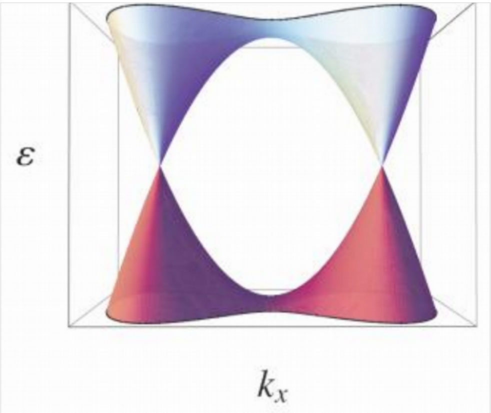
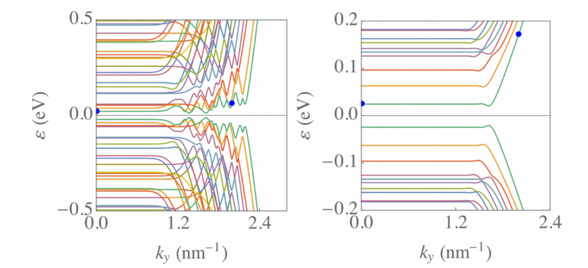
Landau levels and Hall effects in topological semimetals

Enrique Benito Matías, Yuriko Baba, José González, Rafael A. Molina

Instituto de Estructura de la Materia – CSIC (Madrid, Spain)



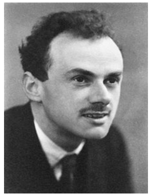


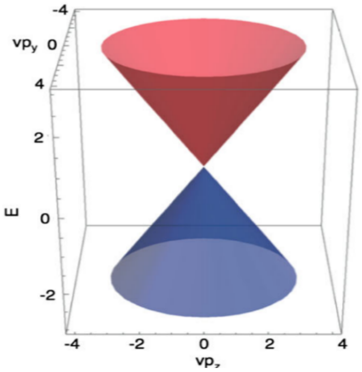
PRL 116, 156803 (2016)
PRB 96, 045437 (2017)
PRL 120, 146601 (2018)
PRB 99, 075304 (2019)
PRB 100, 165105 (2019)
PRB 101, 085420 (2020)
NJP 23, 023008 (2021)

GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN
MINISTERIO DE UNIVERSIDADES
Unión Europea
Fondo Europeo de Desarrollo Regional
"Una manera de hacer Europa"

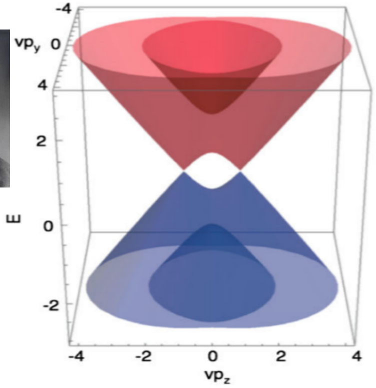
Introduction: topological semimetals

Dirac

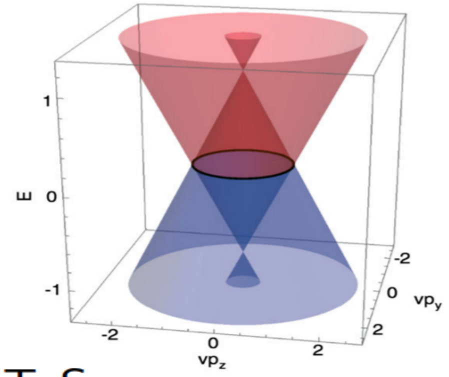




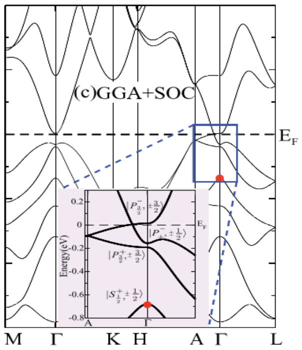
Weyl

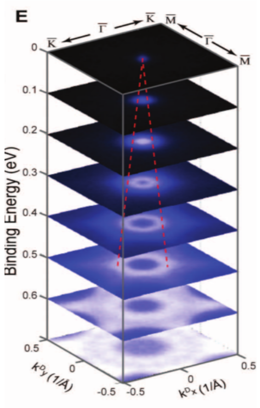


Nodal-line

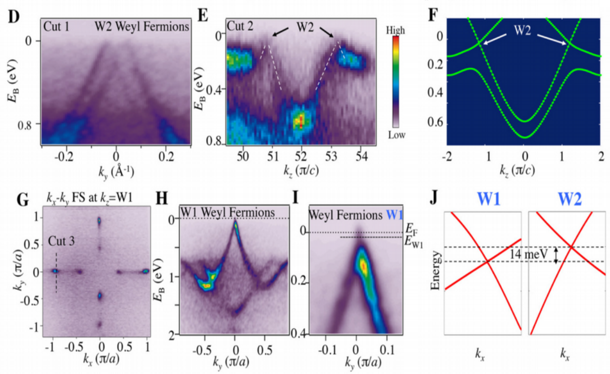


Na_3Bi

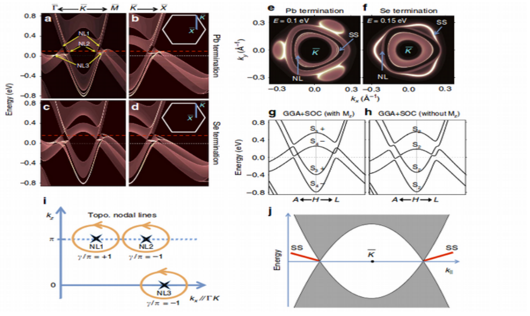




TaAs



$PbTaSe_2$



Z. Wang et al. PRB 85, 195320 (2012) (theory)

Z.K. Liu et al. Science 343, 864 (2014) (experiments)

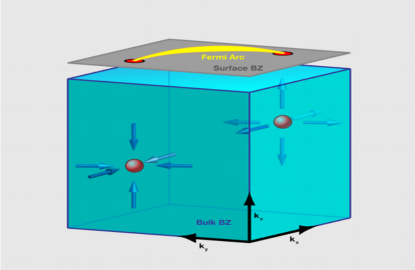
Su-Yang Xu et al. Science 349, 613 (2015)

Guang Bian et al. Nat. Comm. 7, 10556 (2016)

LaSbTe Wang et al. PRB 103, 125131 (2021)

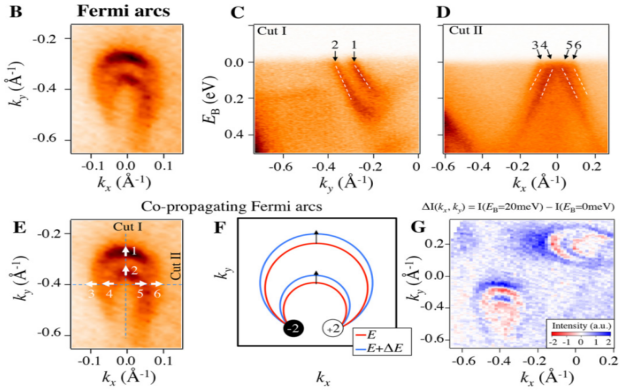
Topological semimetals: surface states

- Fermi arcs



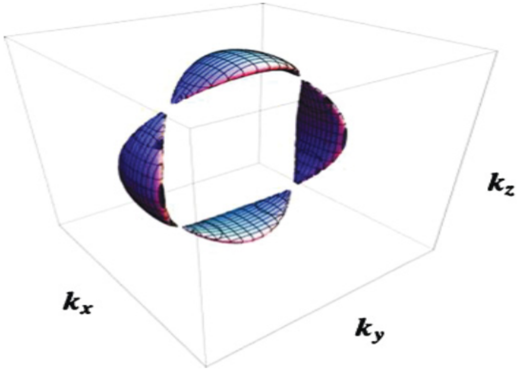
Leon Balents, Weyl electrons kiss, Physics 4, 36 (2011)

TaAs



Su-Yang Xu et al. Science 349, 613 (2015)

- Drumhead states for nodal line semimetals



Burkov, Hook, Balents PRB 84, 235126 (2011)

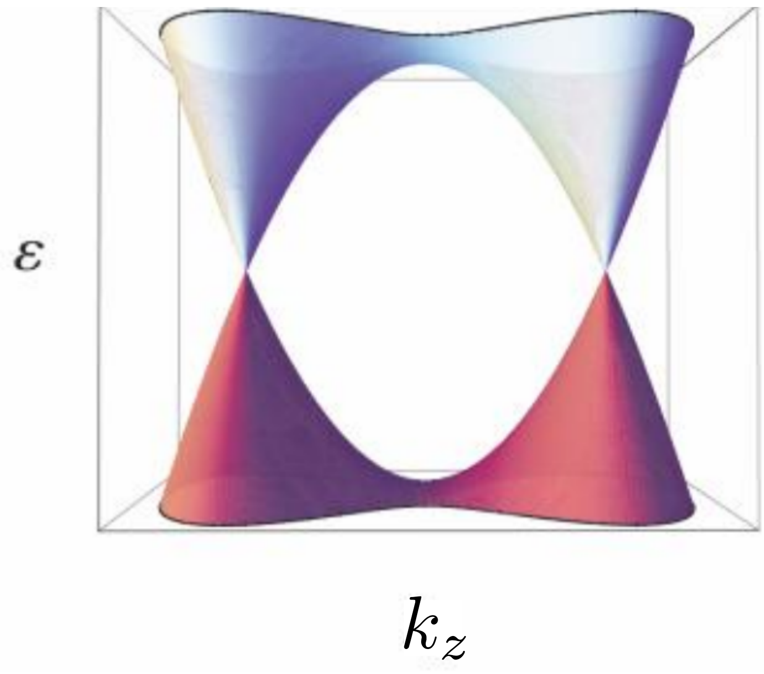
Topological semimetals

Minimal two-band model of a Weyl semimetal

$$\mathrm{H}_W = [m_0 - m_1(k_x^2 + k_y^2 + k_z^2)]\sigma_z + v\sigma_x k_x + \eta v \sigma_y k_y$$

$$\varepsilon_\pm = \pm\sqrt{(m_0 - m_1\mathbf{k}^2)^2 + v^2(k_x^2 + k_y^2)}$$

Weyl nodes: $k_z = \pm\sqrt{\frac{m_0}{m_1}}$ $\quad k_x = 0 \quad k_y = 0$



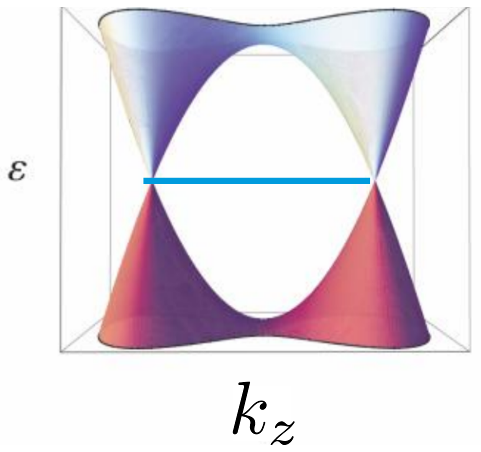
Topological semimetals

Minimal two-band model of a Weyl semimetal

$$\mathrm{H}_W = [m_0 - m_1(k_x^2 + k_y^2 + k_z^2)]\sigma_z + v\sigma_x k_x + \eta v \sigma_y k_y$$

$$\varepsilon_\pm = \pm\sqrt{(m_0 - m_1\mathbf{k}^2)^2 + v^2(k_x^2 + k_y^2)}$$

Weyl nodes: $k_z = \pm\sqrt{\frac{m_0}{m_1}}$ $k_x = 0$ $k_y = 0$



We look for decaying surface states: Fermi arcs

$$\varphi(x,y,z) \sim e^{ik_x x} e^{-\alpha x} f(z,y)$$

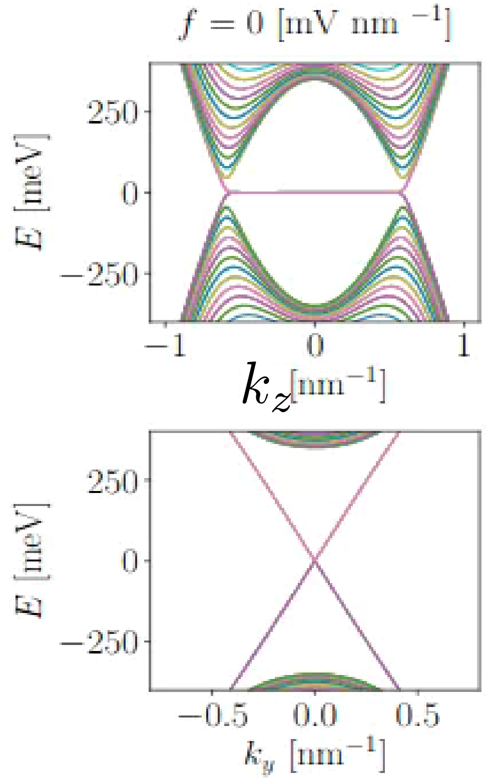
Topological semimetals

Minimal two-band model of a Weyl semimetal

$$\mathrm{H}_W = [m_0 - m_1(k_x^2 + k_y^2 + k_z^2)]\sigma_z + v\sigma_x k_x + \eta v \sigma_y k_y$$

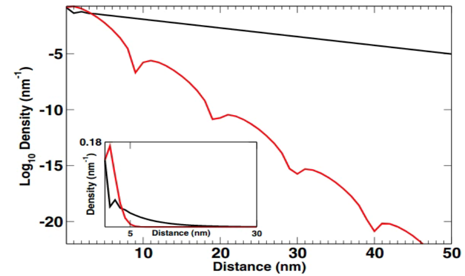
$$\varepsilon_\pm = \pm\sqrt{(m_0 - m_1\mathbf{k}^2)^2 + v^2(k_x^2 + k_y^2)}$$

Weyl nodes: $k_z = \pm\sqrt{\frac{m_0}{m_1}}$ $\quad k_x = 0 \quad k_y = 0$



We look for decaying surface states: Fermi arcs

$$\varphi(x,y,z) \sim e^{ik_x x} e^{-\alpha x} f(z,y)$$

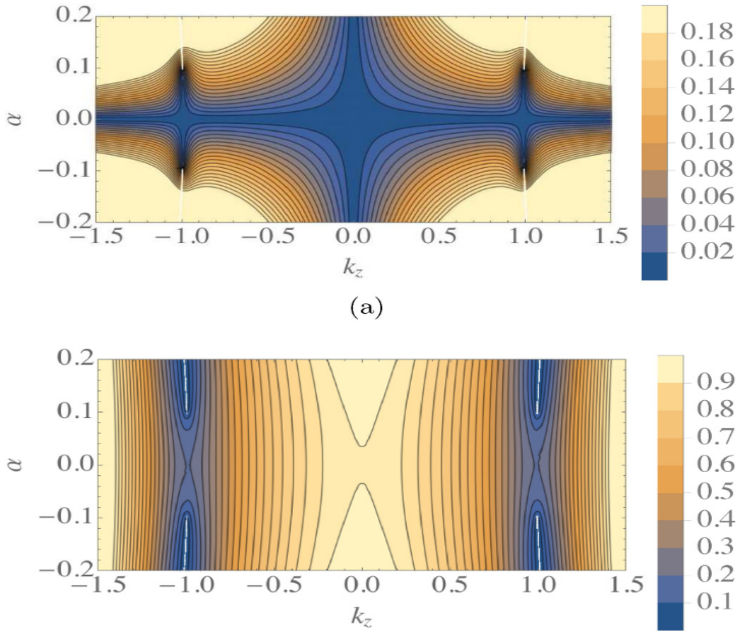


Fermi arcs as exceptional points

$$\lambda = \pm\sqrt{\left(m_0 - m_1(k_x^2 + (k_z + i\alpha)^2)\right)^2 + v^2(k_z + i\alpha)^2}$$

Im

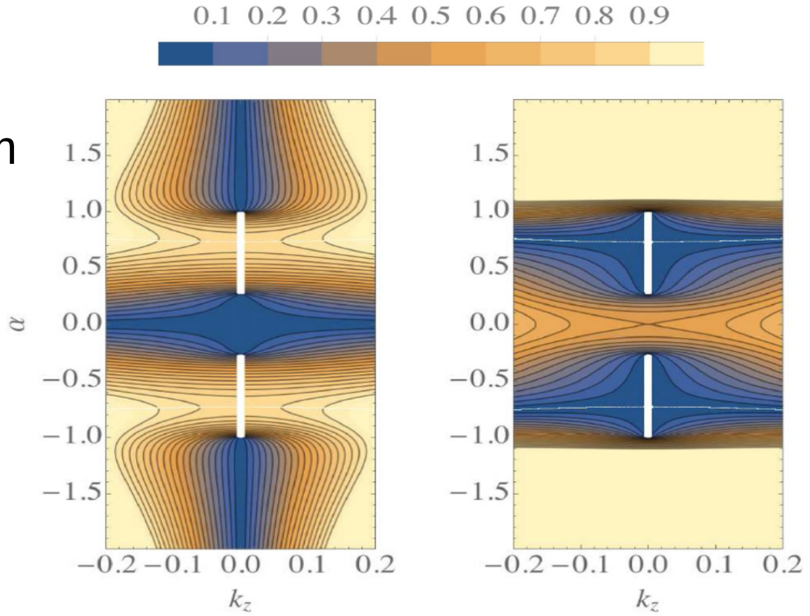
Re



Type A (evanescent plus oscillations)

Im

Re



Type B (pure evanescent)

J. González, RAM, PRB 96, 045437 (2017)

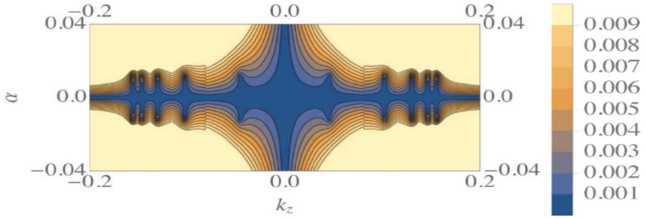
Drumhead states as exceptional points

$$H_{\rm NL} = (m_0 + m_1 \boldsymbol{\nabla}^2)\sigma_z - iv\partial_z\sigma_x$$

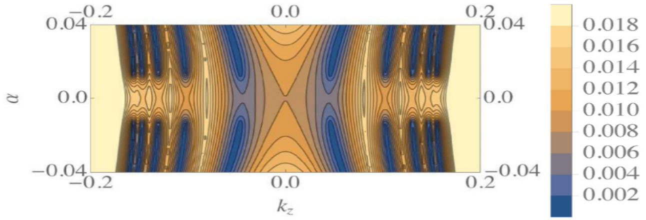
$$\chi(r,\theta,z) \sim e^{ik_z z} e^{-\alpha z} e^{im\theta} f(r)$$

Type A nodal line semimetal $4m_1 m_0 > v^2$

$$\alpha = \frac{v}{2m_1} \qquad k_r = \sqrt{\frac{m_0}{m_1} - k_z^2 - \alpha^2}$$



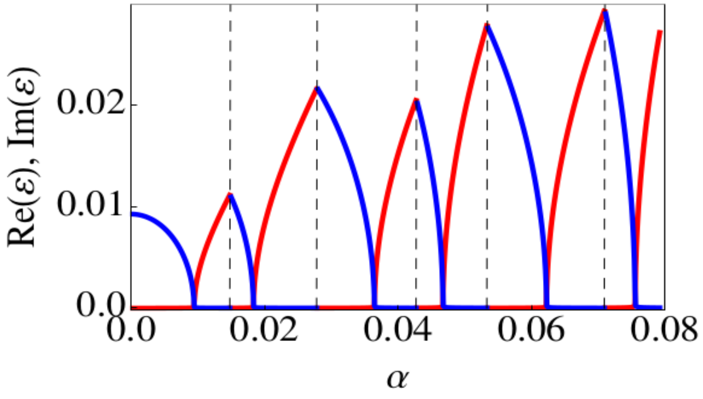
(a)



Type B nodal line semimetal $4m_1 m_0 < v^2$

$$k_z = 0$$

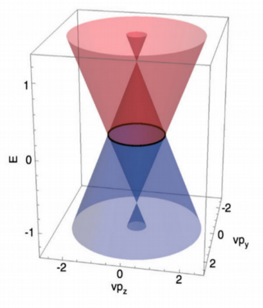
$$\alpha = \frac{v \pm \sqrt{v^2 - 4m_1(m_0 - m_1 k_r^2)}}{2m_1}$$

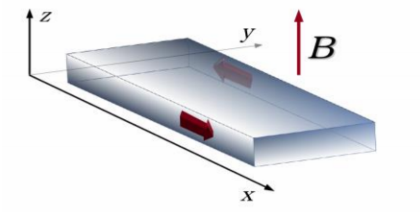


Surface quantum Hall effect in nodal-line semimetals

Magnetic field perpendicular to the plane of the nodal line

$$H_{\rm NL} = (m_0 + m_1 \boldsymbol{\nabla}^2)\sigma_z - iv\partial_z\sigma_x$$





$$\mathbf{A} = (-By, 0, 0)$$

$$\varepsilon = \pm\sqrt{(m_0 - m_1\mathbf{k}^2)^2 + v^2k_z^2}$$

$$k_x^2 + k_y^2 = m_0/m_1 \qquad k_z = 0$$

$$H_\perp = \left[m_0 + m_1\left(-(-i\partial_x - By)^2 + \partial_y^2 + \partial_z^2\right)\right]\sigma_z - iv\partial_z\sigma_x$$

Eigenstates in the bulk are given in terms of the eigenfunctions of a harmonic oscillator centered in $y = k_x/B$

$$\varepsilon_n = \pm\sqrt{[m_0 - m_1k_z^2 - 2m_1B(n+1/2)]^2 + v^2k_z^2}$$

RAM, J. González, PRL 120, 146601 (2018)

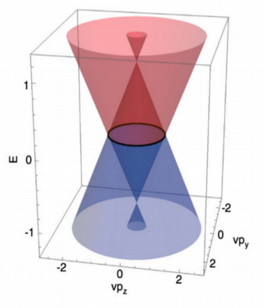
Surface quantum Hall effect in nodal-line semimetals

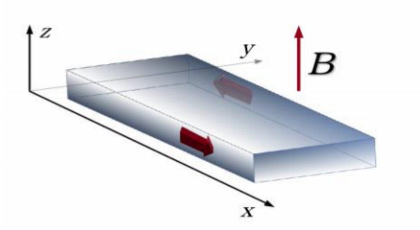
Magnetic field perpendicular to the plane of the nodal line

$$H_{\rm NL} = (m_0 + m_1 \boldsymbol{\nabla}^2)\sigma_z - iv\partial_z\sigma_x$$

$$\varepsilon = \pm\sqrt{(m_0 - m_1\mathbf{k}^2)^2 + v^2 k_z^2}$$

$$k_x^2 + k_y^2 = m_0/m_1 \qquad k_z = 0$$





$$\mathbf{A} = (-By, 0, 0)$$

$$H_\perp = \left[m_0 + m_1\left(-(-i\partial_x - By)^2 + \partial_y^2 + \partial_z^2\right)\right]\sigma_z - iv\partial_z\sigma_x$$

We can look for Landau states decaying from the z surface

$$\Psi \sim e^{iwz}\chi(x,y)\hat{\eta} \qquad \sigma_y\hat{\eta} = \pm\hat{\eta}$$

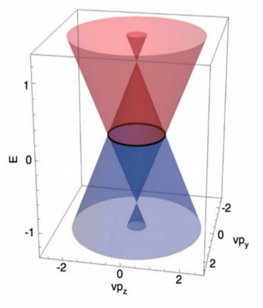
$$4m_0m_1 < v^2 \qquad w = \pm i\,\frac{v \pm \sqrt{v^2 - 4m_1(m_0 - m_1 2B(n+1/2))}}{2m_1}$$

RAM, J. González, PRL 120, 146601 (2018)

Surface quantum Hall effect in nodal-line semimetals

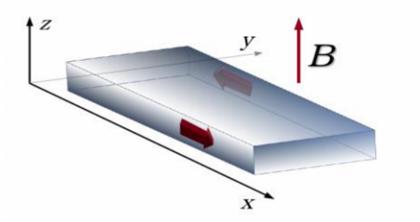
Magnetic field perpendicular to the plane of the nodal line

$$H_{\rm NL} = (m_0 + m_1 \nabla^2)\sigma_z - iv\partial_z\sigma_x$$



$$\varepsilon = \pm\sqrt{(m_0 - m_1\mathbf{k}^2)^2 + v^2k_z^2}$$

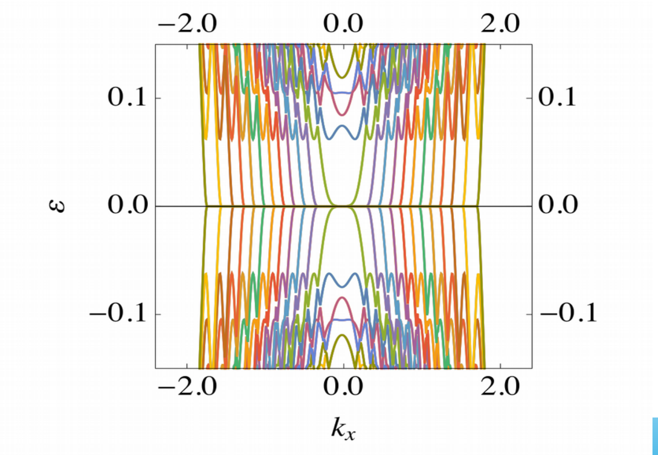
$$k_x^2 + k_y^2 = m_0/m_1 \qquad k_z = 0$$



$$\mathbf{A} = (-By, 0, 0)$$

B=30 T
W=40 nm

$$H_\perp = \left[m_0 + m_1\left(-(-i\partial_x - By)^2 + \partial_y^2 + \partial_z^2\right)\right]\sigma_z - iv\partial_z\sigma_x$$



We can look for Landau states decaying from the z surface

$$\Psi \sim e^{iwz}\chi(x,y)\hat{\eta} \qquad \sigma_y\hat{\eta} = \pm\hat{\eta}$$

$$w = \pm i\,\frac{v \pm \sqrt{v^2 - 4m_1(m_0 - m_1 2B(n+1/2))}}{2m_1}$$

$$4m_1m_0 > v^2$$

RAM, J. González, PRL 120, 146601 (2018)

Surface quantum Hall effect in nodal-line semimetals

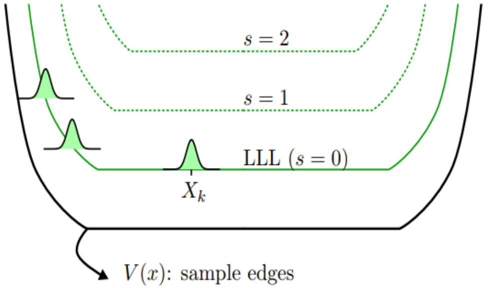
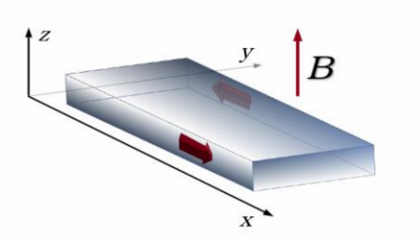
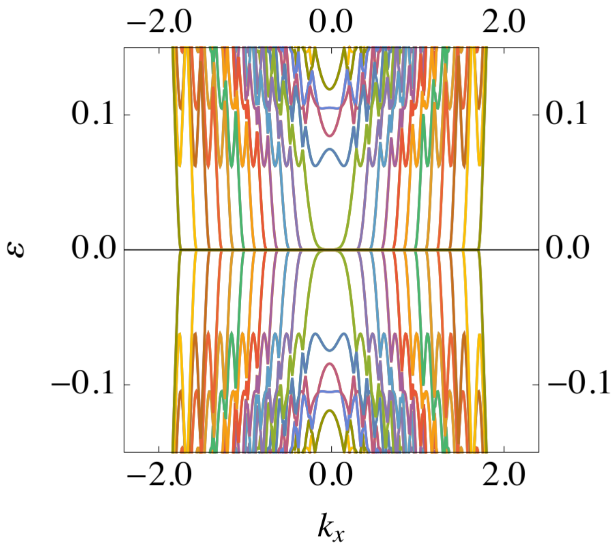


Figure 1.4: Edge states from curved Landau levels.





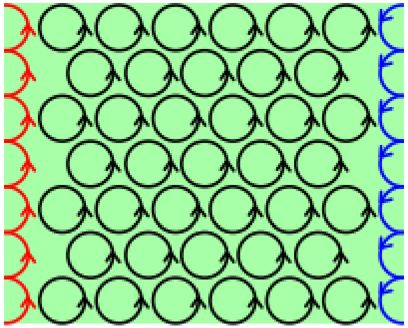
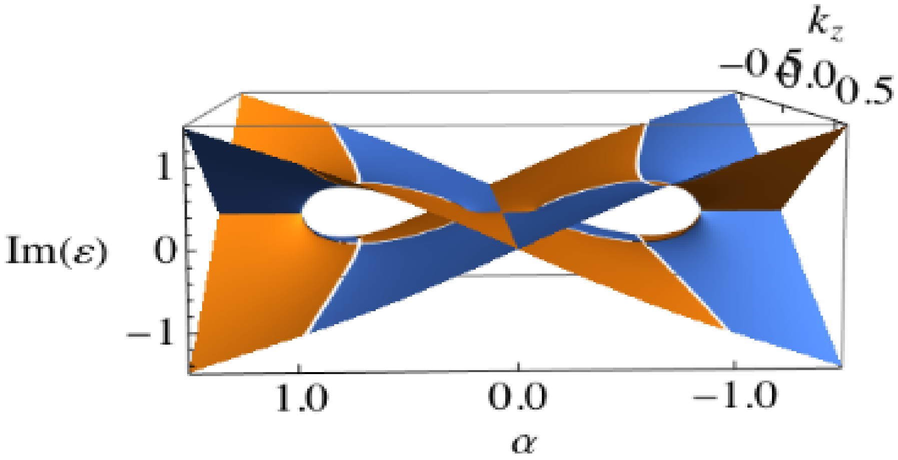


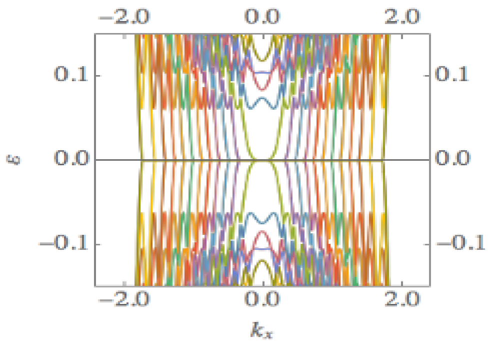
Figure 1.5: Classical skipping orbits.

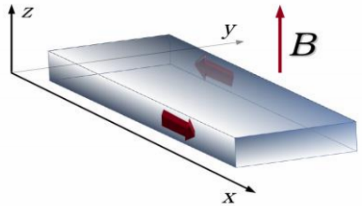
S. Huber

2D Quantum Surface Hall effect

The Landau levels are exceptional points in the complex plane

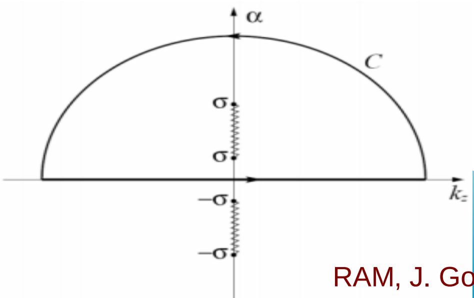






It is possible to define a topological index counting the number of exceptional points in the upper half-plane

$$\nu = \frac{1}{2\pi i} \sum_n{}' \oint_C dw \frac{1}{\varepsilon_n(w)} \frac{d}{dw} \varepsilon_n(w)$$



$$\sigma_{xy} = N(e^2/h)$$

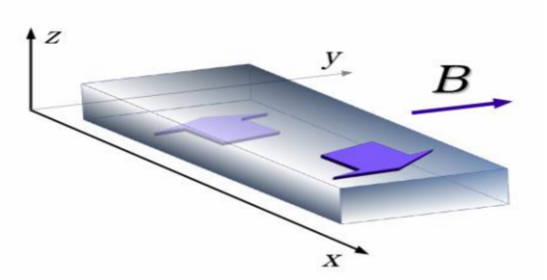
$$N \sim 30 \qquad B = 10 \text{ T}$$

$$m_0 \sim 1 \text{ eV}, \; m_1 \sim 1.0 \text{ eV nm}^2$$

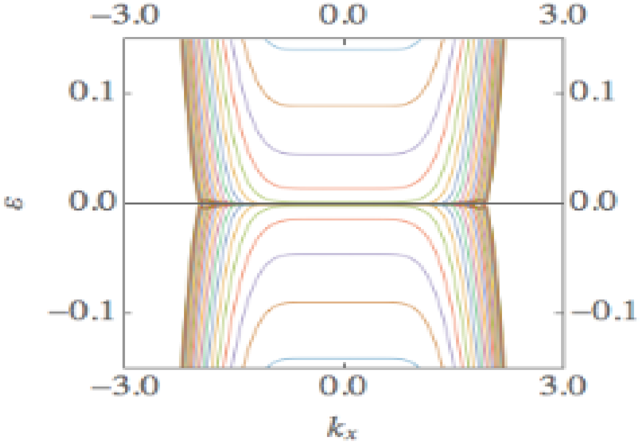
RAM, J. González, PRL 120, 146601 (2018)

3D Quantum Hall Effect

Magnetic field parallel to the line of nodes $H_{\|} = (m_0 + m_1[-(-i\partial_x + Bz)^2 + \partial_y^2 + \partial_z^2])\sigma_z - iv\partial_z\sigma_x.$



B=30 T
W=60 nm



There is no analytical solution but numerical resolution shows zero-energy states in the bulk localized in 2D slices parallel to the nodal plane.

There is a huge degeneracy of the zeroth Landau level coming from the collapse of a number of flat bands with different k_y.

Hall conductance $G = N(e^2/h)$

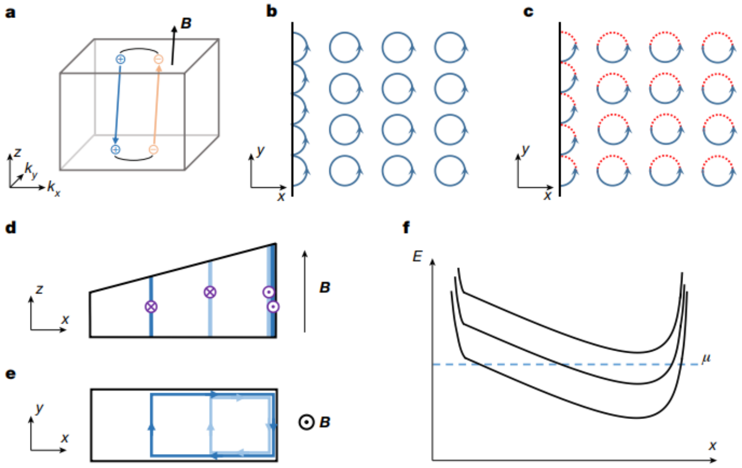
Number of channels (number of zero modes) N ~ $\widetilde{K}_y \Delta y / 2\pi$

RAM, J. González, PRL 120, 146601 (2018)

Conclusions

- Depending on the direction of the magnetic field with respect to the nodal line we have different Quantum Hall effects in nodal line semimetals.
- Surface Quantum Hall effect when the magnetic field is perpendicular to the line of nodes. We can define a topological index from the dispersion relation.
- 3D Quantum Hall effect when the magnetic field is parallel to the line of nodes.
- In both cases the number of channels that dictates the conductance quantization may be quite large.

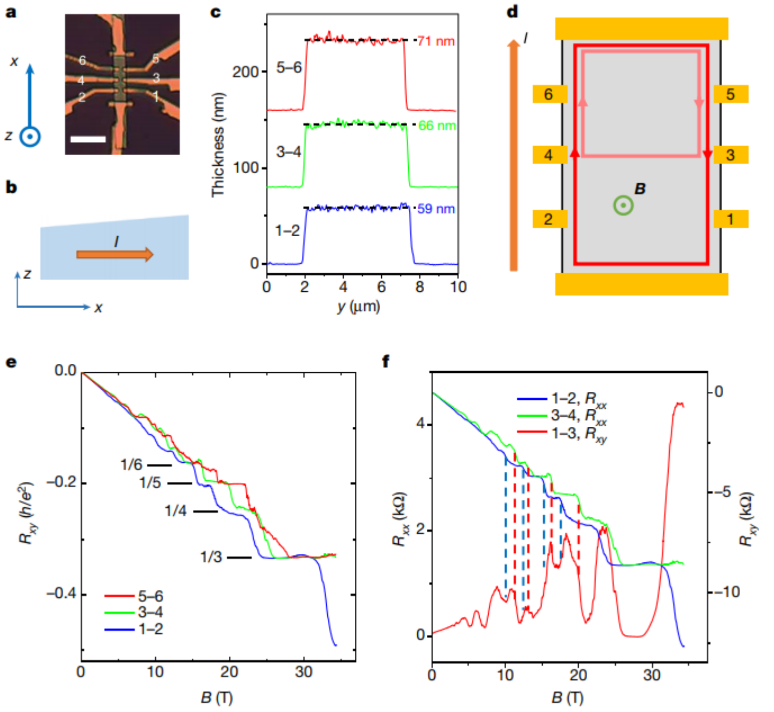
3D Quantum Hall effect through Weyl orbits



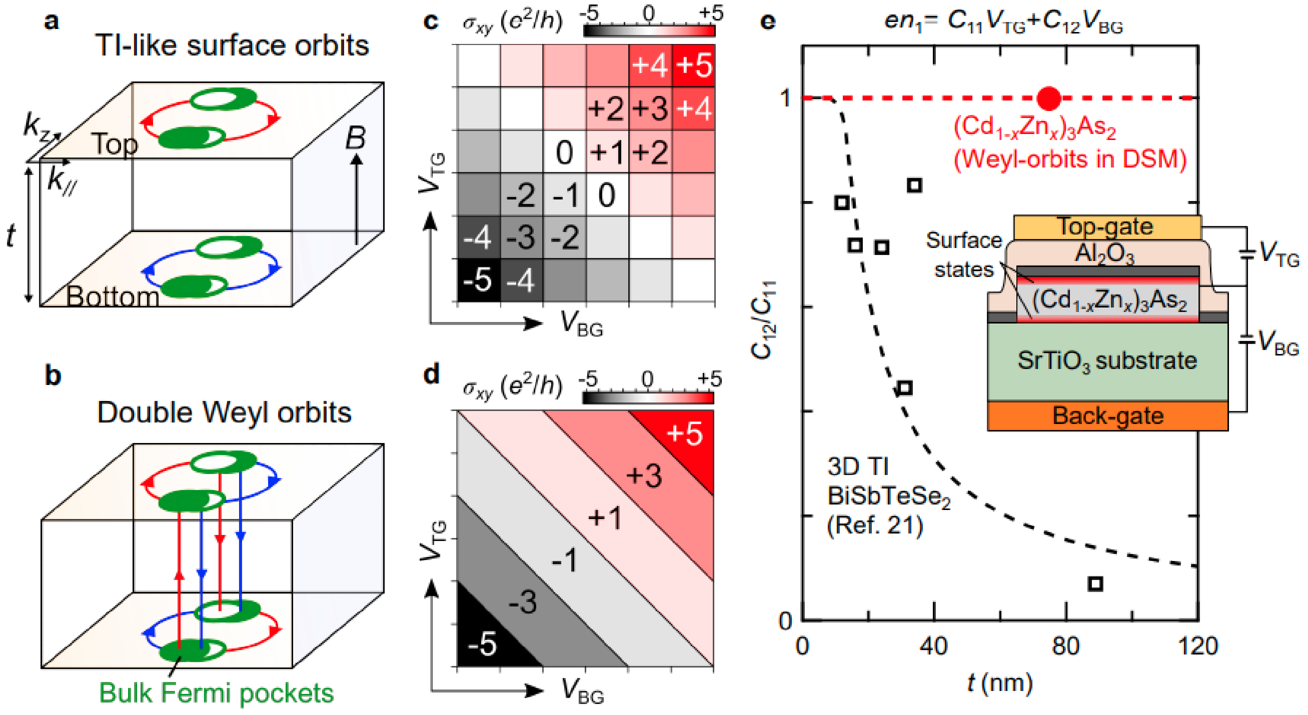
C. Zhang et al. Nature 565, 331 (2019)

Theory: Potter et al. Nat. Communications 5, 5161 (2014).

Cd_3As_2

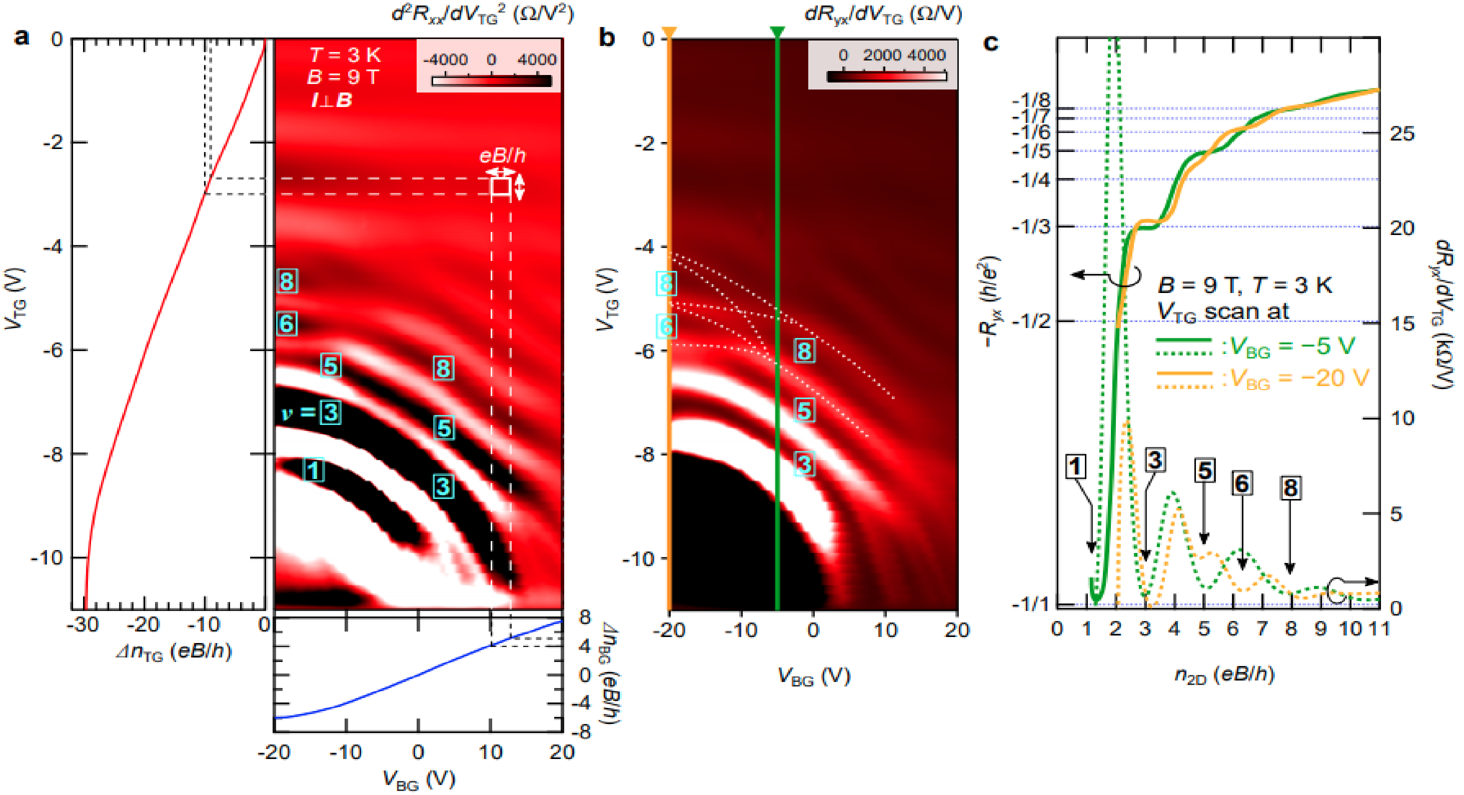


3D Quantum Hall Effect through Weyl orbits



Nishihaya et al.
https://www.researchsquare.com/article/rs-73203/v1

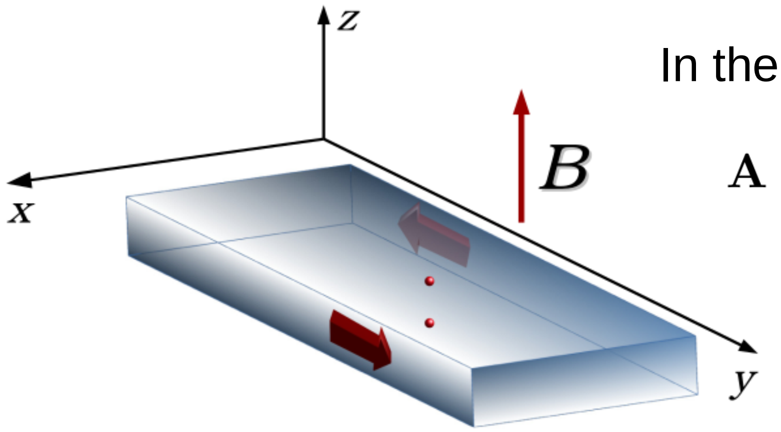
3D Quantum Hall Effect through Weyl orbits



Nishihaya et al.
https://www.researchsquare.com/article/rs-73203/v1

Bulk Landau levels in Weyl semimetals

Magnetic field parallel to the line joining the nodes



In the Landau gauge:

$$\mathbf{A} = (0, Bx, 0)$$

To diagonalize this problem we can use the basis of a harmonic oscillator in the x plane centered at $-k_y/B$ with frequency $\hbar\omega = 2m_1 B$. We can define creation and destruction operators as:

$$a = \frac{-i}{\sqrt{2}}\left(\sqrt{B}(x - k_y/B) + \frac{\partial_x}{\sqrt{B}}\right)$$
$$a^\dagger = \frac{i}{\sqrt{2}}\left(\sqrt{B}(x - k_y/B) - \frac{\partial_x}{\sqrt{B}}\right)$$

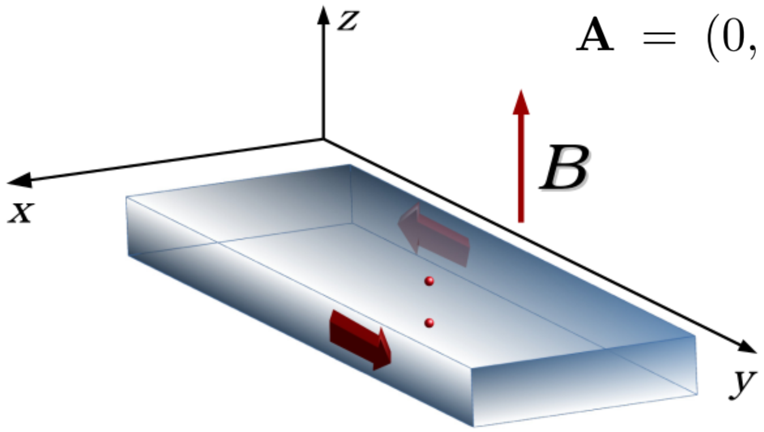
$$H_2 = \{m_0 + m_1[-2B(a^\dagger a + 1/2) + \partial_z^2]\}\sigma_z - iv\sqrt{\frac{B}{2}}\sigma_x(a - a^\dagger) + v\sqrt{\frac{B}{2}}\sigma_y(a + a^\dagger)$$

Lu et al. Phys. Rev. B 92 045203 (2015)

Bulk Landau levels in Weyl semimetals

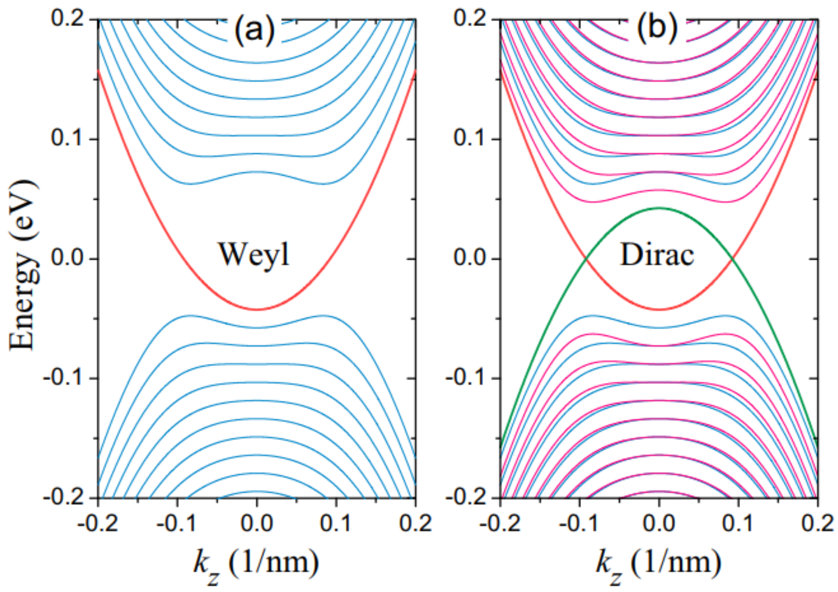
Magnetic field parallel to the line joining the nodes

$$\mathbf{A} = (0, Bx, 0)$$



$$E^0(k_z) = \omega/2 - (m_0 - m_1 k_z^2) \quad |n=0\rangle \propto \begin{pmatrix} 0 \\ |0\rangle \end{pmatrix}$$

$$|n \geq 1 > \propto \begin{pmatrix} |n-1\rangle \\ |n\rangle \end{pmatrix}$$

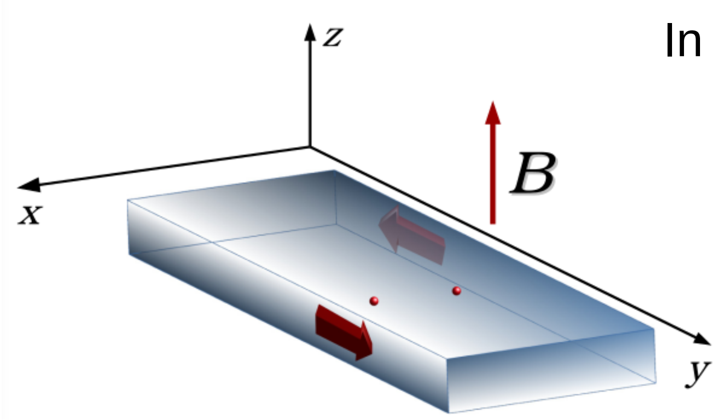


Landau levels keep chirality

Lu et al. Phys. Rev. B 92 045203 (2015)

Bulk Landau levels in Weyl semimetals

Magnetic field perpendicular to the line joining the nodes



In the Landau gauge:

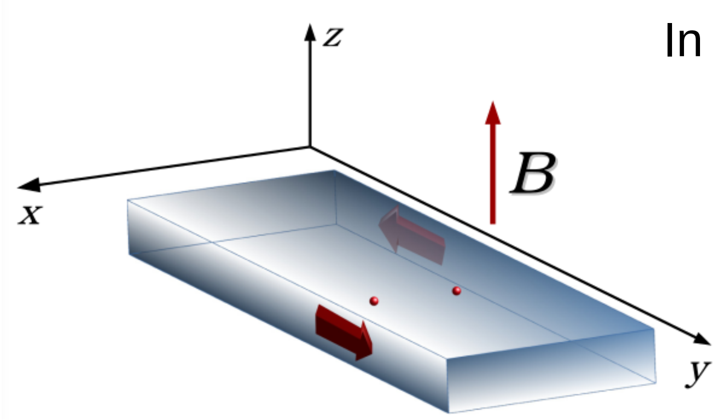
$$\mathbf{A} = (0, Bx, 0)$$

$$a = \frac{1}{\sqrt{2}}\left(\sqrt{B}(x + k_y/B) + \frac{\partial_x}{\sqrt{B}}\right)$$
$$a^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{B}(x + k_y/B) - \frac{\partial_x}{\sqrt{B}}\right)$$

$$H_{Weyl}(B_z) = \left[m_0 - m_1[2B(a^\dagger a + 1/2) + k_z^2]\right] \sigma_z - v\sigma_x k_z + v\sqrt{B/2}\sigma_y(a + a^\dagger)$$

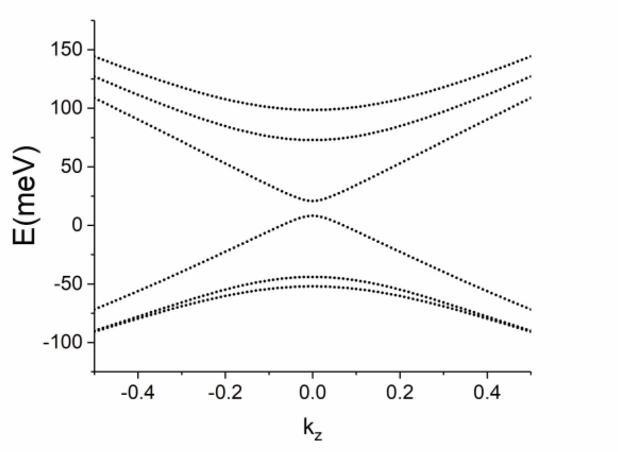
Bulk Landau levels in Weyl semimetals

Magnetic field perpendicular to the line joining the nodes



In the Landau gauge:

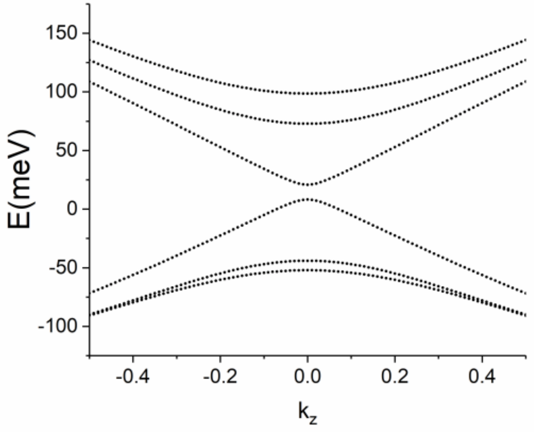
$$\mathbf{A} = (0, Bx, 0)$$



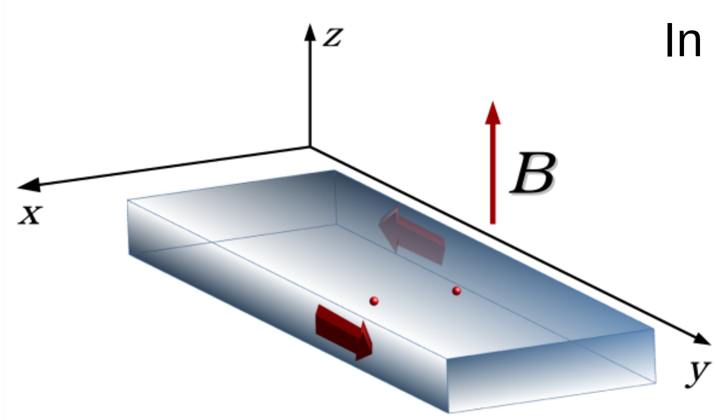
Chiralities mixed in strong magnetic field, a gap opens → Destruction of Weyl nodes

Zhang et al. Magnetic-tunneling induced Weyl node annihilation in TaP Nat. Phys. 13 979 (2017)
Ramshaw et al. Quantum limit transport and destruction of the Weyl nodes in TaAs Nat. Comun. 9, 2217 (2018).

Bulk Landau levels in Weyl semimetals

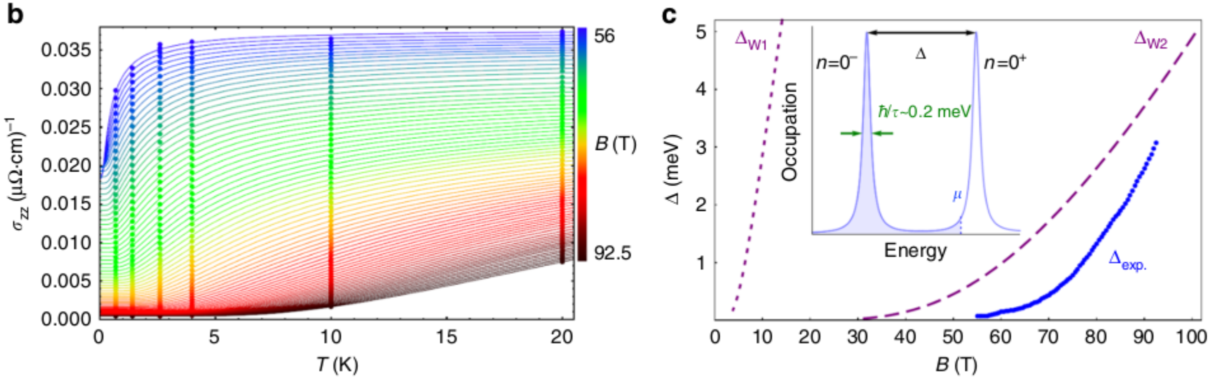


Magnetic field perpendicular to the line joining the nodes



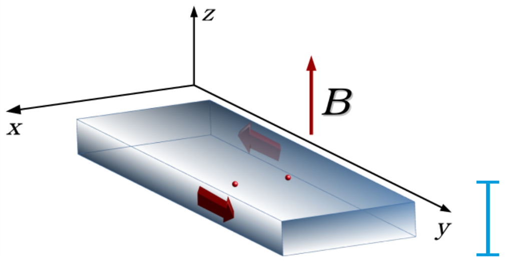
In the Landau gauge:

$$\mathbf{A} = (0, Bx, 0)$$



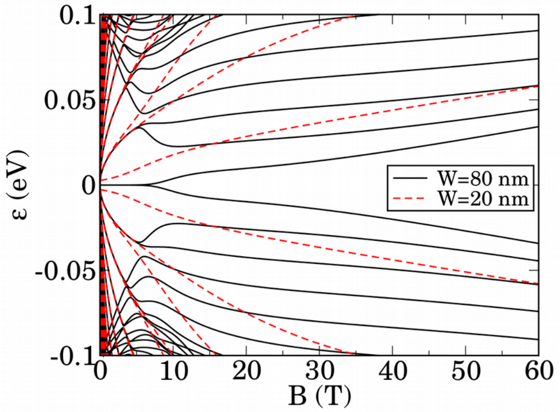
Ramshaw et al. Quantum limit transport and destruction of the Weyl nodes in TaAs Nat. Comun. 9, 2217 (2018).

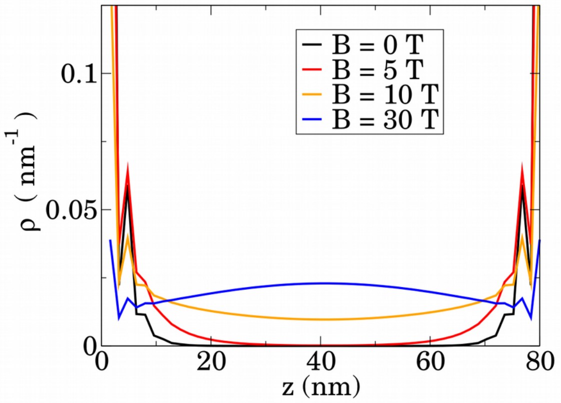
Landau levels from surface states



$$H_1 = \{m_0 + m_1[-2B(a^\dagger a + 1/2) + \partial_z^2]\}\,\sigma_z$$
$$- iv\sigma_x\partial_z + v\sqrt{\frac{B}{2}}\sigma_y(a + a^\dagger).$$

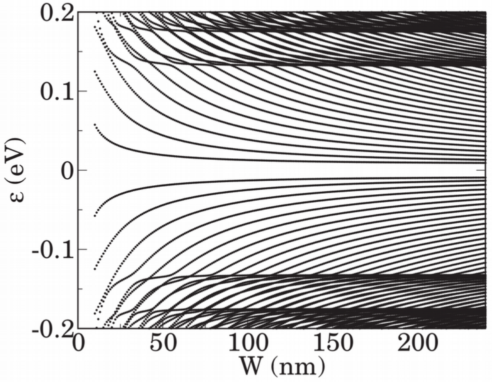
Thin-film vs. 3D regime



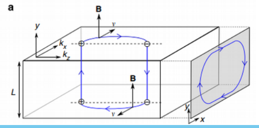


$m_0 = 0.1\,\text{eV}$, $m_1 = 0.2\,\text{eV nm}^2$, and $v = 0.5\,\text{eV nm}$

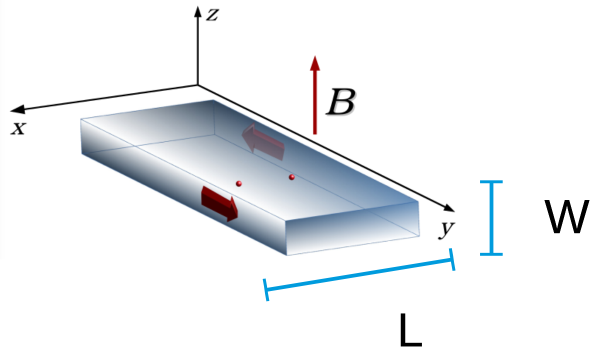
B=30 T



Quantum mechanical equivalent of Weyl orbits.

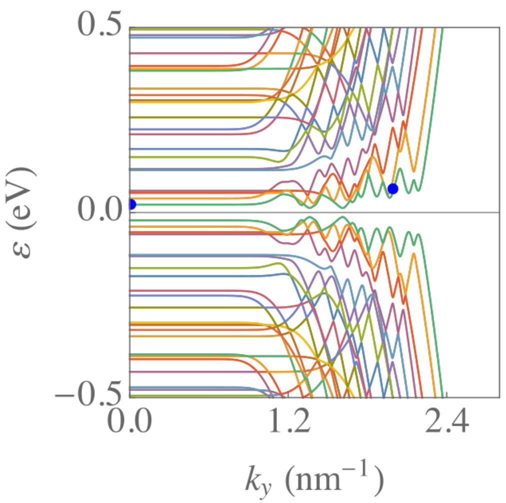


Landau levels from surface states



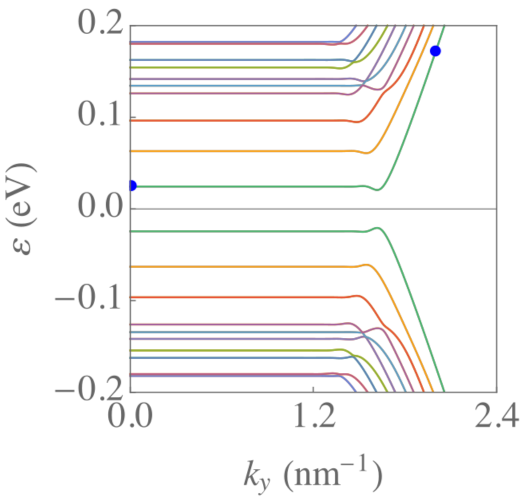
$m_0 - m_1 B \gg v\sqrt{B}$

Inversion regime

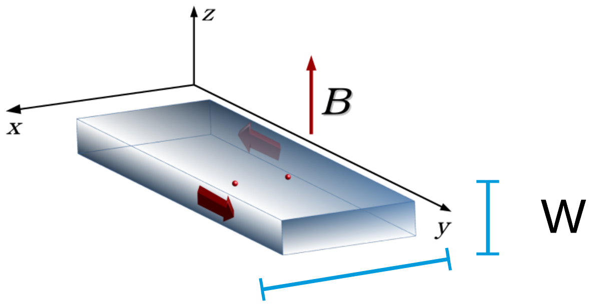


$m_0 - m_1 B \ll v\sqrt{B}$

Weyl cone regime



Landau levels from surface states

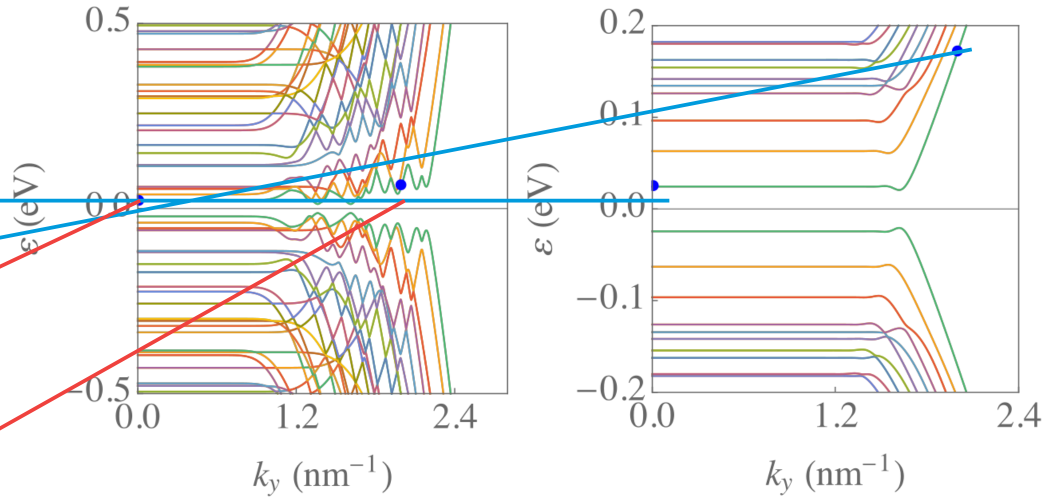


$m_0 - m_1 B \gg v\sqrt{B}$

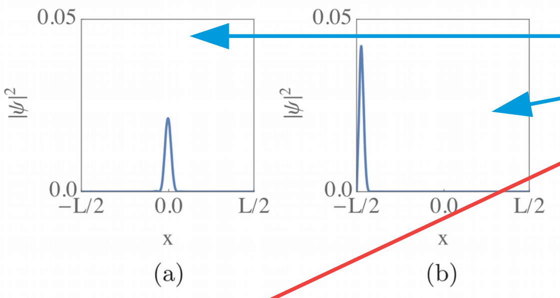
Inversion regime

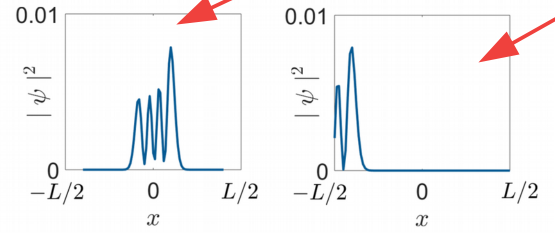
$m_0 - m_1 B \ll v\sqrt{B}$

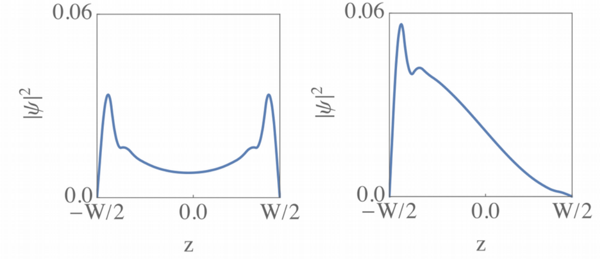
Weyl cone regime



$$G = n(e^2/h)$$

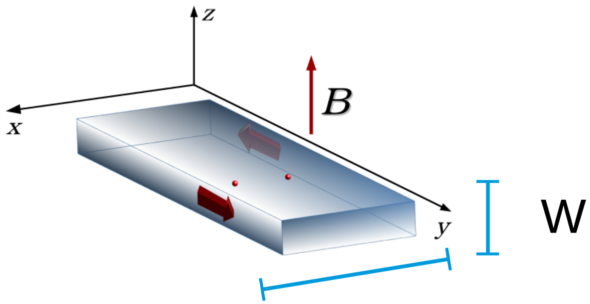


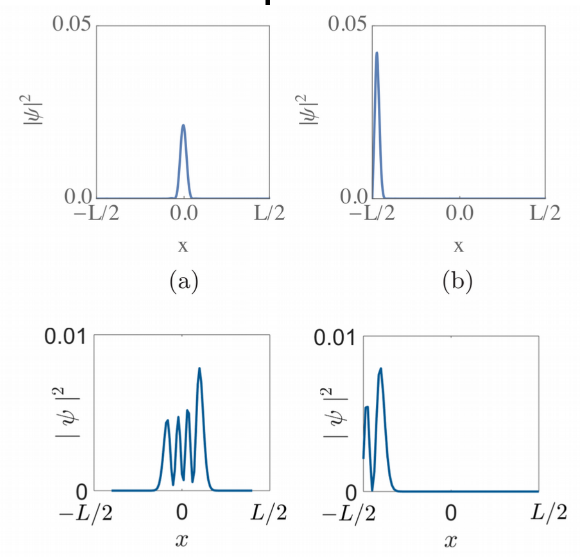




$$I_y = \frac{e}{\hbar} \int_{\text{filled states}} \frac{dk_y}{2\pi} \frac{\partial \varepsilon}{\partial k_y}$$

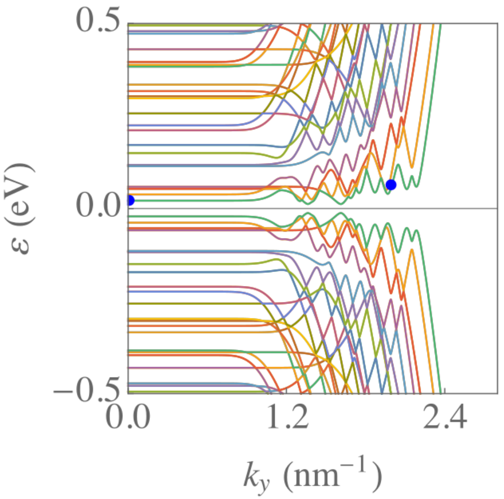
Landau levels from surface states





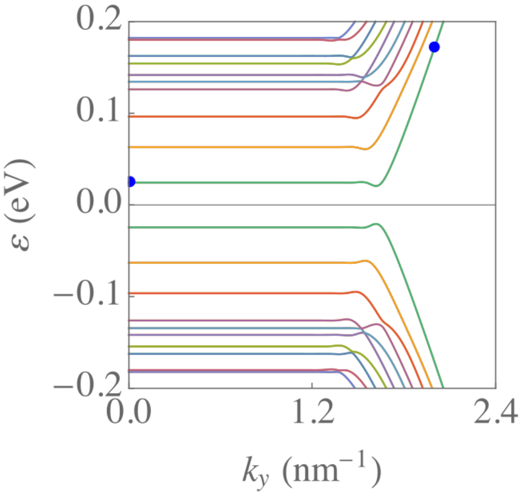
$m_0 - m_1 B \gg v\sqrt{B}$

Inversion regime

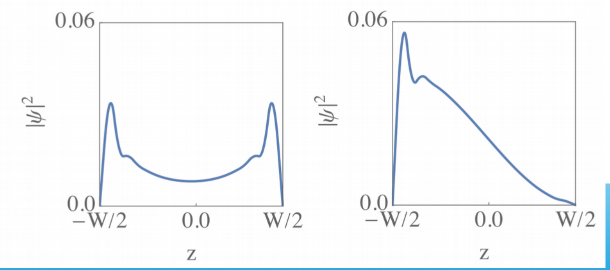


$m_0 - m_1 B \ll v\sqrt{B}$

Weyl cone regime



$G = n(e^2/h)$



$$I_y = \frac{e}{\hbar} \int_{\text{filled states}} \frac{dk_y}{2\pi} \frac{\partial \varepsilon}{\partial k_y}$$

Landau levels from surface states

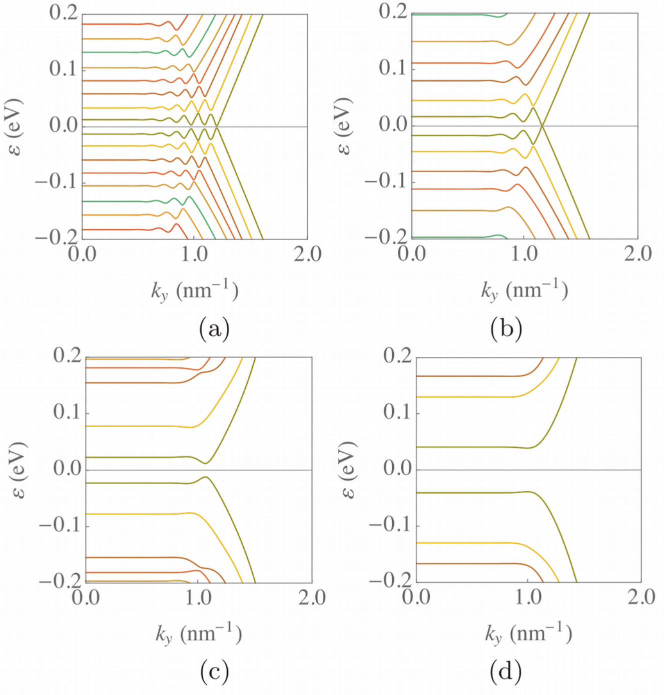


FIG. 6. Energy bands of a thin film of WS in a perpendicular magnetic field in a setup with the line connecting opposite Weyl nodes parallel to the faces of the film. The levels have been computed for a bar with transverse dimension $L = 60\,\text{nm}$, depth $W = 20\,\text{nm}$, and magnetic field $B = 30$ T. The model of WS has parameters $m_1 = 1.0\,\text{eV nm}^2$, $v = 0.5\,\text{eV nm}$, and m_0 taking values, from (a) to (d), equal to 1.2, 0.6, 0.2, and 0.1 eV [leading, respectively, to $(m_0 - m_1 B)/v\sqrt{B} \simeq 10.82, 5.2, 1.45, 0.51$].

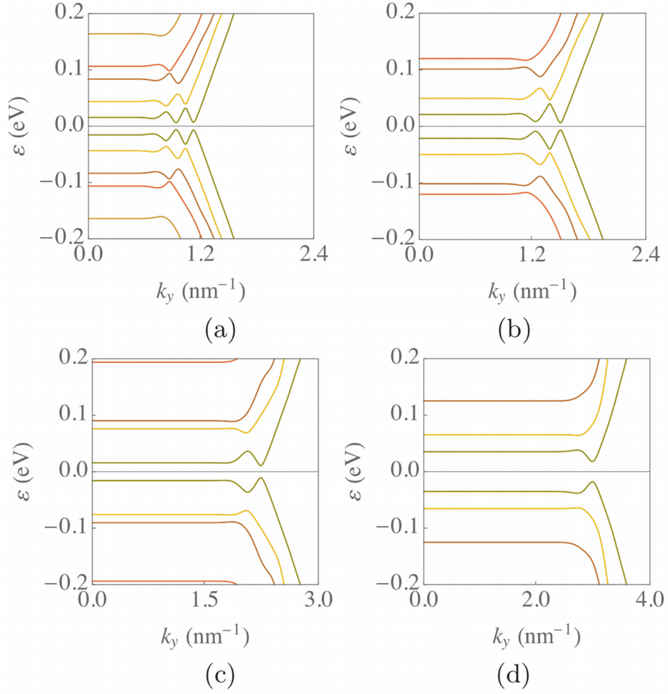
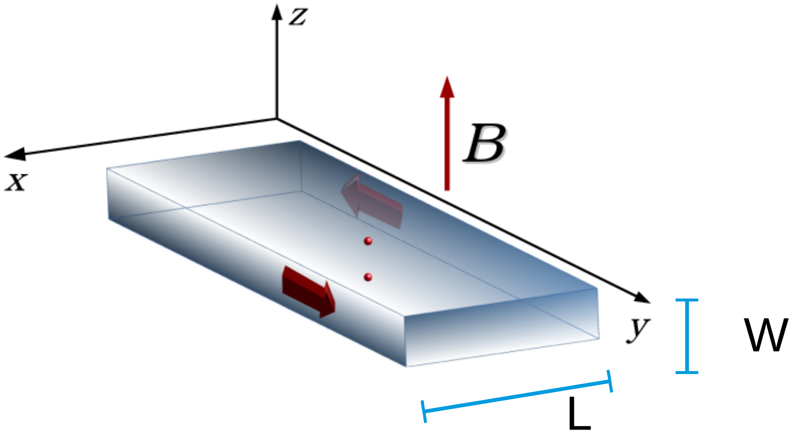
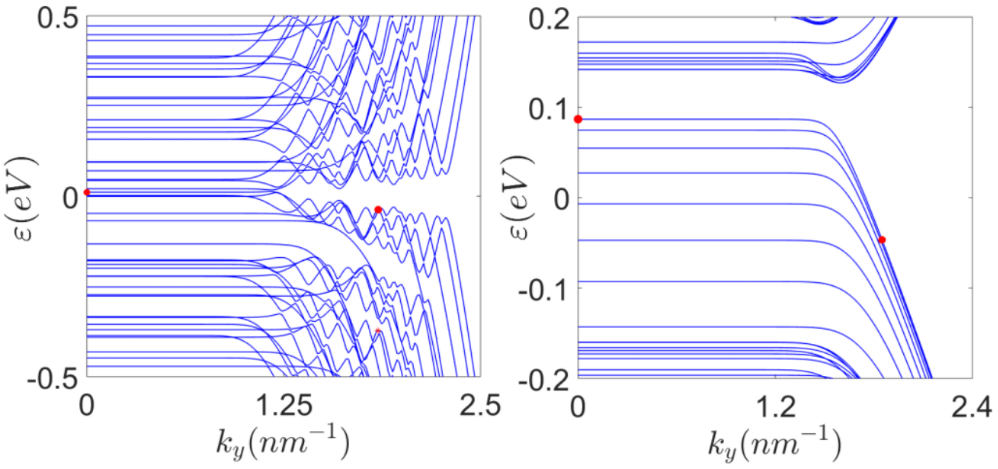


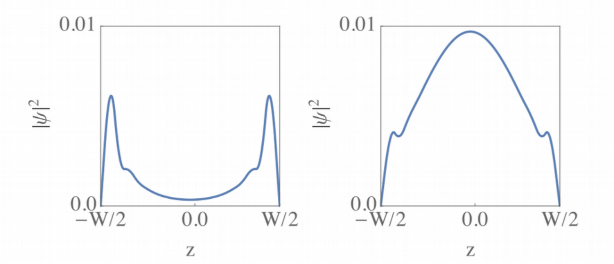
FIG. 5. Energy bands of a thin film of WS in a perpendicular magnetic field in a setup with the line connecting opposite Weyl nodes parallel to the faces of the film. The levels have been computed for a bar with transverse dimension $L = 60\,\text{nm}$ and depth $W = 20\,\text{nm}$, and values of the magnetic field, from (a) to (d), equal to 30, 40, 60, and 80 T. The parameters used to model the WS are $m_0 = 0.8\,\text{eV}$, $m_1 = 1.6\,\text{eV nm}^2$, $v = 0.5\,\text{eV nm}$. The quantity $(m_0 - m_1 B)/v\sqrt{B}$ equals, from (a) to (d), ≈6.82, 5.71, 4.34, 3.48.

Landau levels from bulk states



$$H_2 = \{m_0 + m_1[-2B(a^\dagger a + 1/2) + \partial_z^2]\}\sigma_z - iv\sqrt{\frac{B}{2}}\sigma_x(a - a^\dagger) + v\sqrt{\frac{B}{2}}\sigma_y(a + a^\dagger)$$





Conclusions

- Well ordered sequence of Landau levels in thin films of Weyl semimetals in some parametric regime. Well separated electron- and hole-like levels. This parametric regime is relevant experientally (TaAs, Cd_3As_2, Na_3Bi).
- Deviations from that regime may prevent the observation of conductancte quantization.
- Thin films may provide suitable setups to observe the quantum Hall effect at strong magnetic field with electronic transport taking place at the edges but with quite different profiles at the lateral boundaries depending on the orientation of the line connecting the Weyl nodes with respect to the transverse magnetic field.