Universität Bielefeld
Fakultät für Physik
Theorie der kondensierten Materie

Topological Insulators and Ferromagnets: appearance of flat surface bands

Thomas Dahm
University of Bielefeld

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)

T. Paananen et al, New J. Phys. **16**, 033019 (2014)

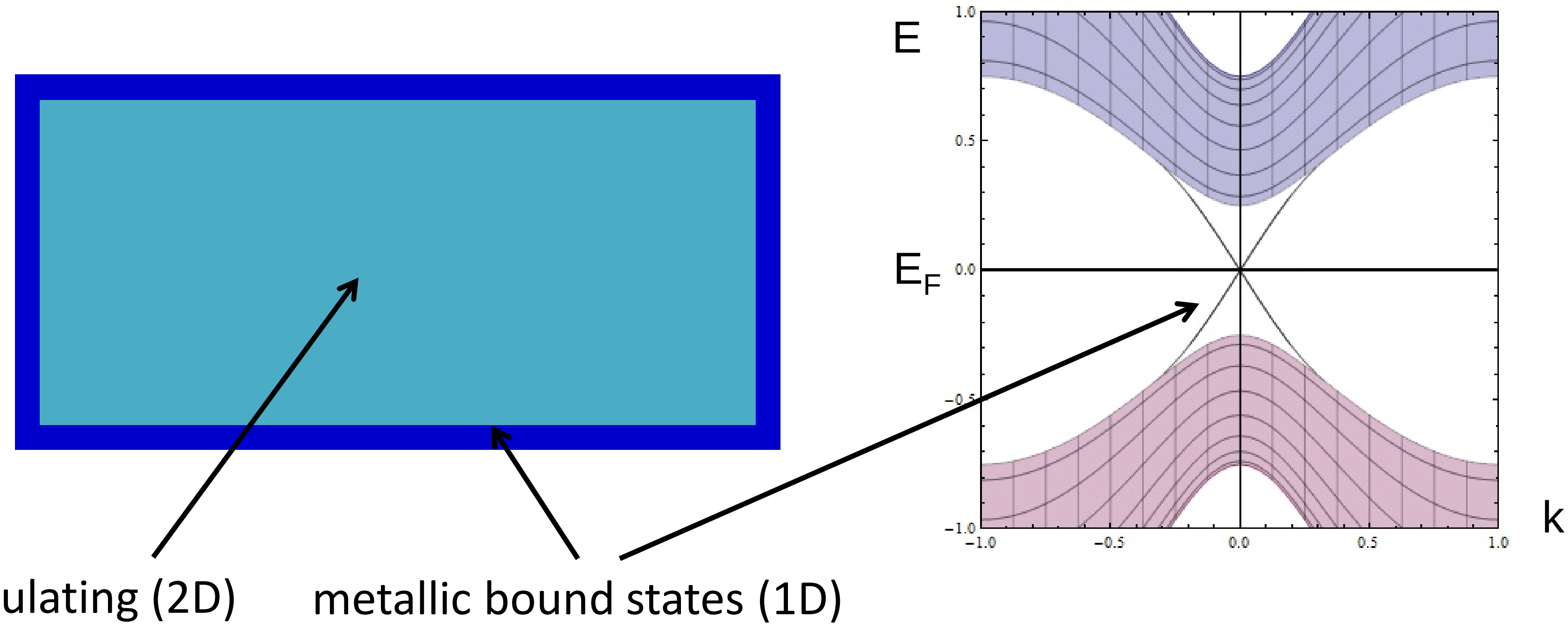
Overview

- Introduction: topological insulator
- Modification of surface states by a ferromagnetic exchange field
- Surface flat bands
- Summary

Introduction: topological insulators

What is a topological insulator ?

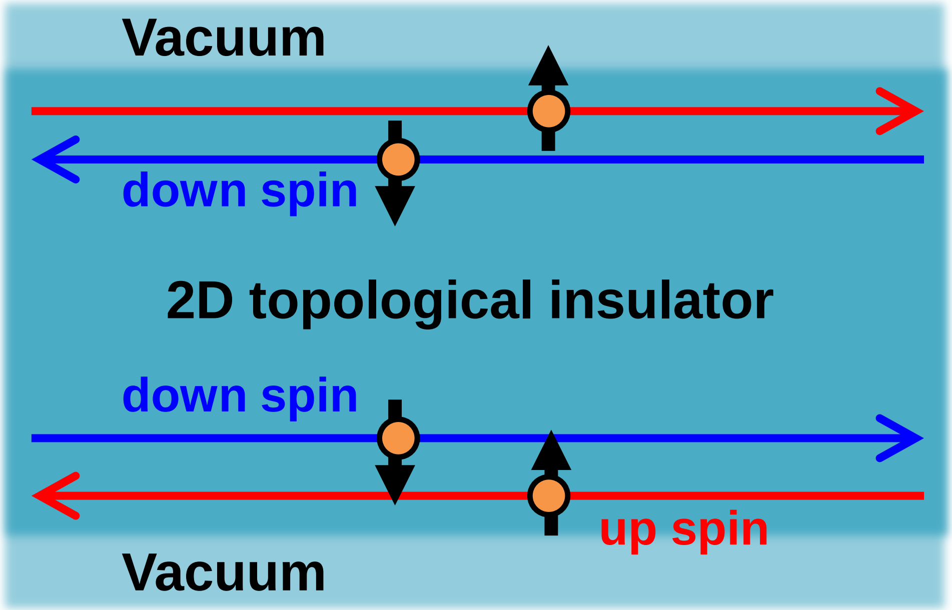
In a topological insulator we have an insulating bulk, but metallic surface states with a linear dispersion.



The existence of the surface states is guaranteed by a topological quantum number

Properties of the surface states

Spin-orbit coupling leads to a spin-momentum locking of the surface states.

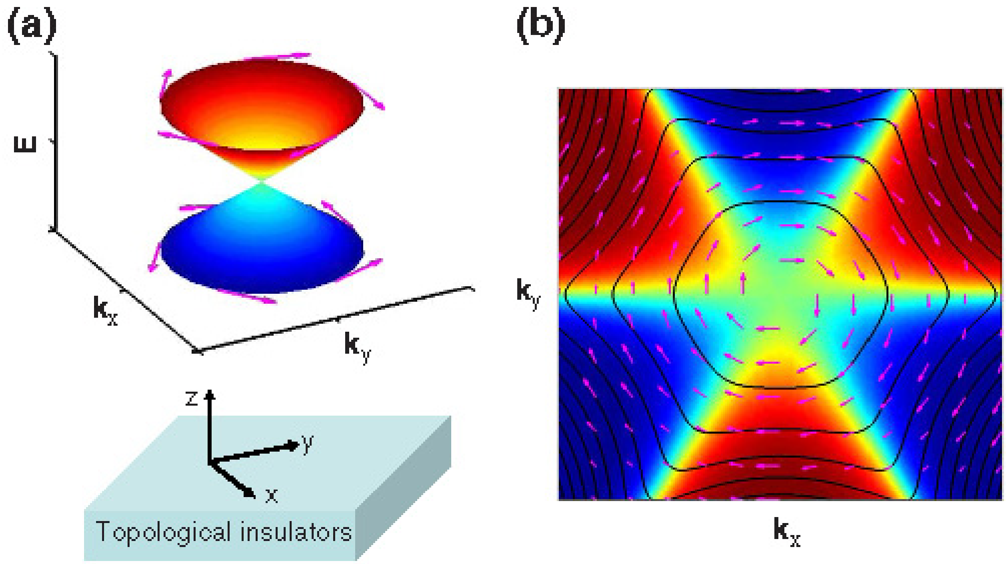


Backscattering between these two channels is forbidden as long as time-reversal symmetry is preserved.

➢ Interesting for spintronics

Properties of the surface states

In a 3D topological insulator the surface states form a massless 2D electron system.



The dispersion forms a Dirac cone, like relativistic fermions.
(In graphene we have two Dirac cones).

Topological insulators and ferromagnets

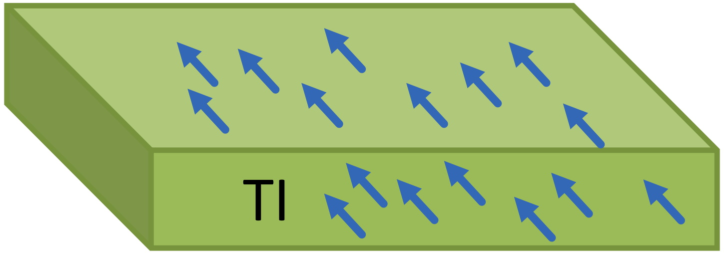
When time-reversal symmetry is respected, the surface states are topologically protected.

What happens, if we break time-reversal symmetry?
Can we control the surface states by a ferromagnet?

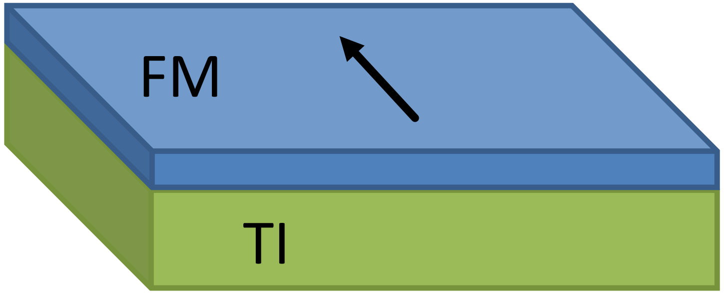
Consider a topological insulator with a Zeeman field

How could this be done?

A ferromagnetic topological insulator ?



Doping by magnetic impurities
Y.L.Chen et al, Science 2010
Mg doped Bi_2Se_3

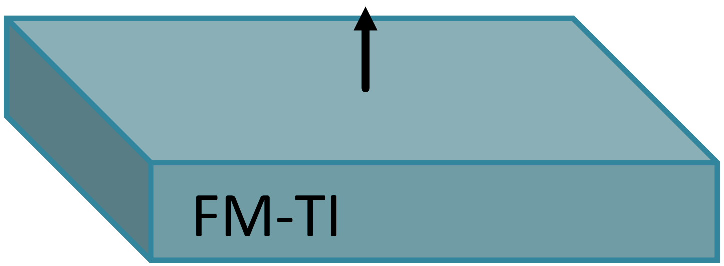


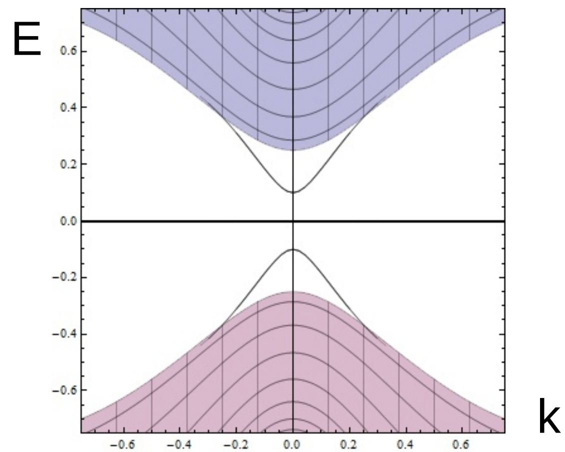
Induction by magnetic proximity effect
P. Wei et al, PRL 2013
EuS on Bi_2Se_3 thin films

What happens to the surface states in a Zeeman field?

R.L. Chu et al, PRB **84**, 085312 (2011)

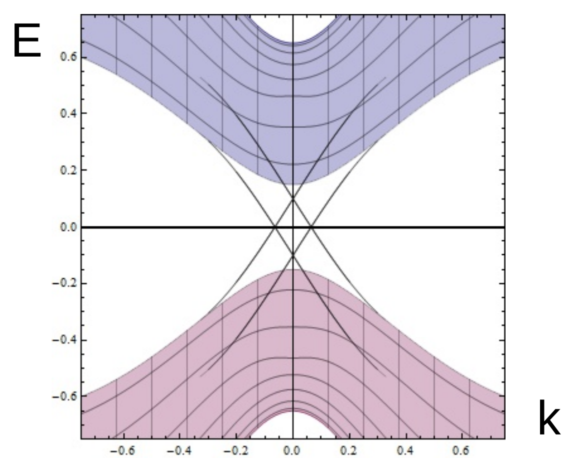
Perpendicular polarization





Surface states become gapped

Parallel polarization

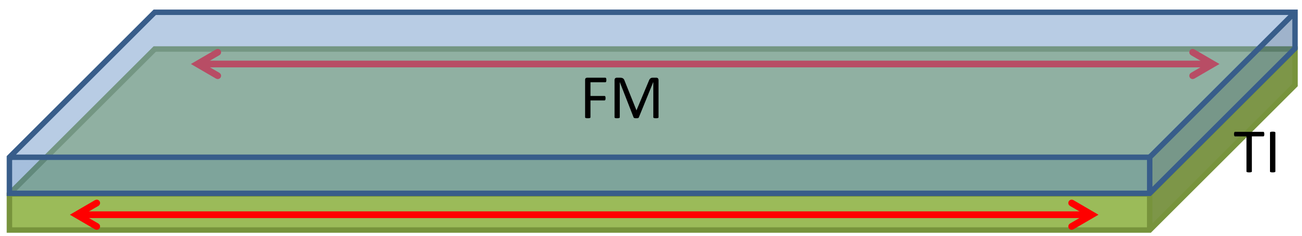


Surface states are shifted, but survive.

Surface flat bands

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)



Standard Hamiltonian for Bi_2Se_3, 2 orbital and 2 spin degrees of freedom:

$$H = \varepsilon_k \mathbb{1}_{4\times4} + \sum_{i=0}^{3} m_i\left(\vec{k}\right)\Gamma^i + \sum_{\alpha\in\{x,y,z\}} V_\alpha \sigma_\alpha \otimes \mathbb{1}_{2\times2}$$

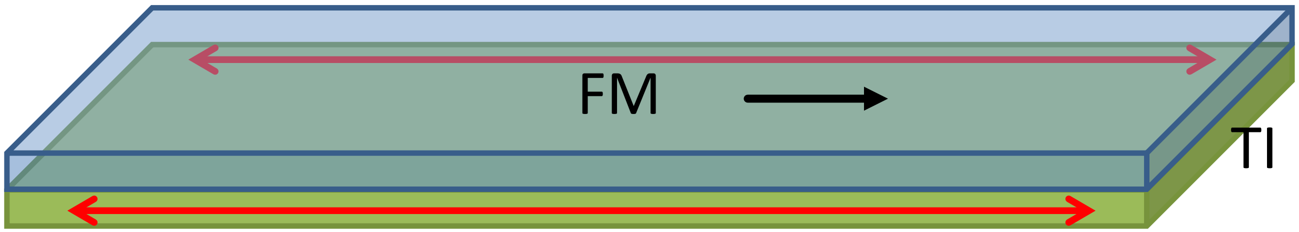
$$m_0(k) = M - 2B_2\left(1-\cos k_x\right) - 2B_2\left(1-\cos k_y\right) - 2B_1\left(1-\cos k_z\right)$$

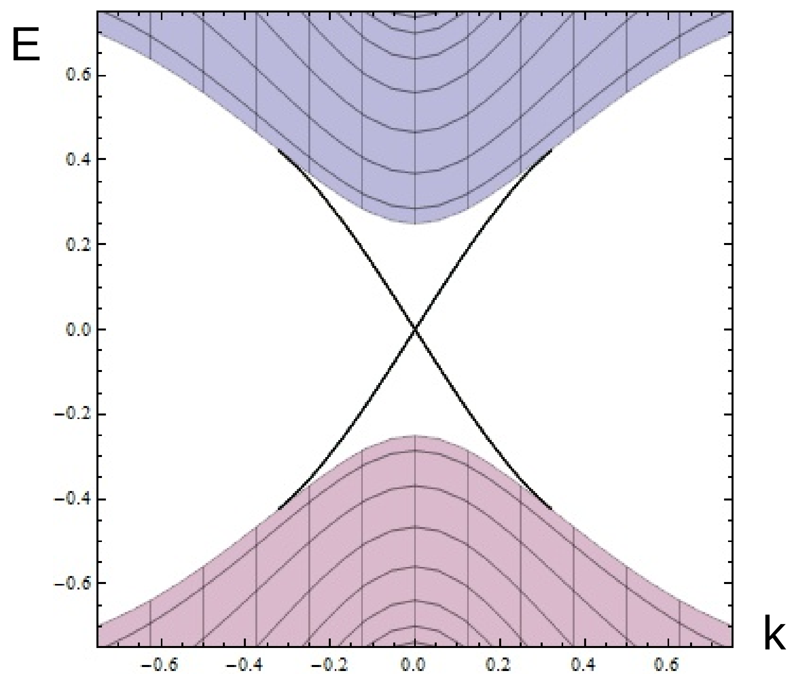
$$m_1(k) = 2A_2 \sin k_x \quad m_2(k) = 2A_2 \sin k_y \quad m_3(k) = 2A_1 \sin k_z$$

In the following we set ε_k=0.

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)





V=0

What happens to the surface states in a Zeeman field?

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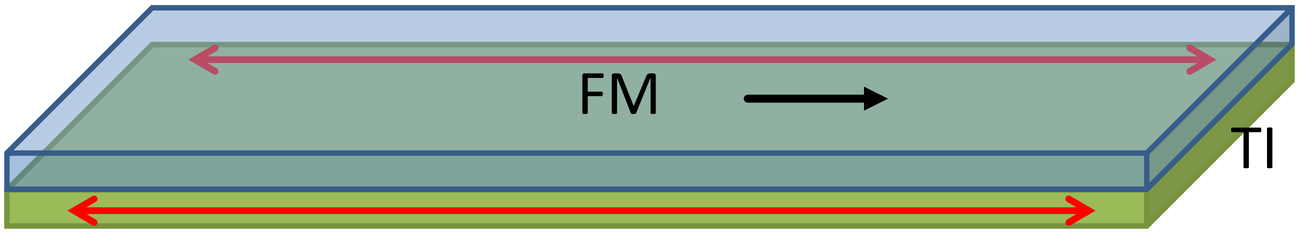
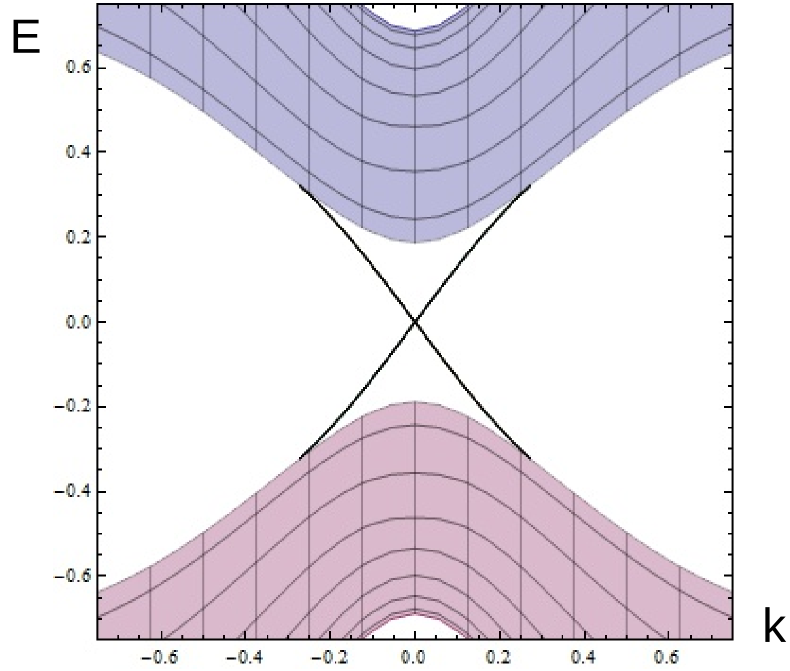
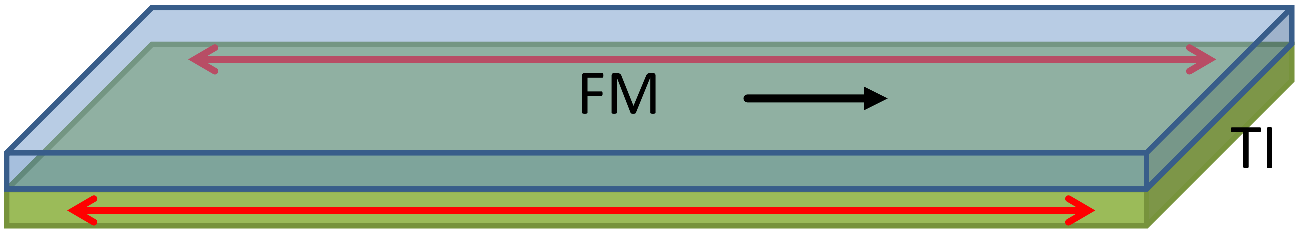


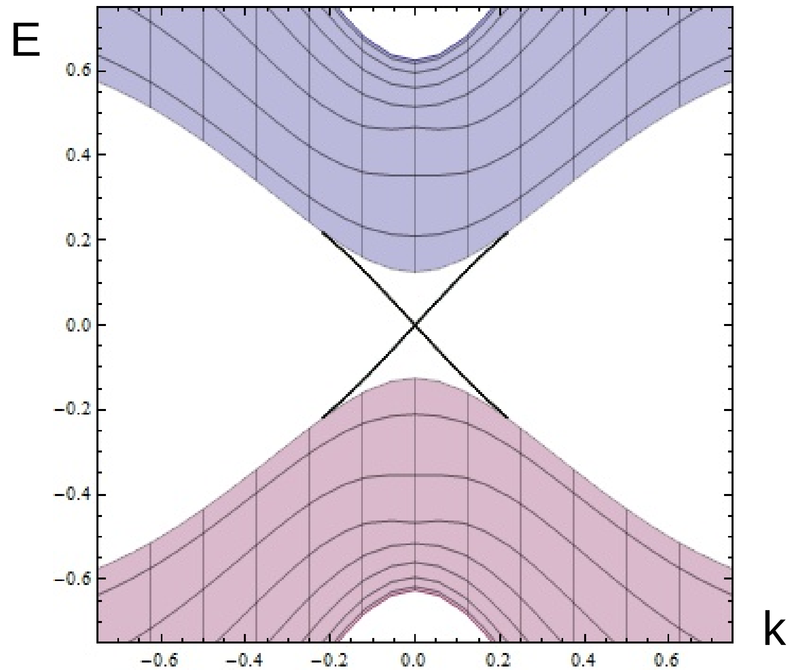


V=0.25 M

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)

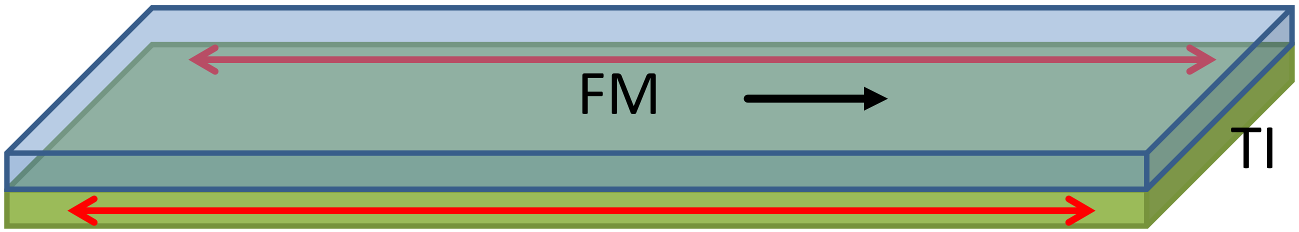


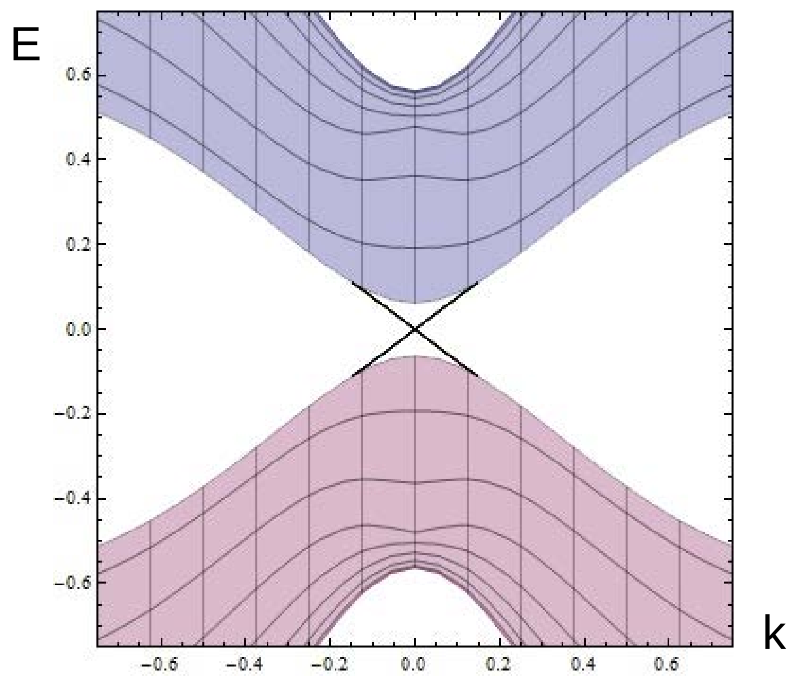


V=0.5 M

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)

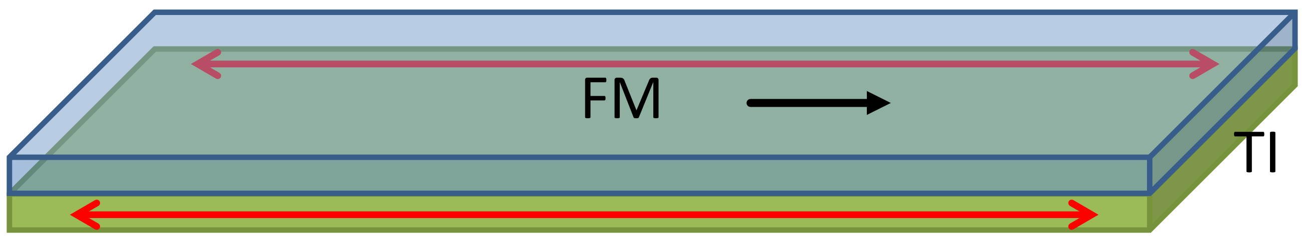


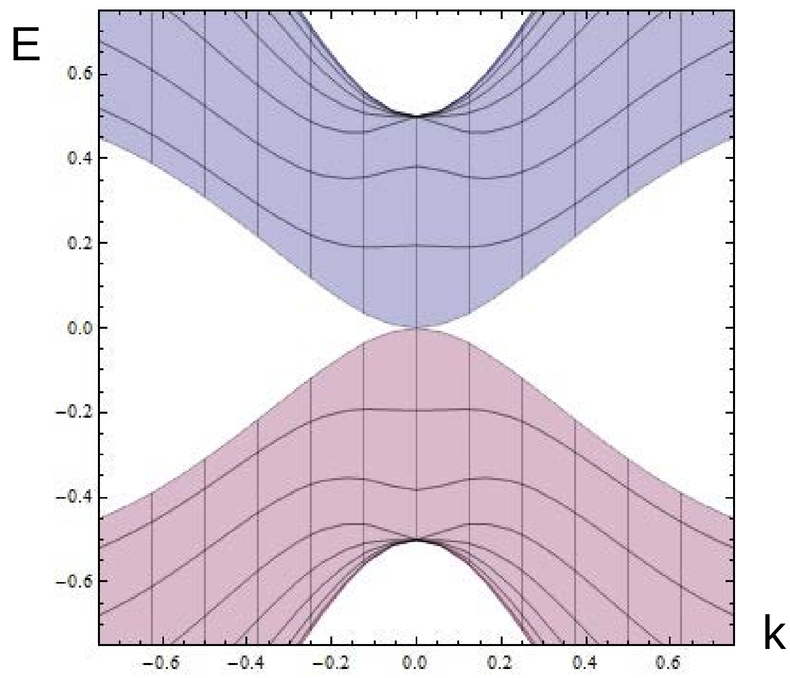


V=0.75 M

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)





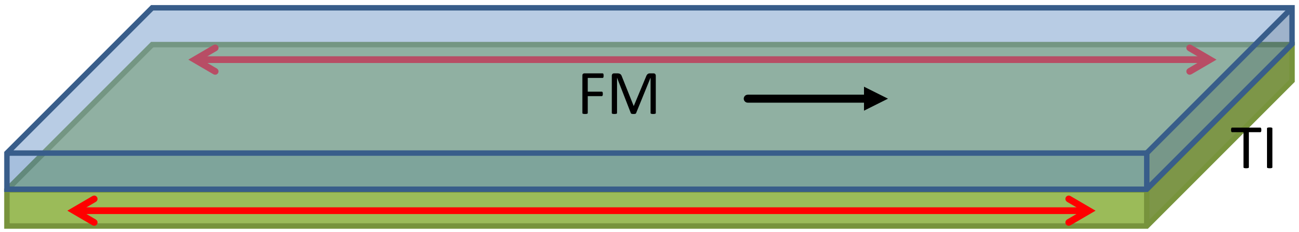
V=1.0 M

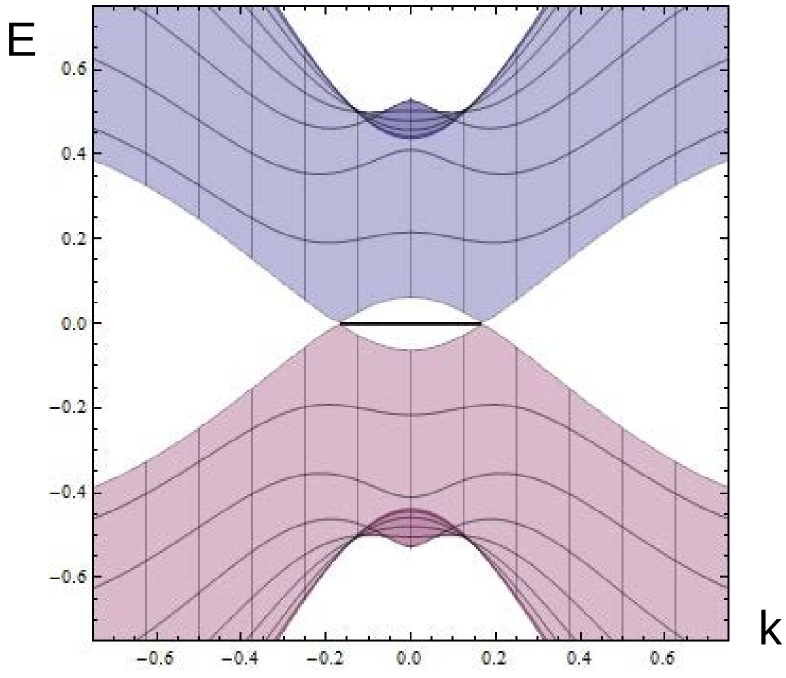
V=bulk gap

Semi-metal

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)

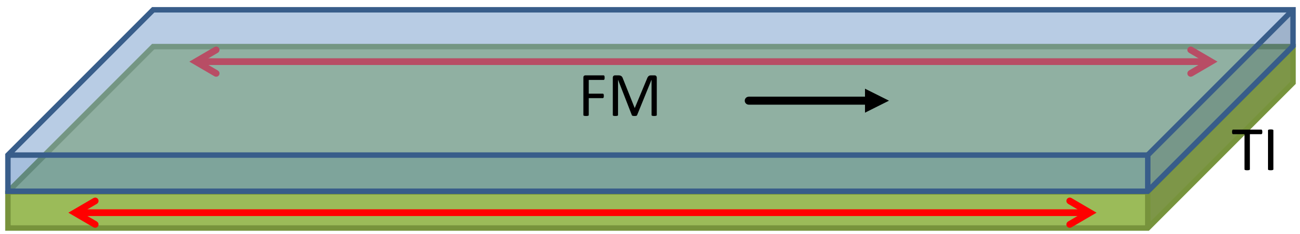


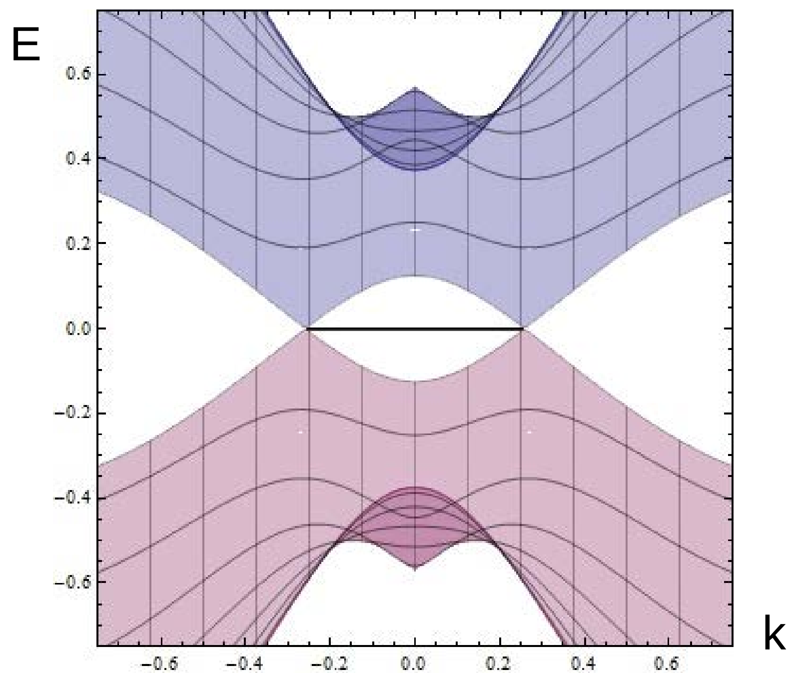


V=1.25 M

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)

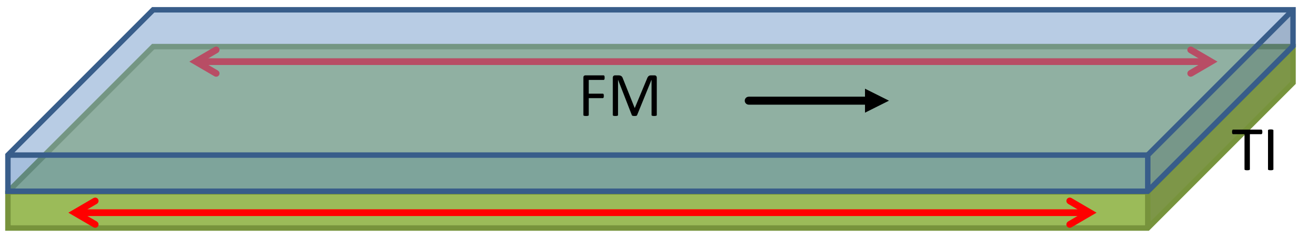


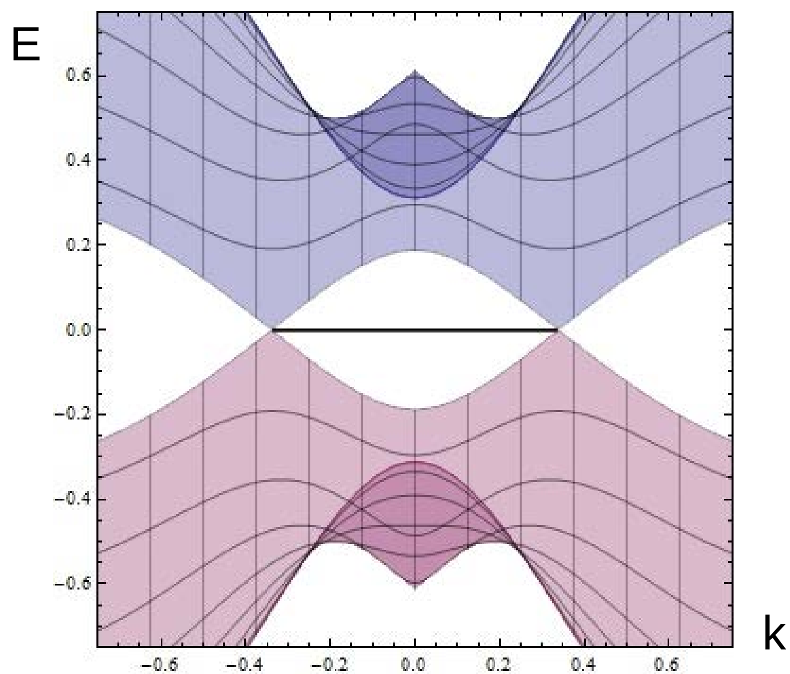


V=1.5 M

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)





V=1.75 M

What happens to the surface states in a Zeeman field?

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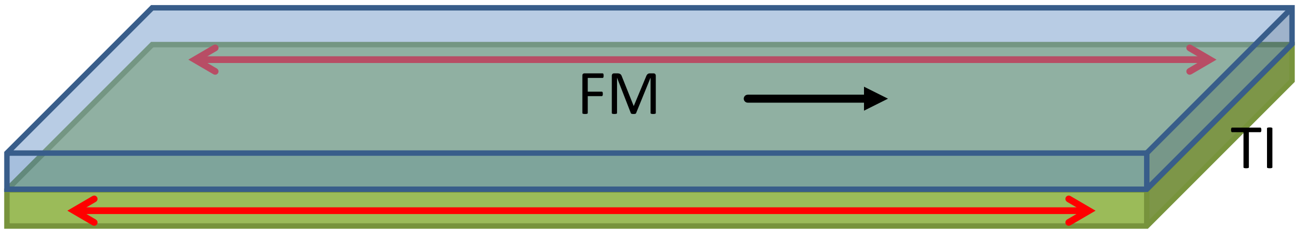
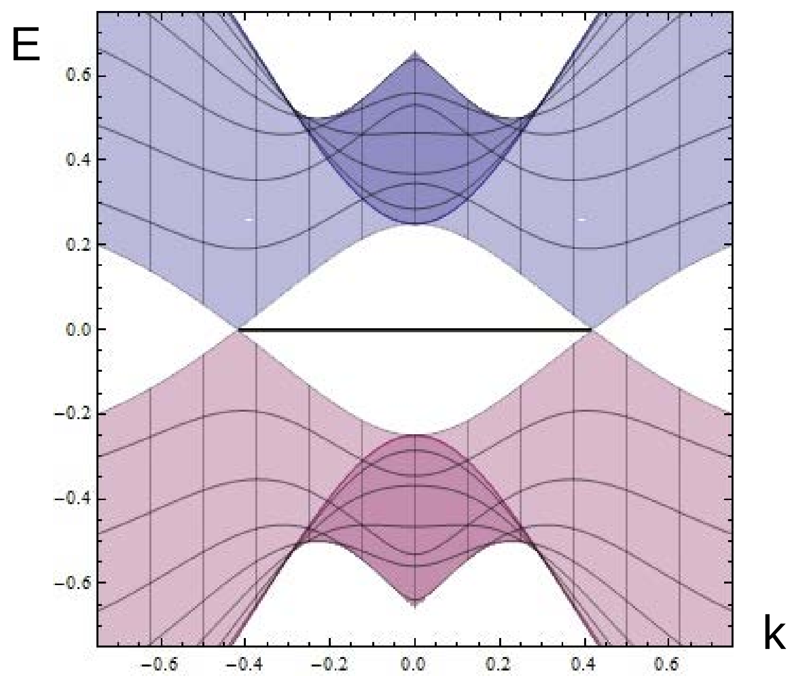
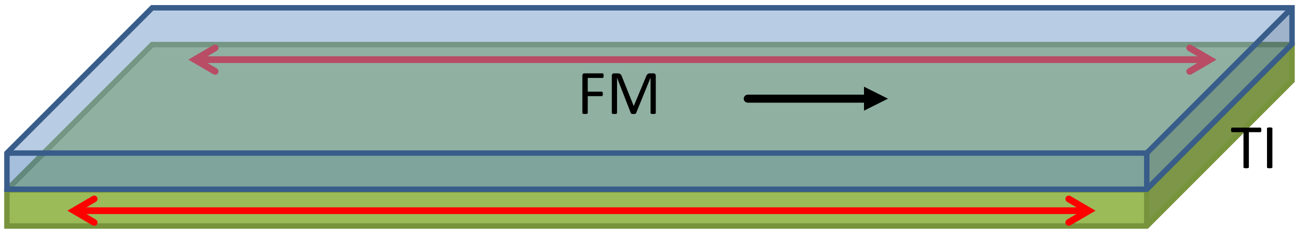




V=2.0 M

What happens to the surface states in a Zeeman field?

T. Paananen and T. Dahm, PRB **87**, 195447 (2013)

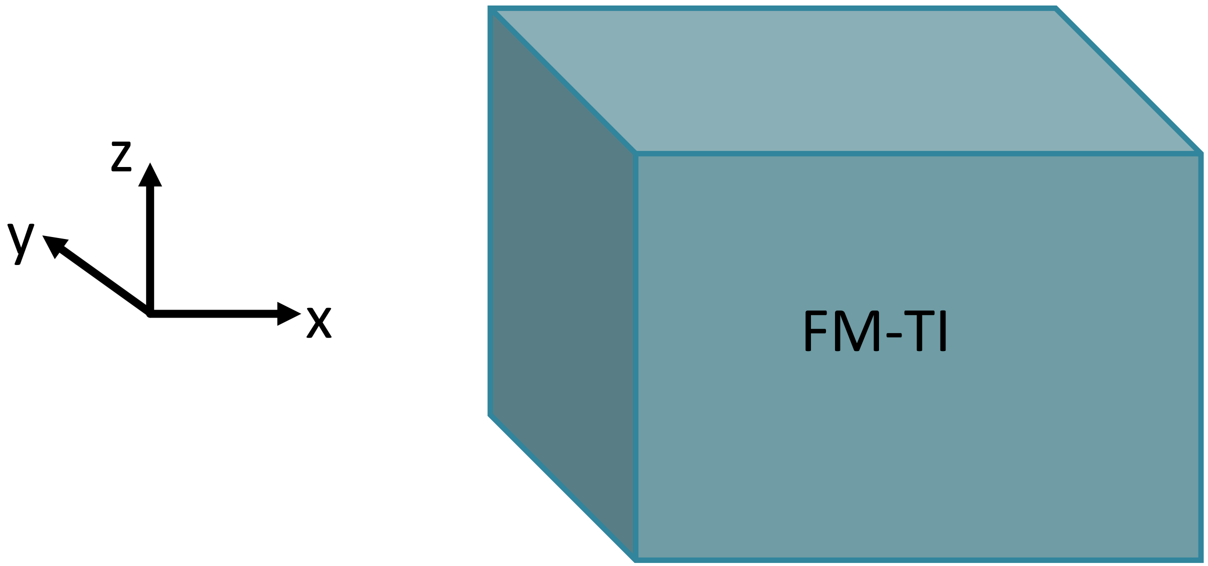


- No splitting of the surface states
- Group velocity can be tuned by the Zeeman field
- No gap
- Appearance of a flat band at zero energy when V>M
- Seems to contradict Chu et al.

3D Topological Insulator

Consider a three dimensional system

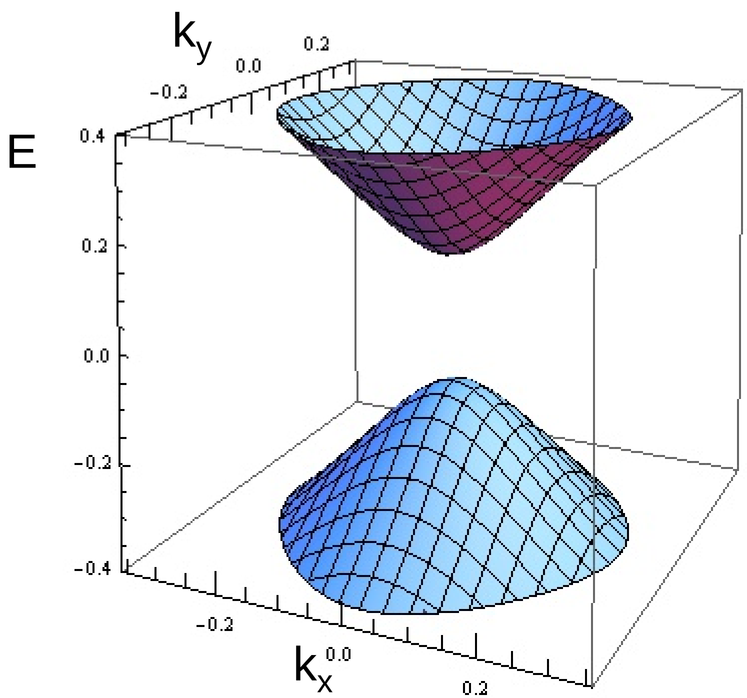
T. Paananen, H. Gerber, M. Götte, and T.Dahm, New J. Phys. (2014)



- Layered, anisotropic materials
- Surfaces are inequivalent

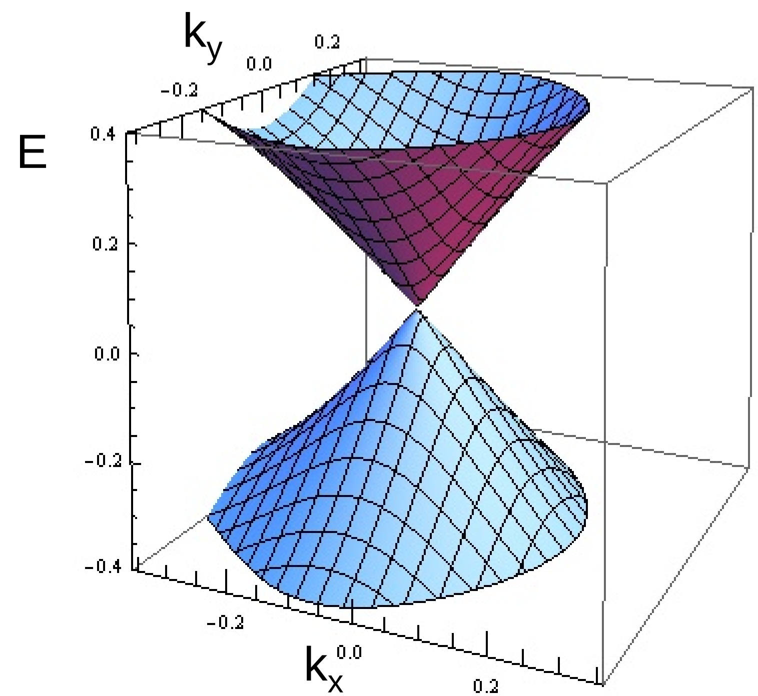
On the top surface we find agreement with Chu et al

V_z=0.5 M



The Dirac cone is gapped

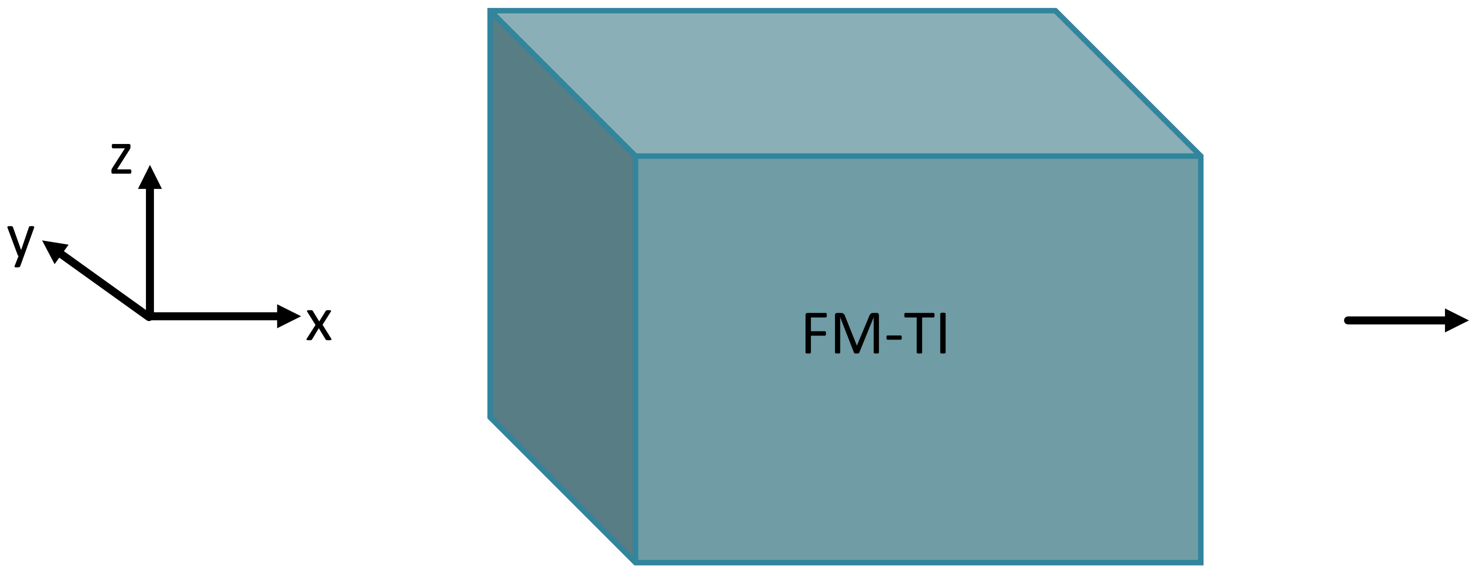
V_x=0.5 M



The Dirac cone is shifted

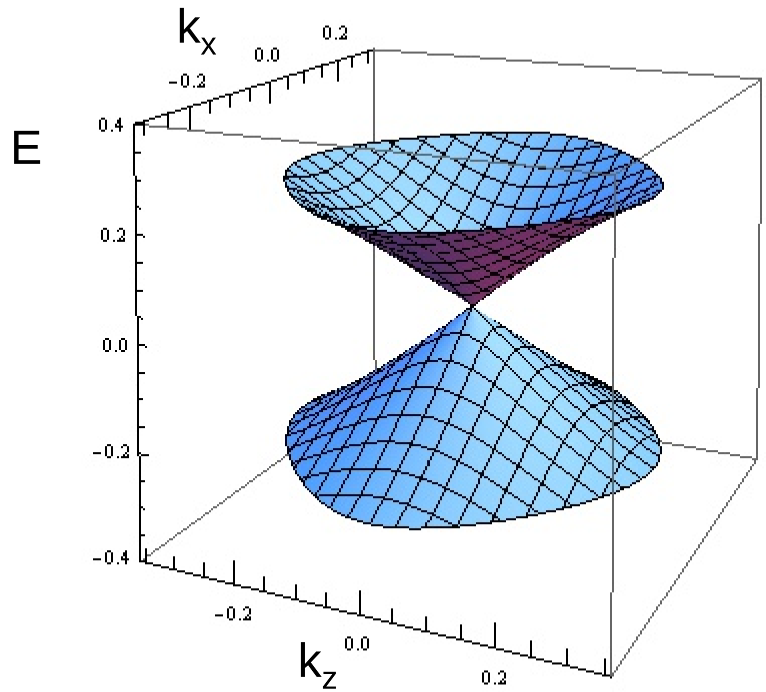
No flat band appears

Front surface: Zeeman field in x-direction



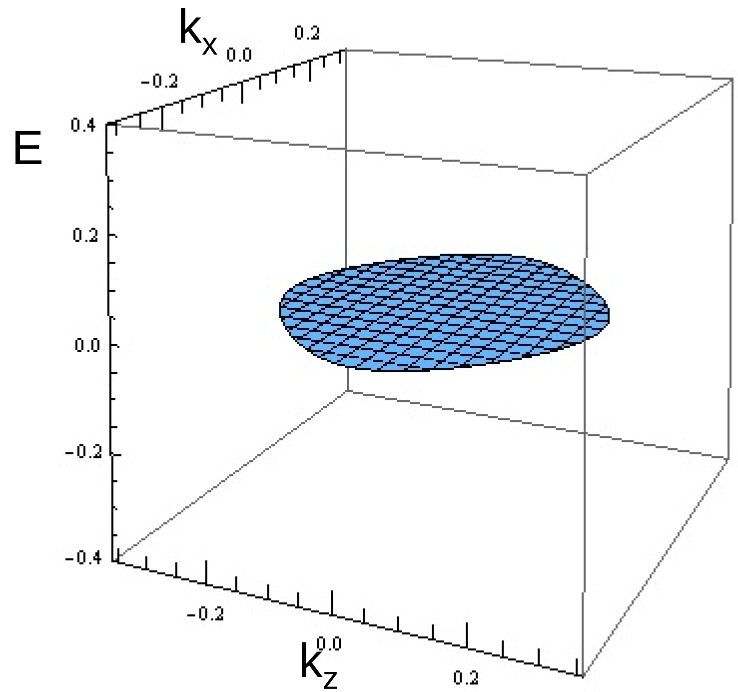
On the front surface the behavior is different

V_x=0.7 M



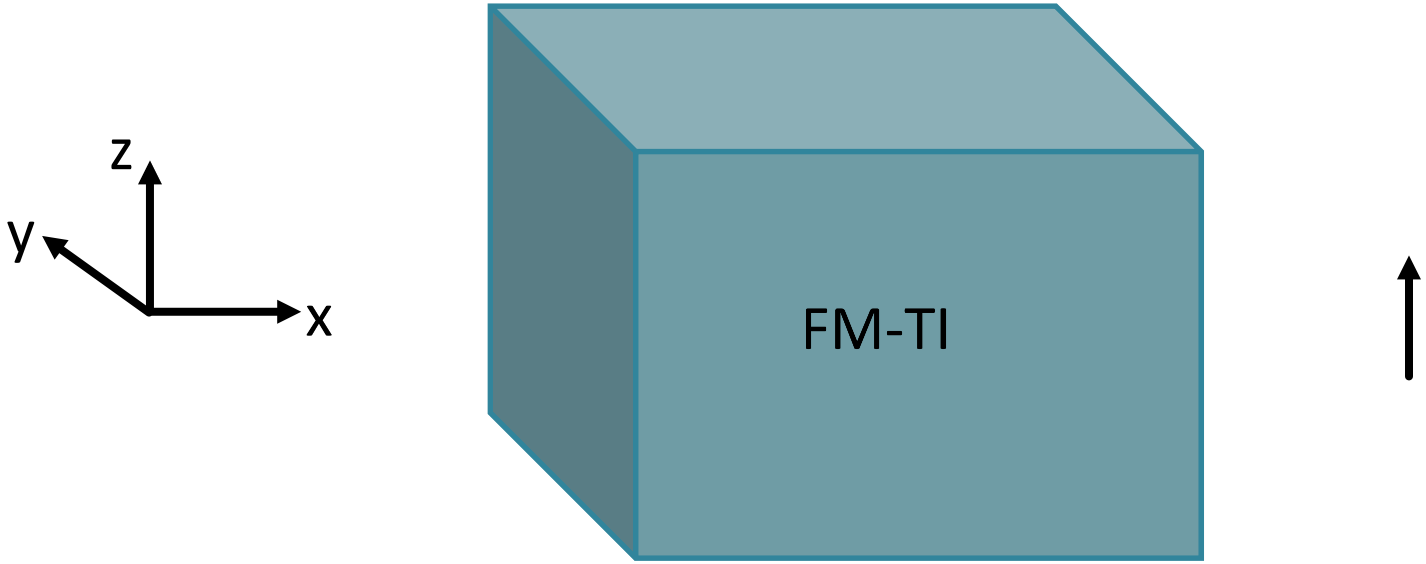
The Dirac cone is isotropically suppressed, tuning of the velocity, no gap

V_x=1.5 M



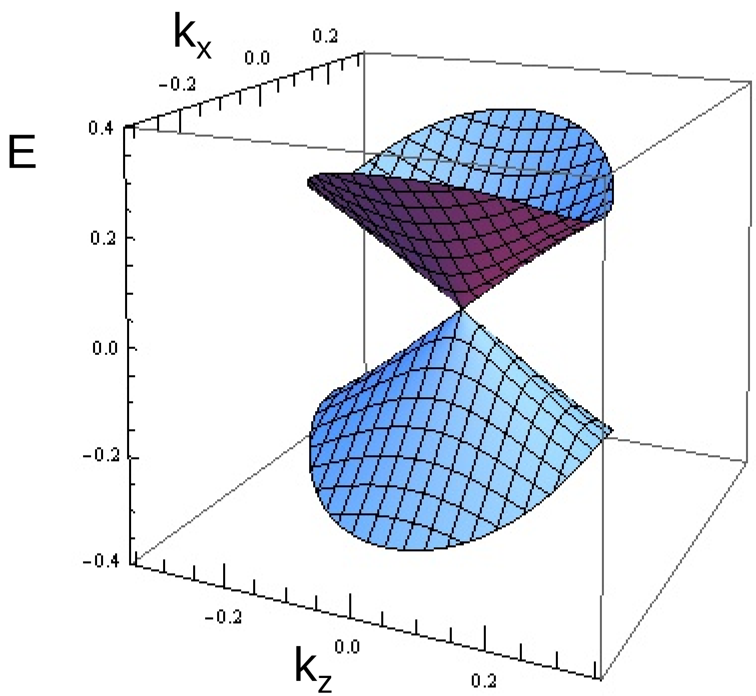
A 2D flat band appears

Front surface: Zeeman field in z-direction



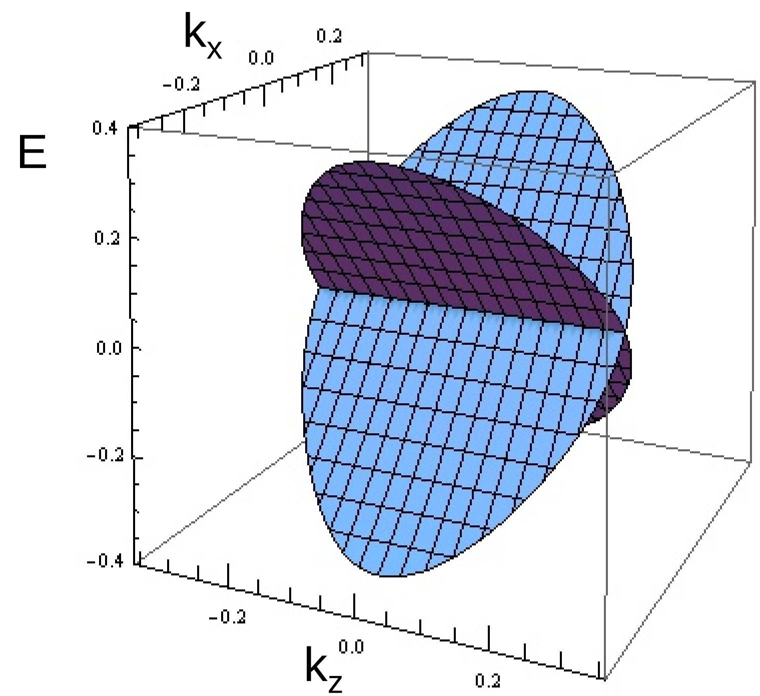
On the front surface the behavior is different

V_z=0.7 M



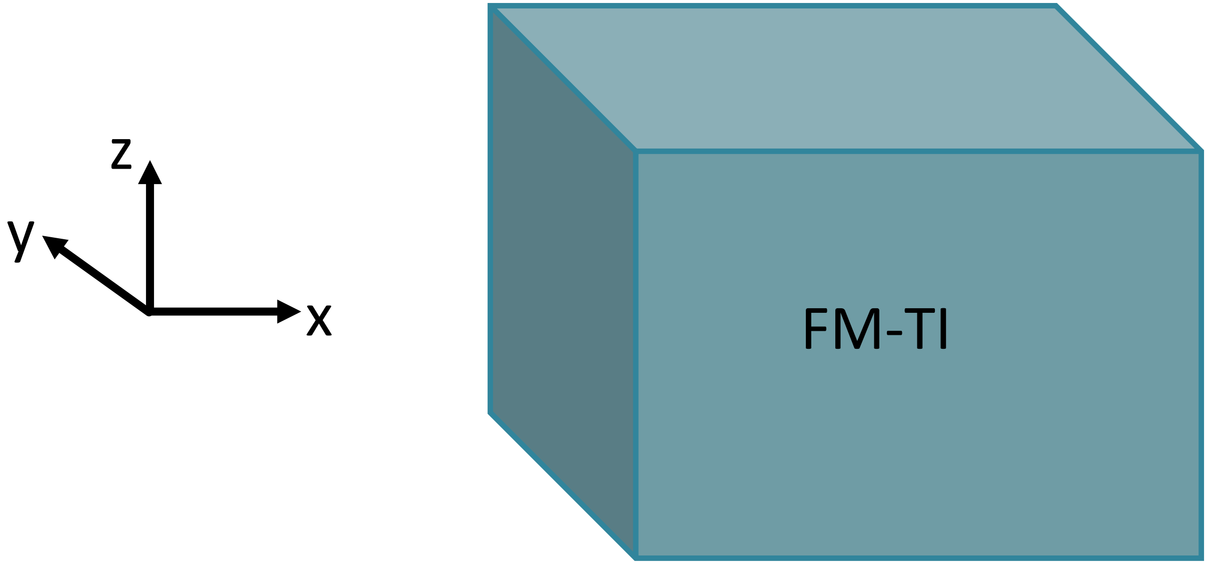
The Dirac cone is anisotropically suppressed, tuning of the velocity, no gap

V_z=1.5 M



A 1D flat band appears

On the front surface the behavior is different



- No gap
- Isotropic suppression and 2D flat band for V_x
- Anisotropic suppression and 1D flat band for V_z

How can we understand the appearance of flat surface bands ?

Bulk-boundary correspondence

Classification of surface states in gapless systems:
S. Matsuura et al, New J. Phys. **15**, 065001 (2013)

If the Hamiltonian possesses a chiral symmetry S, i.e.

$$\{H, S\} = 0$$

a winding number can be defined that tells, if a zero energy surface state exists or not.

We have checked that for all our flat band cases such a chiral symmetry exists and the winding number correctly reproduces the position of the flat bands in momentum space.

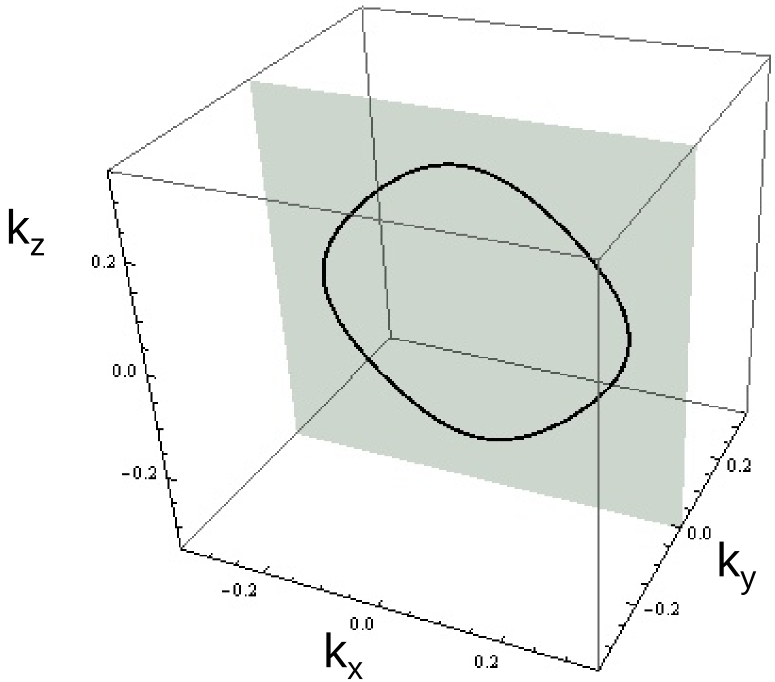
According to Matsuura et al, boundaries of the flat bands are the projection of the Fermi surface onto the surface Brillouin zone.

The dimension of the flat band is the dimension of the Fermi surface plus one.

Let's check this.

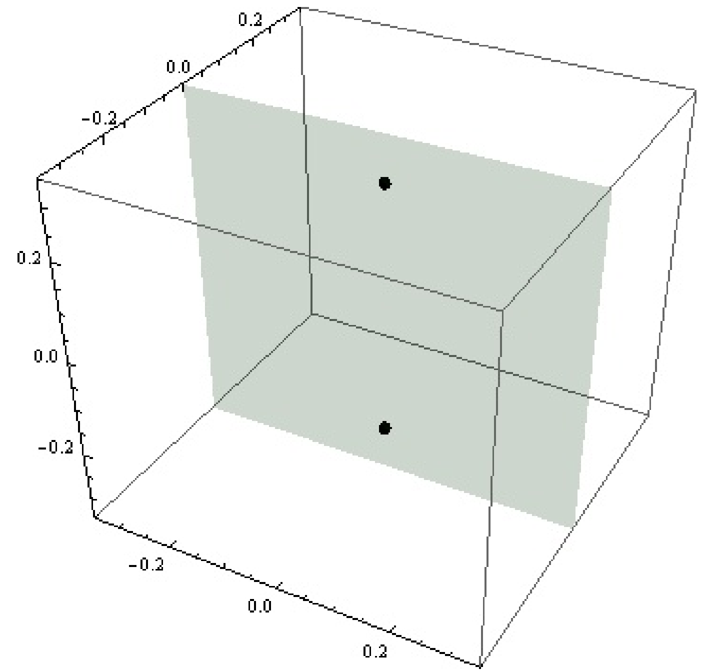
Fermi surface for V>M: semimetal

$V_z=0$



1D Fermi surface
Projection onto k_y plane yields
2D flat band

$V_z\neq 0$



Two Fermi points
Projection onto k_y plane yields
1D flat band, extended along k_z

Weyl semimetal

3D generalization of graphene

Just two bands touch at the Weyl nodes

Has recently been proposed for pyrochlore iridates

Possesses open “Fermi arcs” at the surface BZ

Selected for a Viewpoint in *Physics*

PHYSICAL REVIEW B **83**, 205101 (2011)

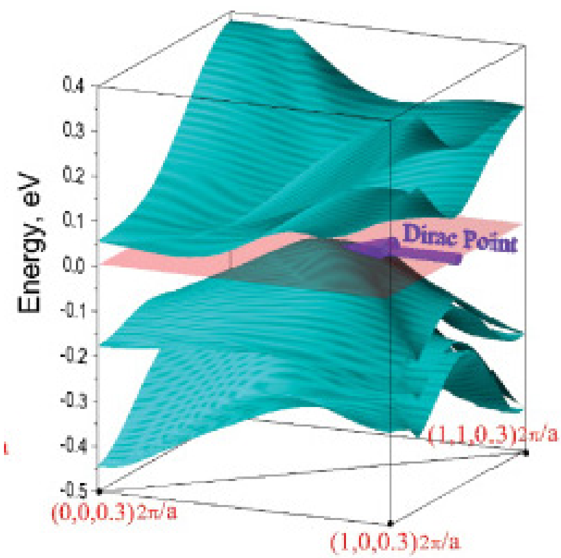
Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates

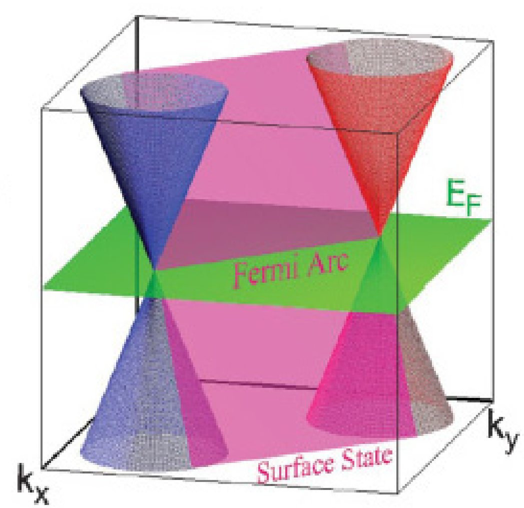
Xiangang Wan,[1] Ari M. Turner,[2] Ashvin Vishwanath,[2,3] and Sergey Y. Savrasov[1,4]

[1]*National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China*
[2]*Department of Physics, University of California, Berkeley, California 94720, USA*
[3]*Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
[4]*Department of Physics, University of California, Davis, One Shields Avenue, Davis, California 95616, USA*
(Received 23 February 2011; published 2 May 2011)

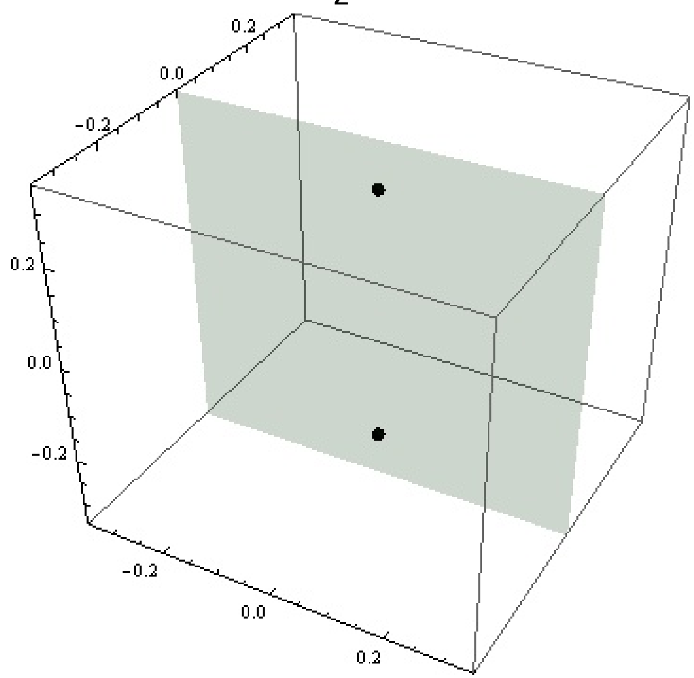
We investigate novel phases that emerge from the interplay of electron correlations and strong spin-orbit interactions. We focus on describing the topological semimetal, a three-dimensional phase of a magnetic solid, and argue that it may be realized in a class of pyrochlore iridates (such as $Y_2Ir_2O_7$) based on calculations using the LDA + U method. This state is a three-dimensional analog of graphene with linearly dispersing excitations and provides a condensed-matter realization of Weyl fermions that obeys a two-component Dirac equation. It also exhibits remarkable topological properties manifested by surface states in the form of Fermi arcs, which are impossible to realize in purely two-dimensional band structures. For intermediate correlation strengths, we find this to be the ground state of the pyrochlore iridates, coexisting with noncollinear magnetic order. A narrow window of magnetic "axion" insulator may also be present. An applied magnetic field is found to induce a metallic ground state.

DOI: 10.1103/PhysRevB.83.205101 PACS number(s): 71.27.+a, 03.65.Vf





$V_z \neq 0$



The bulk is a Weyl semimetal for nonzero V_z

The flat bands are “Fermi arcs”

Only visible at the side surfaces

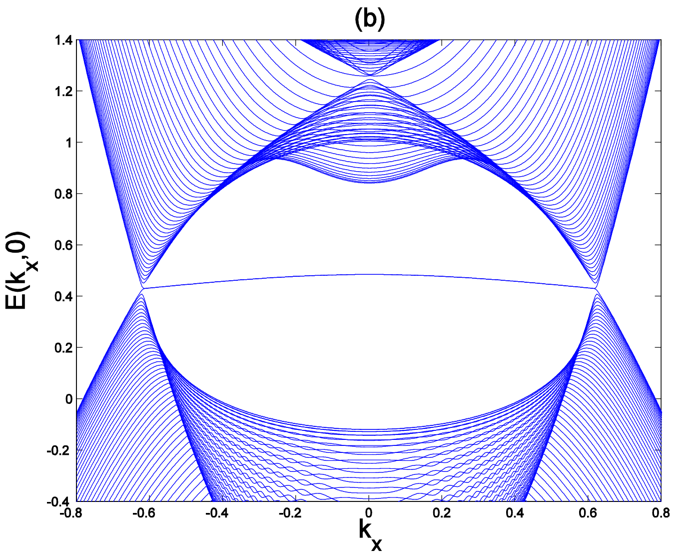
Realistic parameters

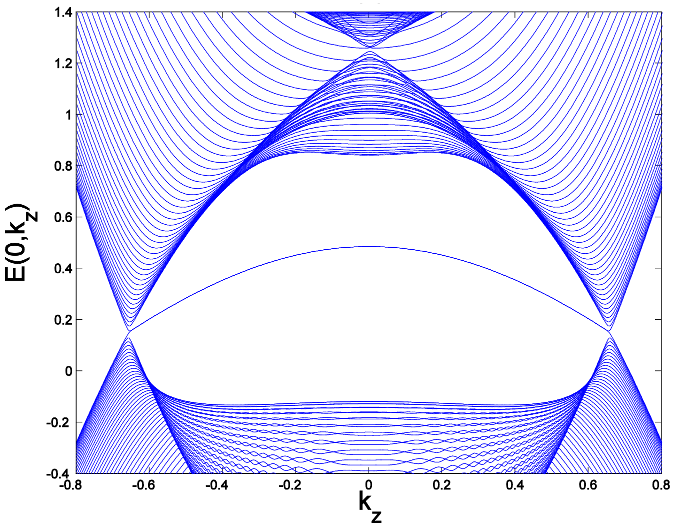
$$H = \varepsilon_k \mathbb{1}_{4\times 4} + \sum_{i=0}^{3} m_i\left(\vec{k}\right)\Gamma^i + \sum_{\alpha\in\{x,y,z\}} V_\alpha \sigma_\alpha \otimes \mathbb{1}_{2\times 2}$$

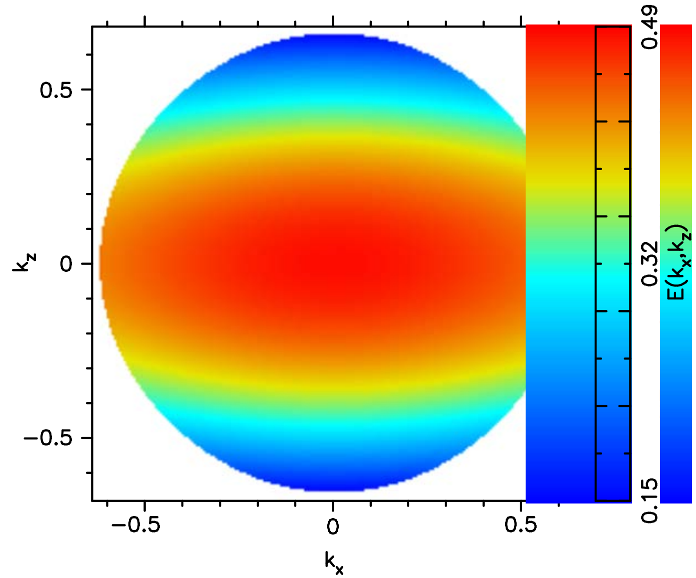
The ε_k term breaks the chiral symmetry S.

What are the consequences for Bi_2Se_3 ?

Realistic parameters for Bi_2Se_3







The flat band gets dispersive, but still exists and remains separated from the bulk.

The system for $V_z \neq 0$ is still a Weyl semimetal.

M=280 meV

Summary

- In the presence of a TRS breaking Zeeman field the surface states are not necessarily removed.

- Topologically protected flat bands appear at the side surfaces if V>M.

- The TI in a Zeeman field becomes a Weyl semimetal for V>M. The surface flat bands create Fermi arcs. The unconventional nature of this phase cannot be seen on the top surface.

- Flat bands at room temperature

- Combination of TIs and ferromagnets promises interesting spintronics applications, as the surface states can be tuned.