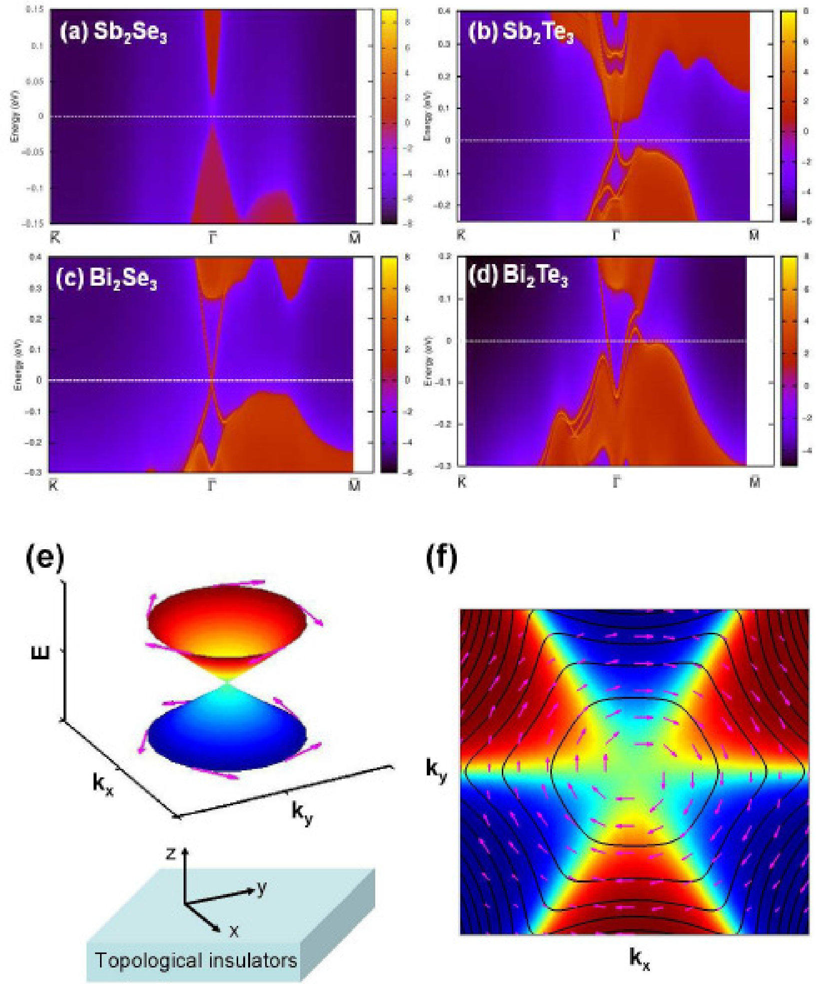



FIG. 20 (a)-(d) Energy and momentum dependence of the local density of states for the $Bi_2Se_3$ family of materials on the [111] surface. A warmer color represents a higher local density of states. Red regions indicate bulk energy bands and blue regions indicate a bulk energy gap. The surface states can be clearly seen around Γ point as red lines dispersing inside the bulk gap. (e) Spin polarization of the surface states on the top surface, where the $z$ direction is the surface normal, pointing outwards. Adapted from Zhang *et al.*, 2009 and Liu *et al.*, 2010.

# 3D topological insulators. Bi2Se3. Effect of magnetic impurities

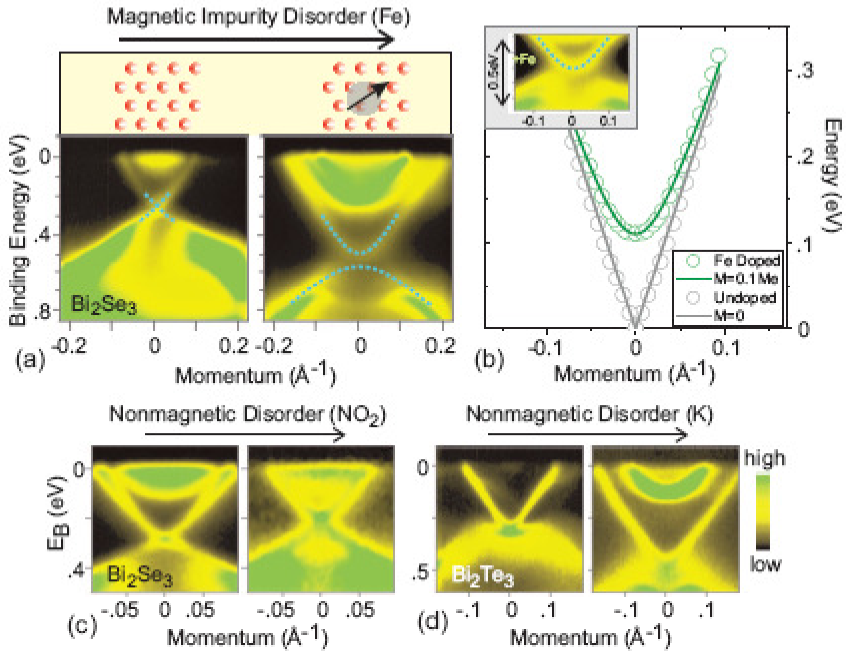



FIG. 15 Protection by time-reversal symmetry: Topological surface states are robust in the presence of strong non-magnetic disorder but open a gap in the presence of time-reversal breaking magnetic impurities and disorder. (a) Magnetic impurity such as Fe on the surface of $Bi_2Se_3$ opens a gap at the Dirac point. The magnitude of the gap is set by the interaction of Fe ions with the Se surface and the time-reversal breaking disorder potential introduced on the surface. (b) A comparison of surface band dispersion with and without Fe doping. (c) Non-magnetic disorder created via molecular absorbent $NO_2$ or alkali atom adsorption (K or Na) on the surface leaves the Dirac node intact in both $Bi_2Se_3$ and $Bi_2Te_3$ (Hsieh, *et al.*, 2009b; Xia, *et al.*, 2009b; Wray, *et al.*, 2010).

# 3D topological insulators.

## *Electromagnetic effects caused by the surface states with broken time-reversal symmetry*

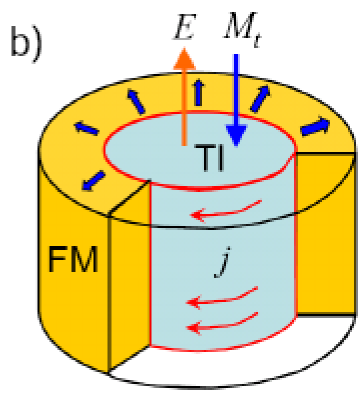
Applied magnetic field

$$\sigma_{xy} = (n + 1/2)e^2/h$$

Proximity to a magnetic material

$$H_{\mathrm{surf}}(\mathbf{k}) = A_2\sigma^x k_y - A_2\sigma^y k_x + m_z\sigma^z$$

$$\sigma_H = \frac{m_z}{|m_z|}\frac{e^2}{2h}$$




$$\mathbf{j} = \frac{m}{|m|}\frac{e^2}{2h}\hat{\mathbf{n}} \times \mathbf{E}$$

# 3D topological insulators. *Magnetic monopole*

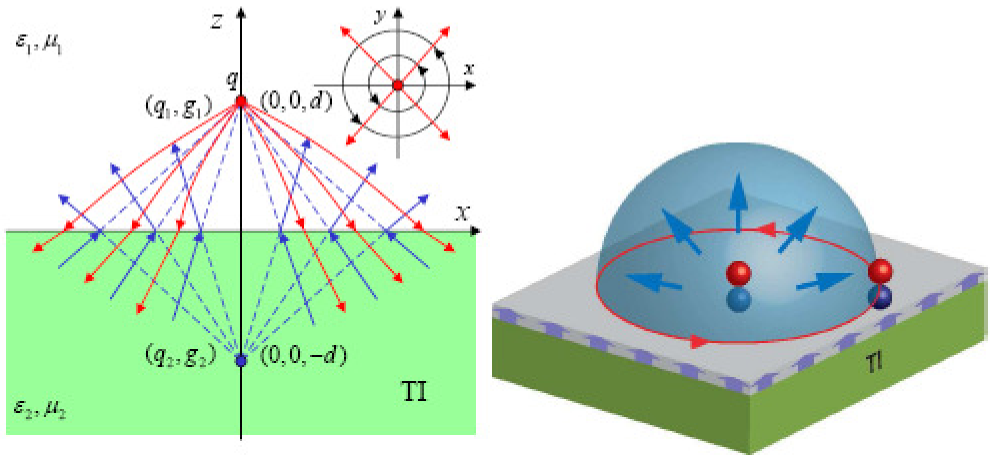



FIG. 23 (a) Image electric charge and image magnetic monopole due to an external electric point charge. The lower half-space is occupied by a topological insulator (TI) with dielectric constant $\epsilon_2$ and magnetic permeability $\mu_2$. The upper half-space is occupied by a topologically trivial insulator (e.g. vacuum) with dielectric constant $\epsilon_1$ and magnetic permeability $\mu_1$. An electric point charge $q$ is located at $(0,0,d)$. Seen from the lower half-space, the image electric charge $q_1$ and magnetic monopole $g_1$ are at $(0,0,d)$. Seen from the upper half-space, the image electric charge $q_2$ and magnetic monopole $g_2$ are at $(0,0,-d)$. The red (blue) solid lines represent the electric (magnetic) field lines. The inset is a top-down view showing the in-plane component of the electric field on the surface (red arrows) and the circulating surface current (black circles). (b) Illustration of the fractional statistics induced by the image monopole effect. Each electron forms a "dyon" with its image monopole. When two electrons are exchanged, a Aharonov-Bohm phase factor is obtained, which is deter- mined by half of the image monopole flux, independently of the exchange path, leading to the phenomenon of statistical transmutation. From Qi *et al.*, 2009.

# Some conclusions

- New type of insulators with metallic layer at the surface
- bulk-boundary correspondence
- Suppression of backscattering in quantum channels

# Some references

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A Short Course on
Topological Insulators

Edited by Frank Ortmann, Stephan Roche, and Sergio O. Valenzuela

Topological Insulators

Fundamentals and Perspectives

With a Foreword by Laurens W. Molenkamp

## *Some problems to be solved after lectures*

1. Solve the Volkov-Pankratov problem (find localized states at the interface with the band inversion) for the particular case of the step-like profile

$$\varepsilon_g(z) = sign(z)$$

2. Solve the Andreev equation (find the subgap localized state) in the step-like gap profile

$$\Delta(z) = sign(z)$$

3. Solve them and send to

melnikov@ipmras.ru