Topological materials:
Optical and magneto-optical properties

Milan Orlita

Laboratoire National des Champs Magnétiques Intenses
CNRS
Grenoble, France

Outline:

- Topological materials – introduction
- Topological materials – optical response at $B=0$
- Topological materials – magneto-optical response
- Conclusions

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- **Topological materials – introduction**
- Topological materials – optical response at B=0
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Topological materials - timeline

2007: 2D topological insulators

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

2008: 3D topological insulators

D. Hsieh et al., Nature 452, 970 (2008)

2012: 3D topological crystalline insulators

P. Dziawa et al. , Nature Mater. 11, 1023 (2012)

2014: 3D Dirac semimetals

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

2015: 3D Weyl semimetals

B. Q. Lv et al., Nature Phys. 11, 724 (2015)

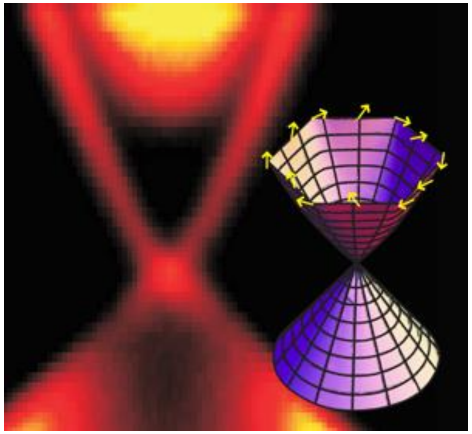
2016: Nodal line/loop Dirac semimetals

Wu, Y. et al., Nature Phys. 12, 667 (2016)

2019: Multifold massless electrons

D. S. Sanchez et al., Nature 567, 501 (2019)

2024: …



M. Z. Hasan and C. L. Kane, RMP 82, 3045 (2010)

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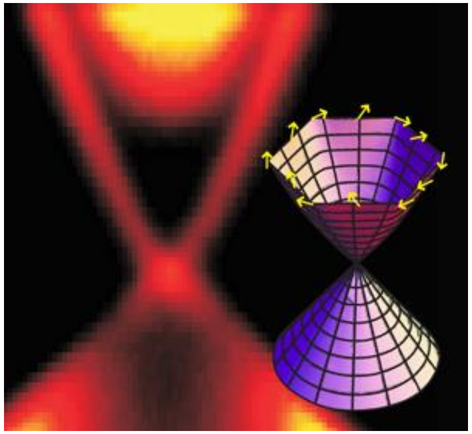

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Relativistic-like electrons in conical bands

(dimensionality, valley and spin degeneracy, protection by symmetry…)

Solids with conical bands: Examples

	Conical band dimensionality		
	1D	2D	3D
Spin degenerated		**HgTe QW** (critical thickness) Büttner et al., Nature Phys. 2011	**3D Dirac semimetals** (w/o symmetry protection!) (gapless HgCdTe, $ZrTe_5$) MO et al., Nature Phys. 2014 Chen et al., PRL 2015
Spin degenerated; Valley degenerated	**Metallic carbon nanotubes** see, e.g. Ando, SST 2000	**Graphene** Novoselov et al., Nature 2005	**3D Dirac semimetals** (Cd_3As_2, Na_3Bi) Liu et al., Science 2014 Liu et al, Nature Mater. 2014
Valley degenerated		**Topological crystalline insulator** (PbSnSe, PbSnSe, SnTe) Dziawa et al., Nature. Mater. 2012	**3D Weyl semimetals** (e.g., TaAs, NbAs, TaP) Lv et al., Nature Phys. 2015 Xu et al., Nature Phys. 2015
	2D topological insulators **inverted HgTe QWs** König et al., Science 2007 **InAs/GaSb QWs** Knez et al., PRL 2011	**3D topological insulators** ($Bi_{1-x}Sb_x$, Bi_2Se_3, Bi_2Te_3) Hsieh et al. , Nature 2008	

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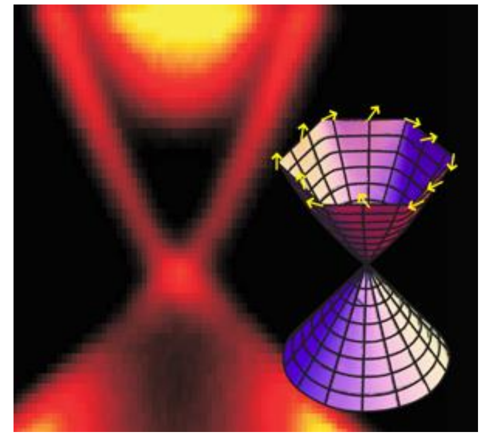

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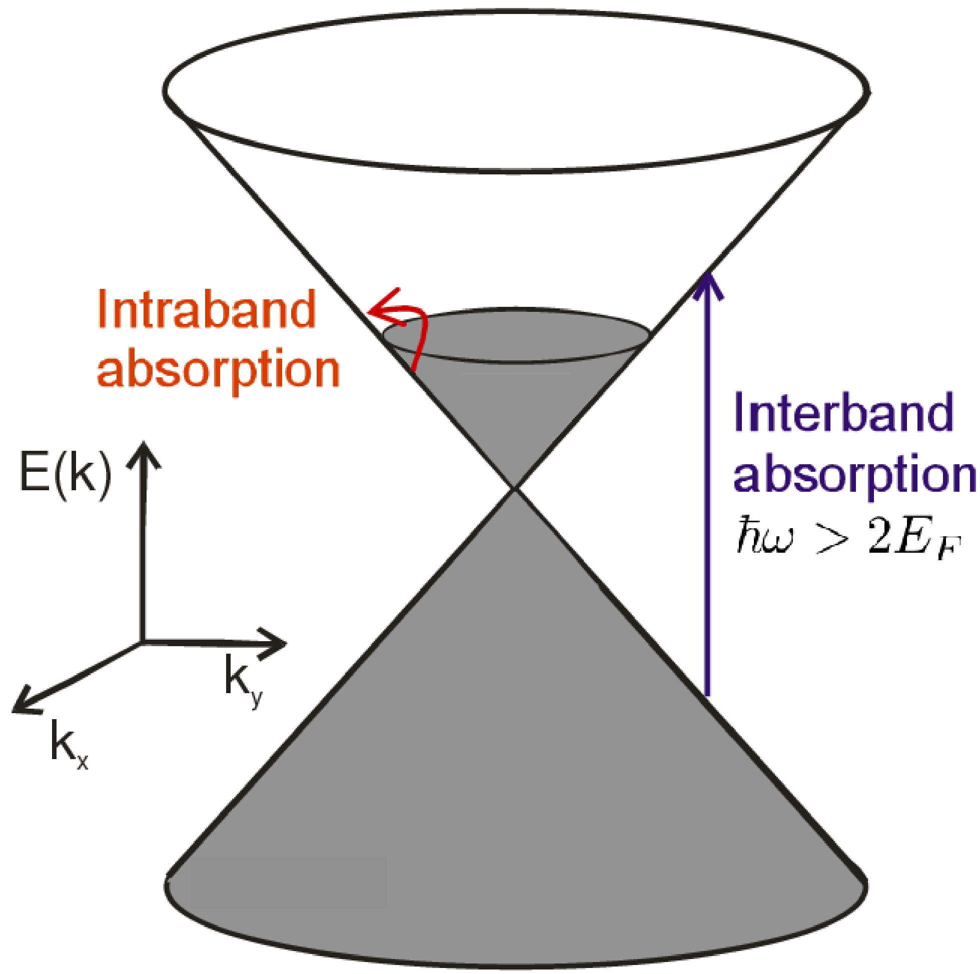
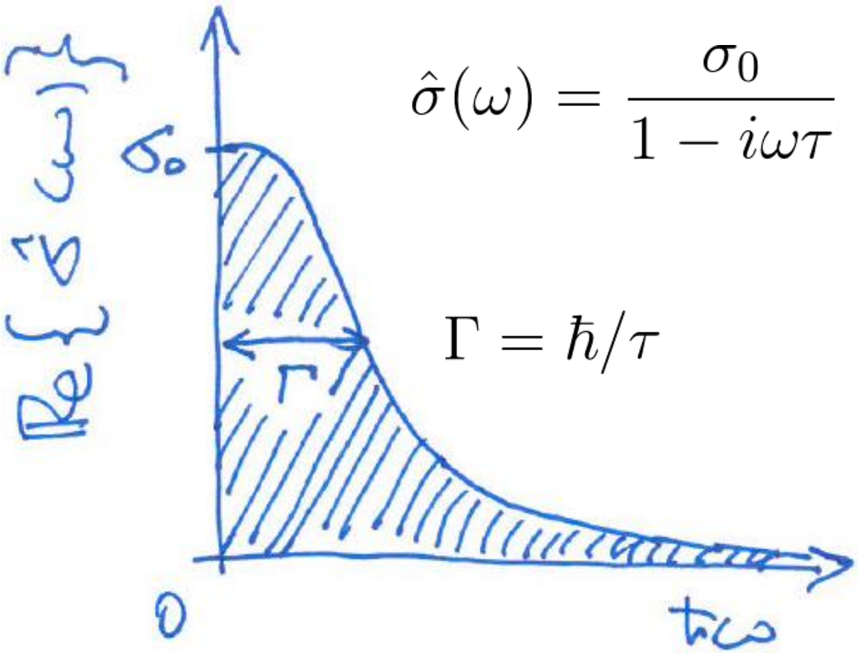
Optical response of electrons in conical bands



1st order, electric-dipole excitations considered only

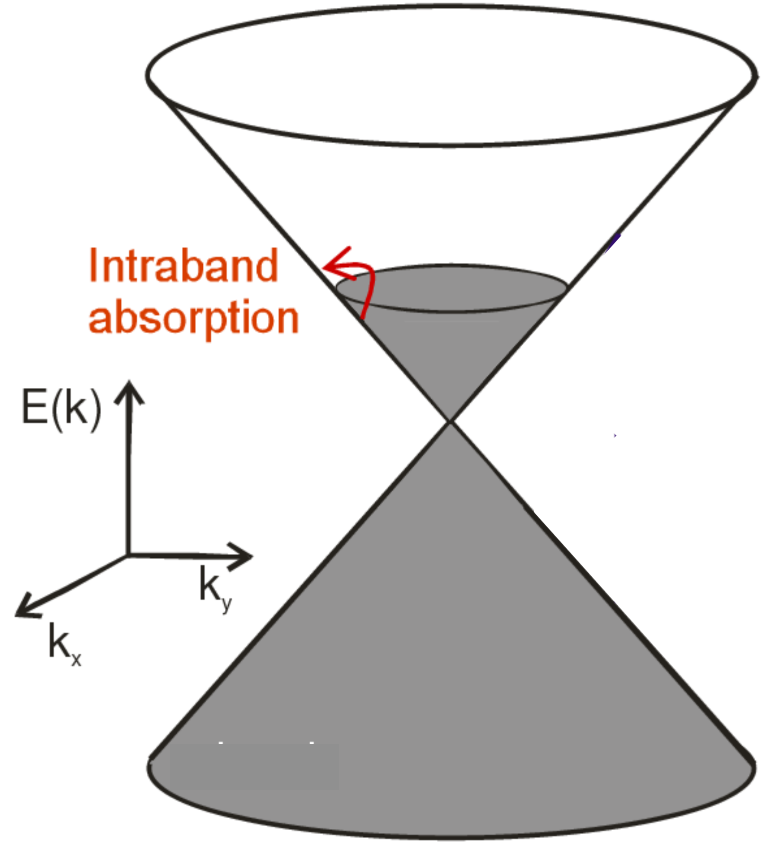
Conical bands: Absorption of light by free carriers

Classical Drude model for (optical) conductivity



$$\hat{\sigma}(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

$$\Gamma = \hbar/\tau$$



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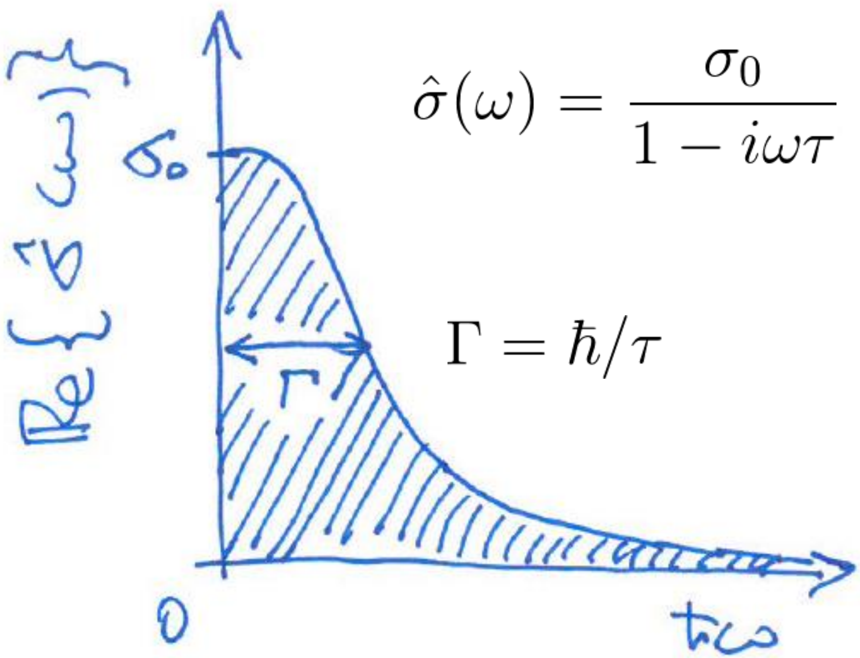

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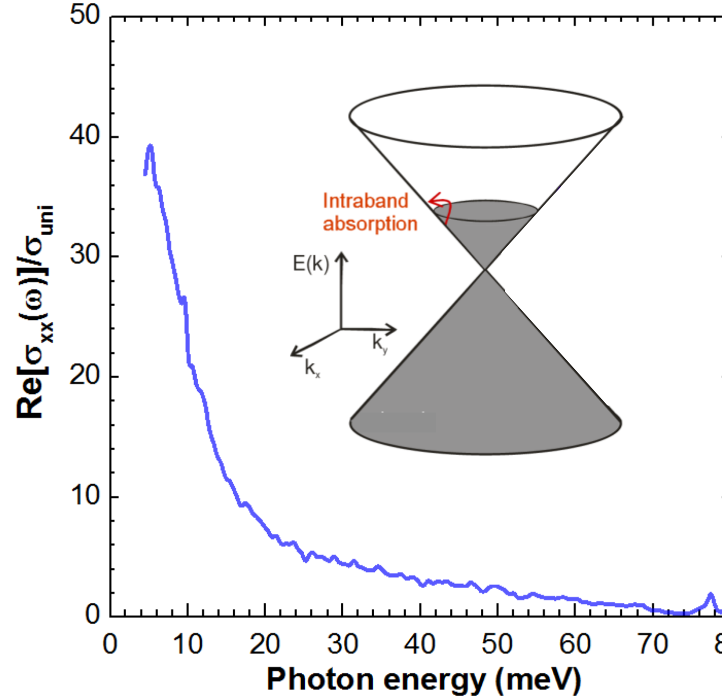
Free-carrier absorption in epitaxial graphene on SiC



MO et al., New. J. Phys. 14, 095008 (2012)

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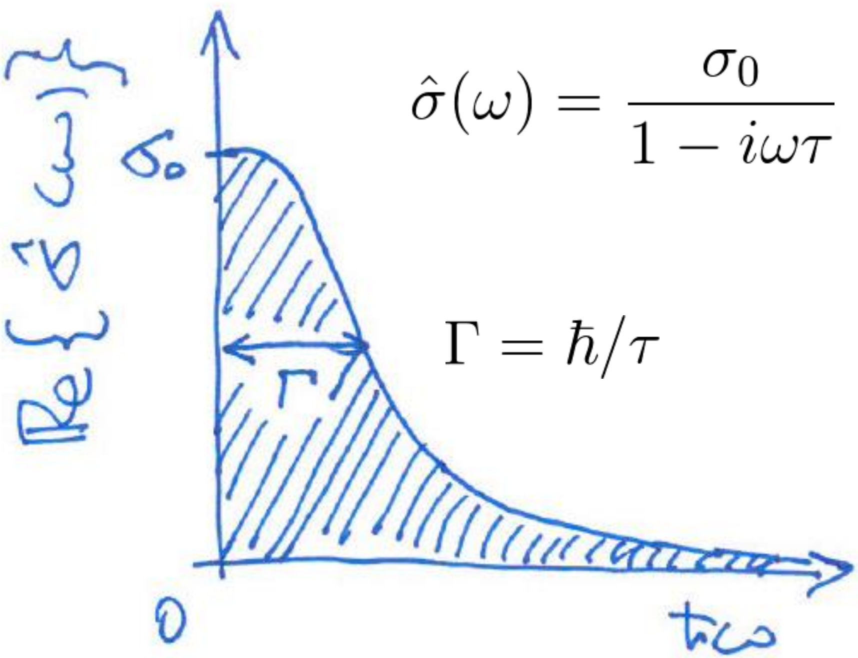

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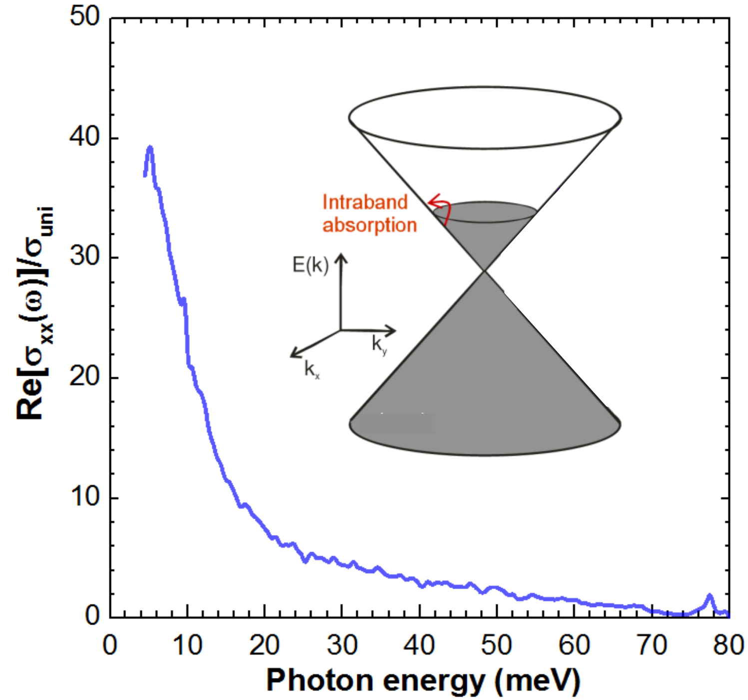

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dc conductivity

$$\sigma_0 = \frac{e\tau n}{m}$$

Conical bands: Absorption of light on free carriers

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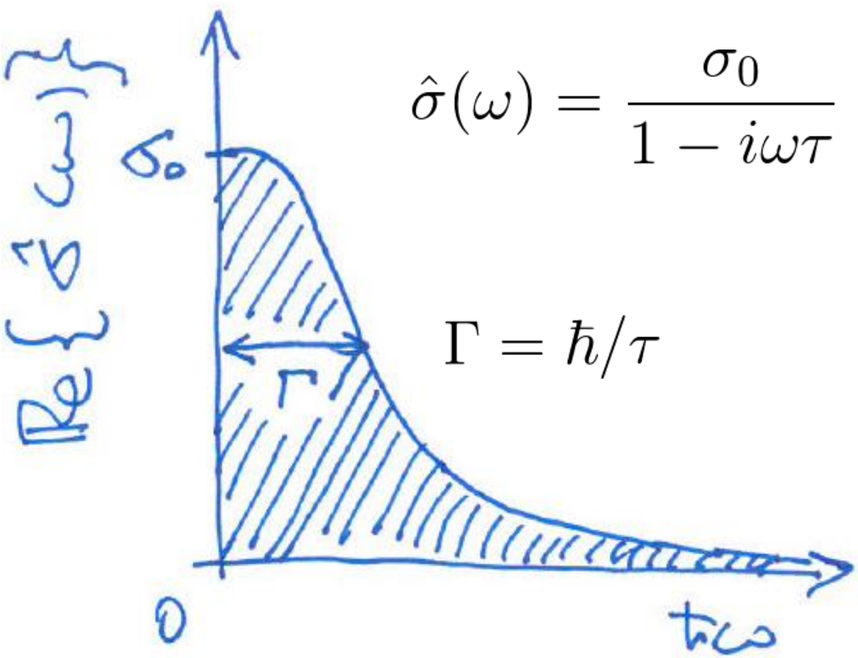

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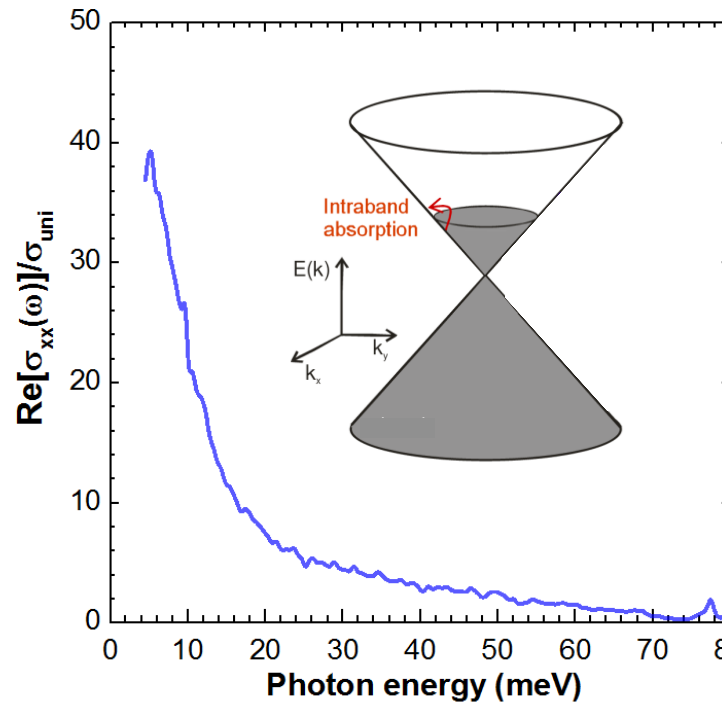
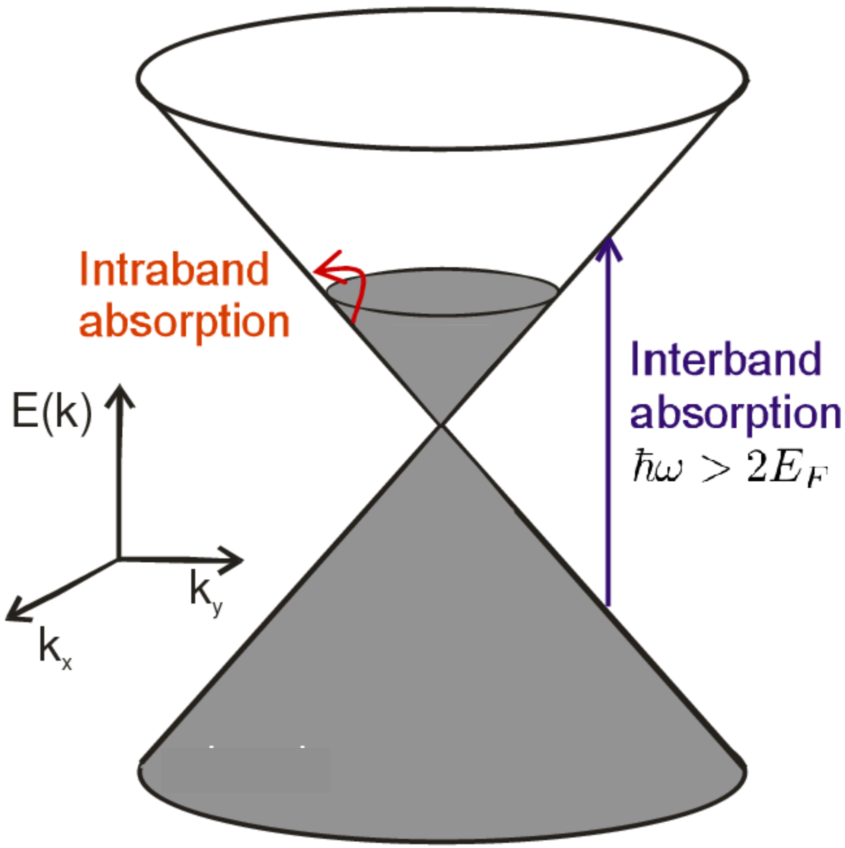


dc conductivity

$$\sigma_0 = \frac{e\tau n}{m} \propto \boxed{\frac{n}{m}}$$

Drude (optical) weight

Interband excitations in conical bands



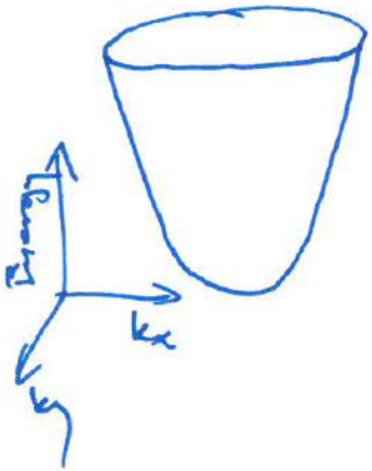
Optical band gap (zero T, finite doping) $2E_F$

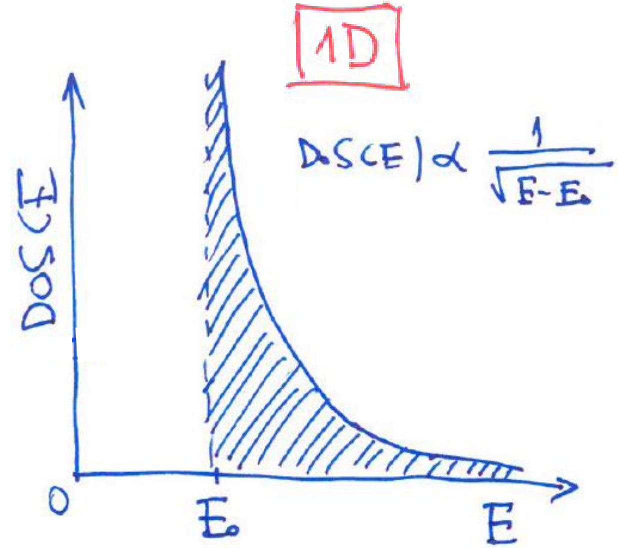
Absorption of light in solids (Fermi's golden rule & electric dipole excitations):

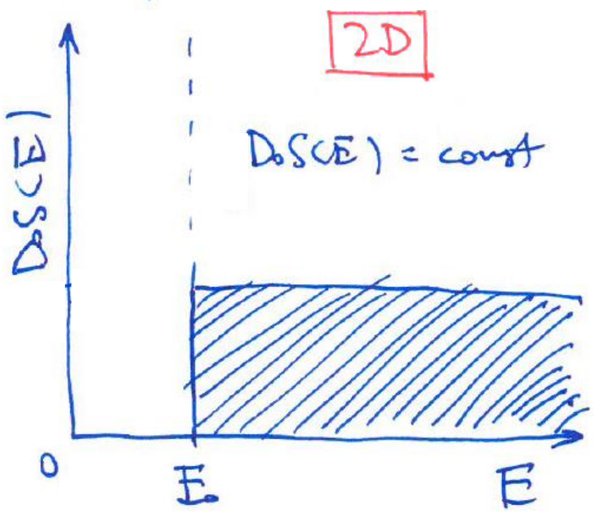
joint density of states

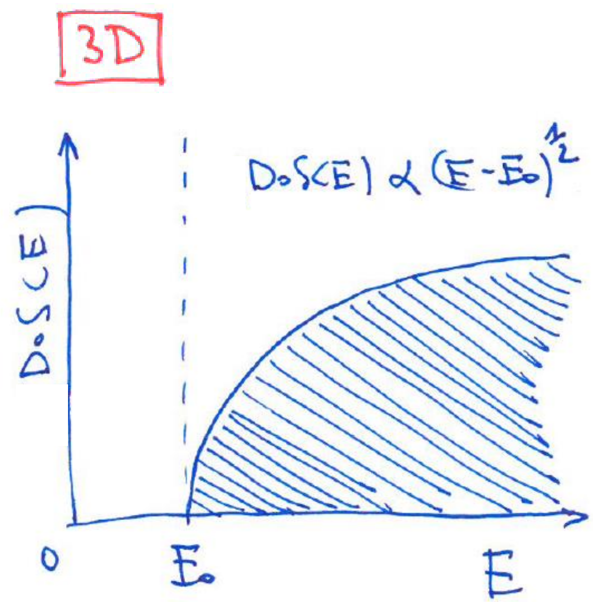
$$\lambda(\omega) \propto \frac{\mathcal{D}(\omega)}{\omega}$$

Density of states: conventional systems

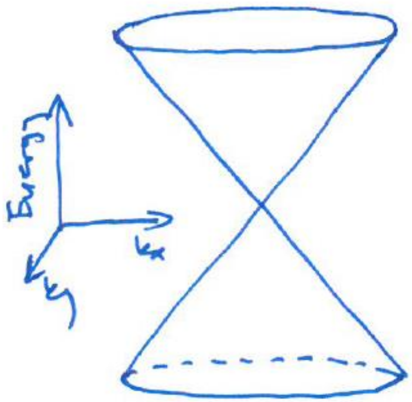


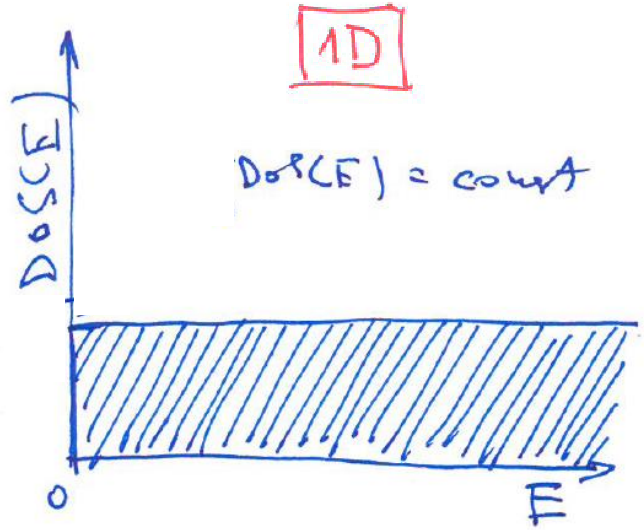


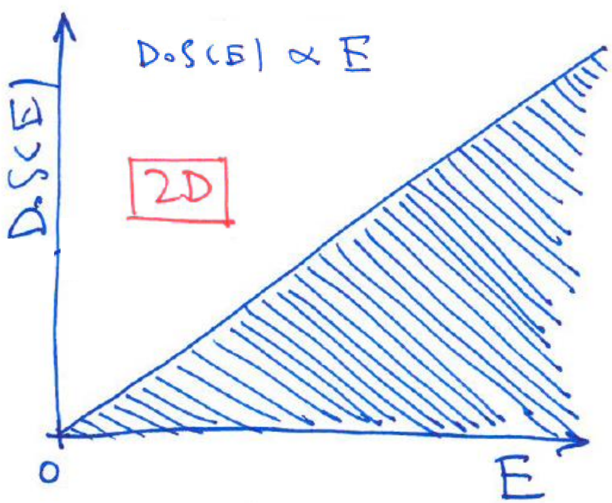


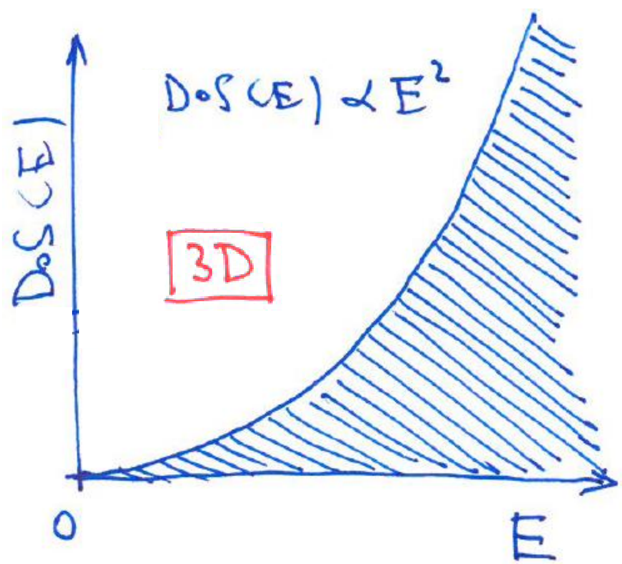


Density of states: conical bands

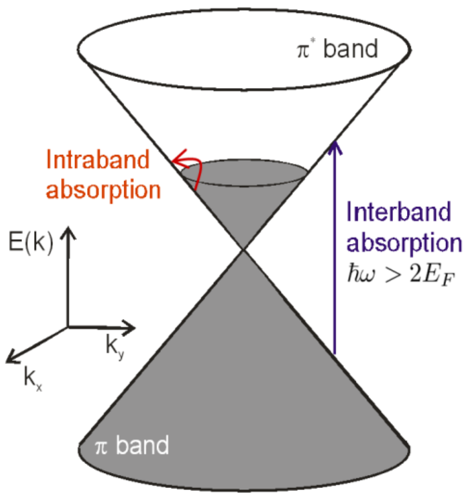


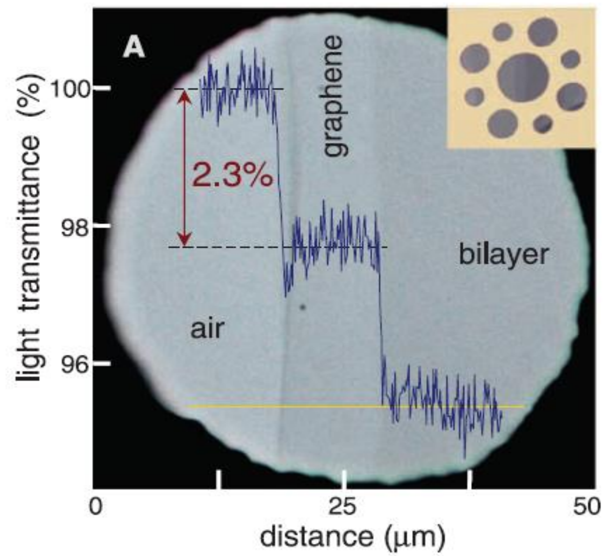


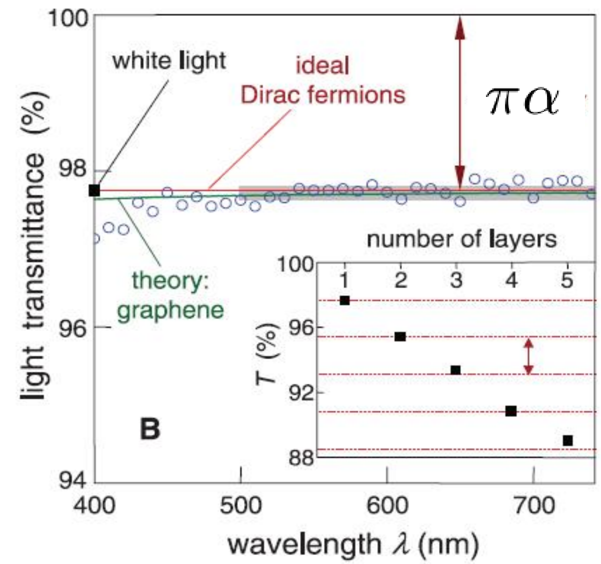




Interband excitations in conical bands





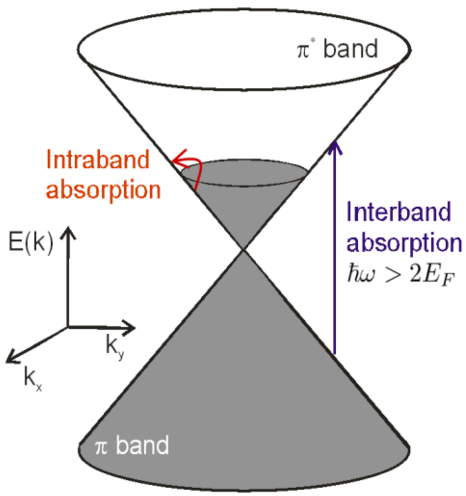


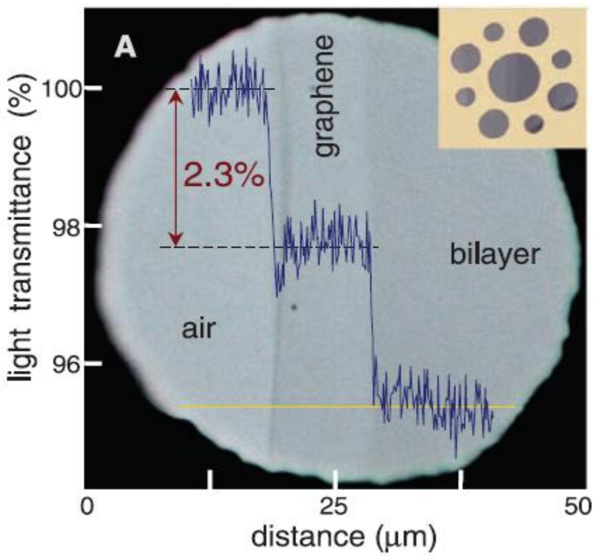
“Flat” absorption of light (2.3%) defined only by the fine structure constant:

$$\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \doteq \frac{1}{137}$$

R. R. Nair et al., Science 320, 1308 (2008)
A. B. Kuzmenko et al., Phys. Rev. Lett. 100, 117401 (2008)

Interband excitations in conical bands





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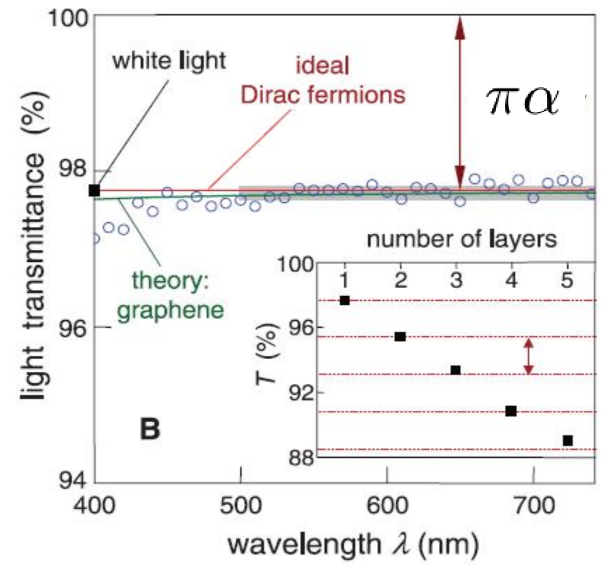


Absorption coefficient:

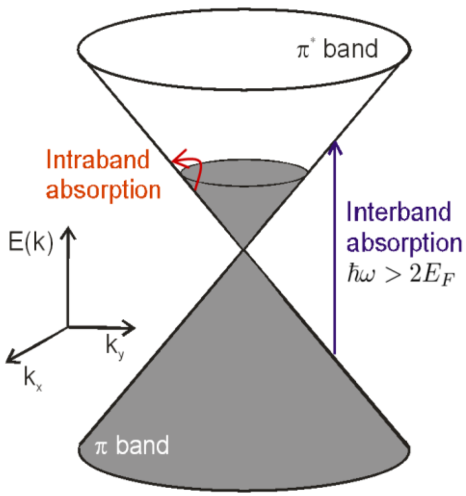
$$\lambda(\omega) \propto \frac{\mathcal{D}(\omega)}{\omega}$$

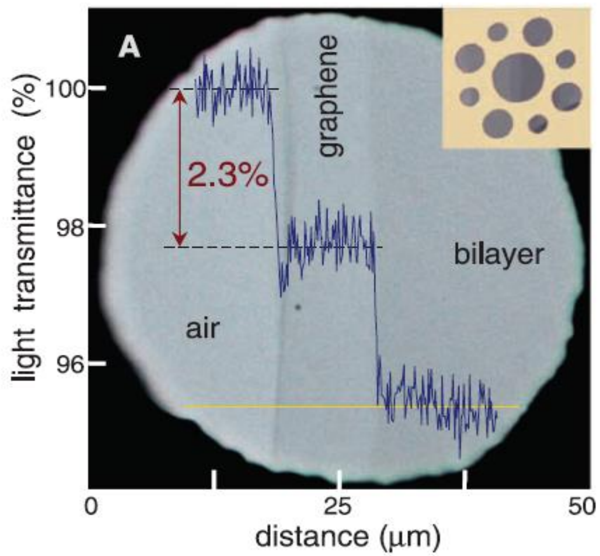
For conical bands in 2D:

$$\mathcal{D}(\omega) \propto \omega$$

Dispersionless and universal interband absorption of light!

Interband excitations in conical bands





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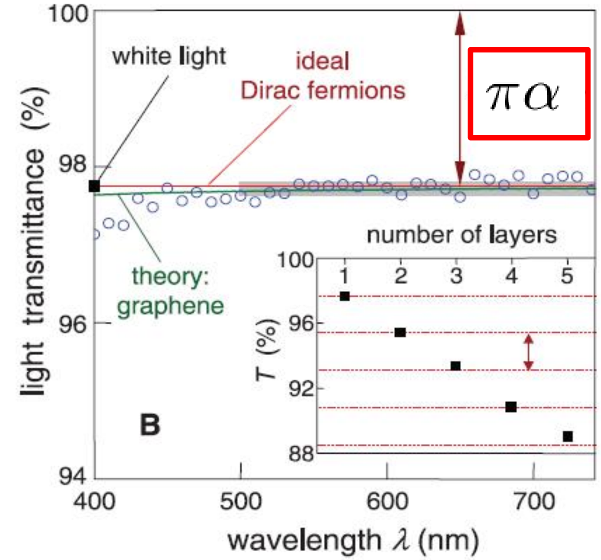

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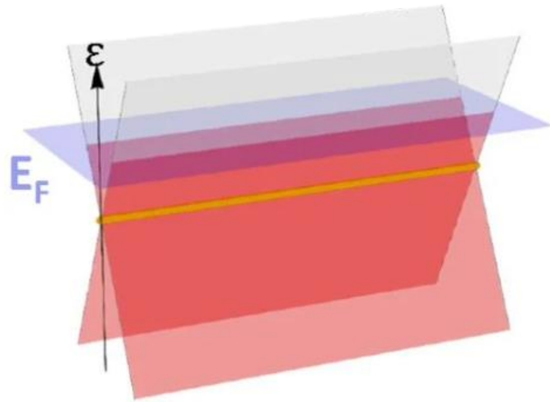
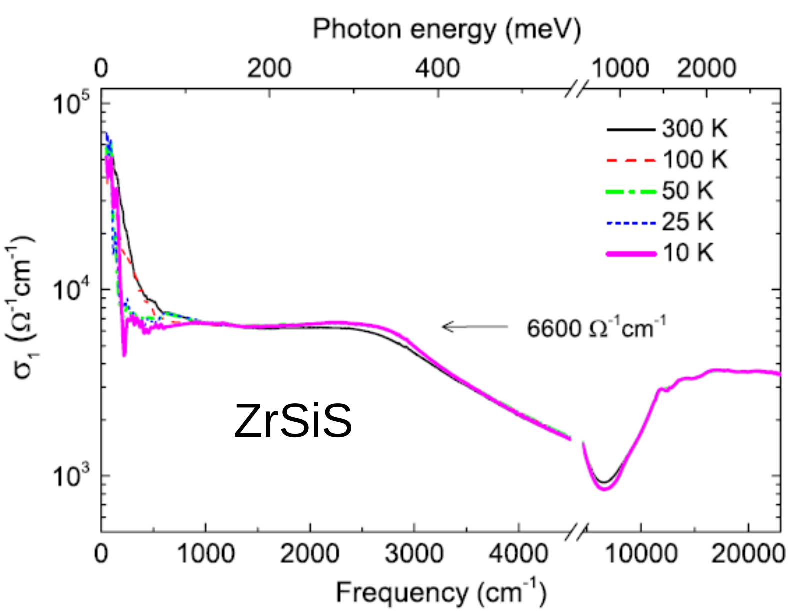
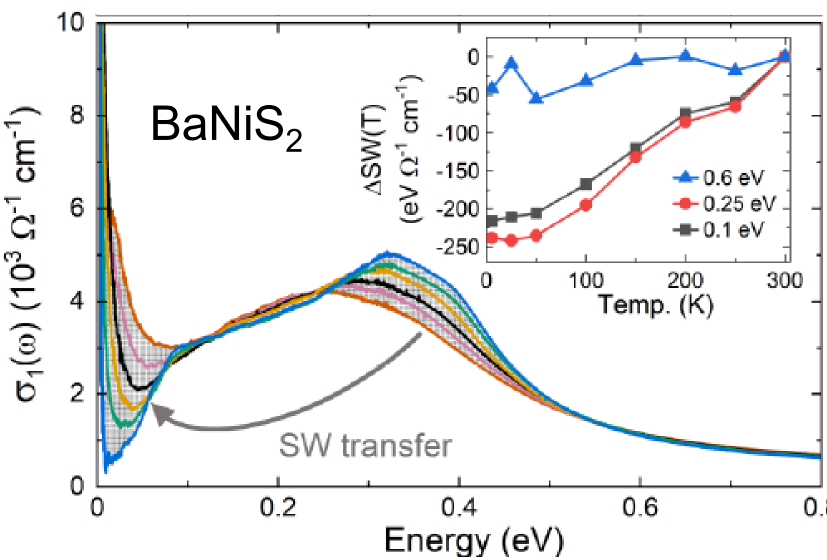
Dirac nodal-line semimetals



(Nearly) dispersionless and but not universal interband absorption of light



M. B. Schilling et al., Phys. Rev. Lett. 119, 187401 (2017)



D. Santos-Cottin et al., Phys. Rev. B 104, L201115 (2021)

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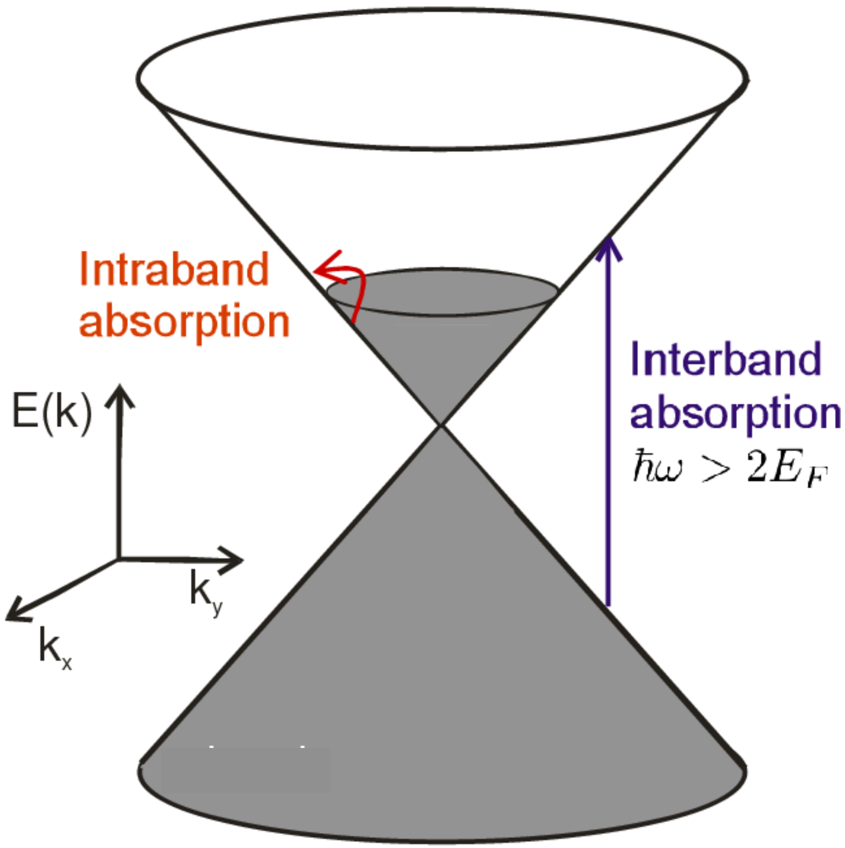

Optical band gap (zero T, finite doping) $2E_F$

Absorption of light in solids (Fermi's golden rule & electric dipole excitations):

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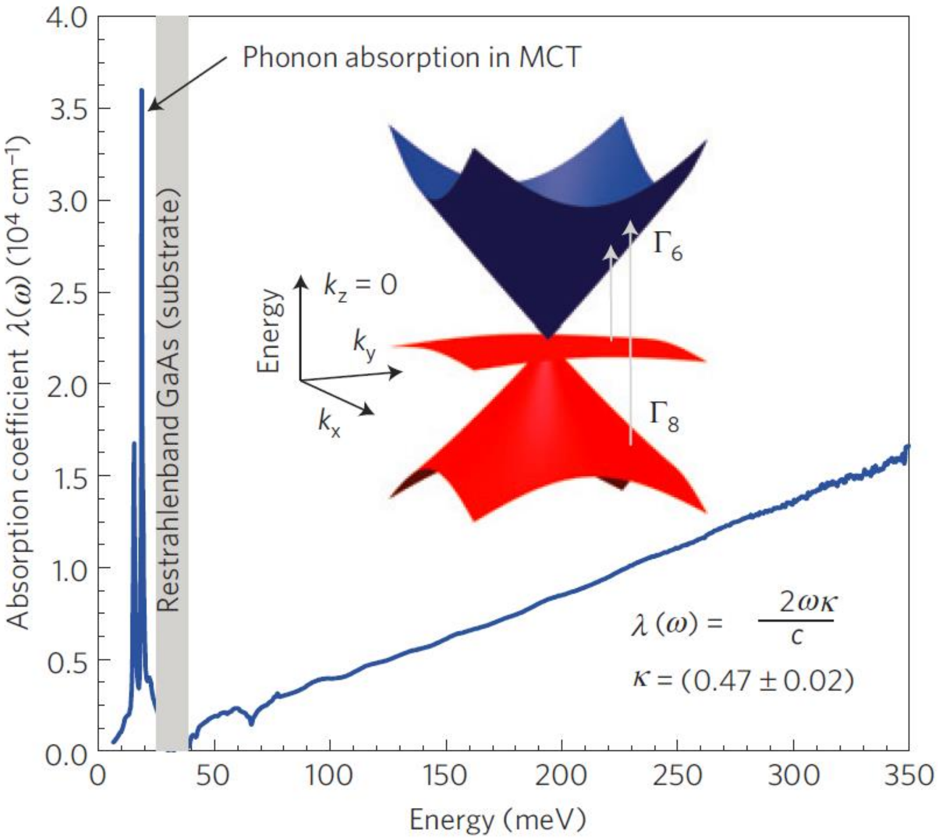
3D conical band: optical conductivity

Gapless HgCdTe:



MO et al., Nature Phys. 10, 233 (2014)

Absorption of light in solids (e.g., Fermi's golden rule):

$$\lambda(\omega) \propto \frac{\mathcal{D}(\omega)}{\omega}$$

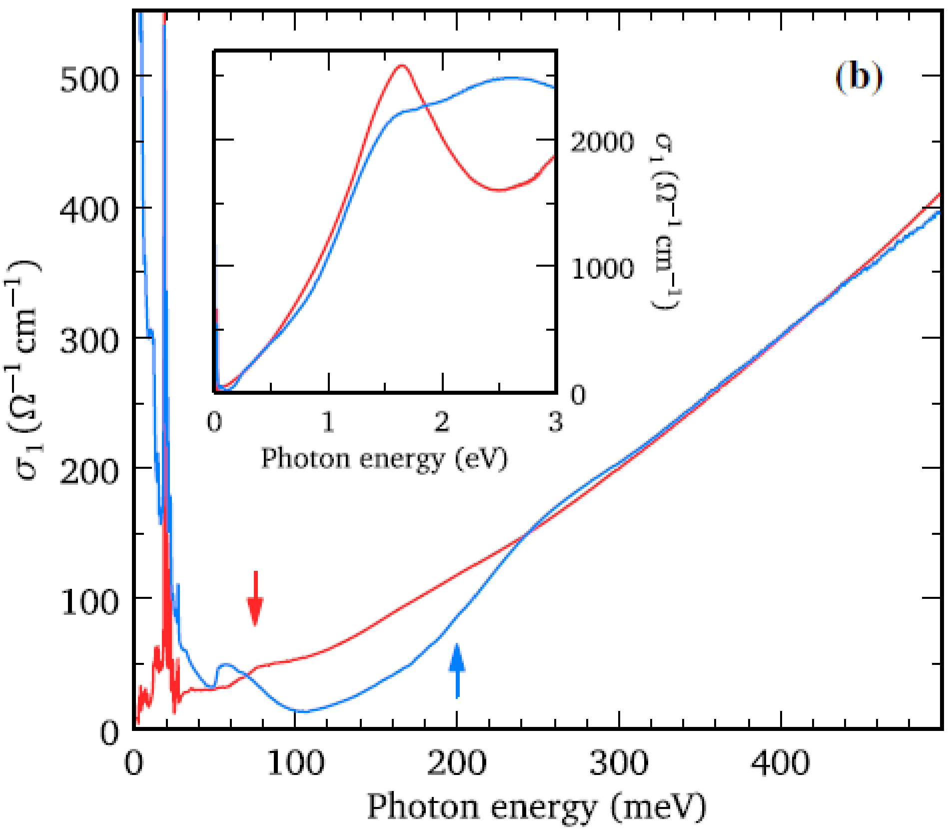
For conical bands in 3D:

$$\mathcal{D}(\omega) \propto \omega^2$$

Absorption coefficient linear in photon frequency!

3D conical band: optical conductivity

Cd_3As_2:



A. Akrap et al., Phys. Rev. Lett. 117, 136401 (2016)

Absorption of light in solids (e.g., Fermi's golden rule):

joint density of states

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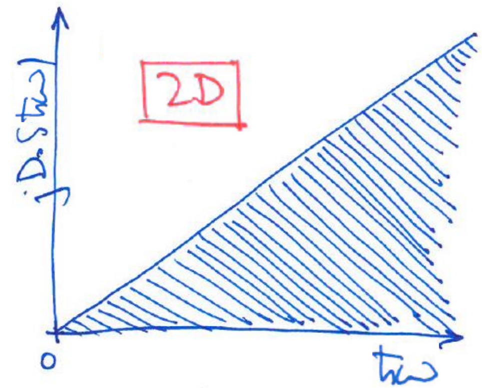
For conical bands in 3D:

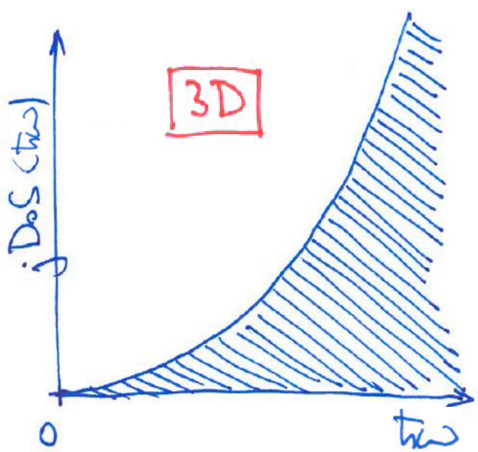
$$\mathcal{D}(\omega) \propto \omega^2$$

Absorption coefficient linear in photon frequency

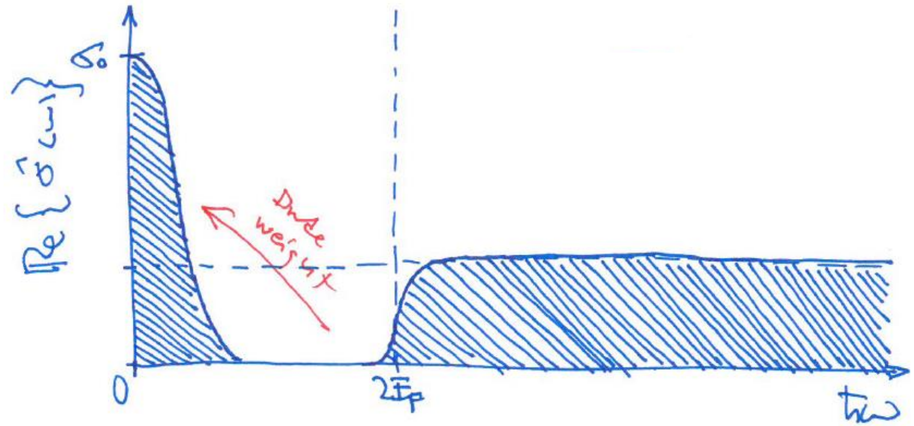
Optical conductivity of a conical band: summary

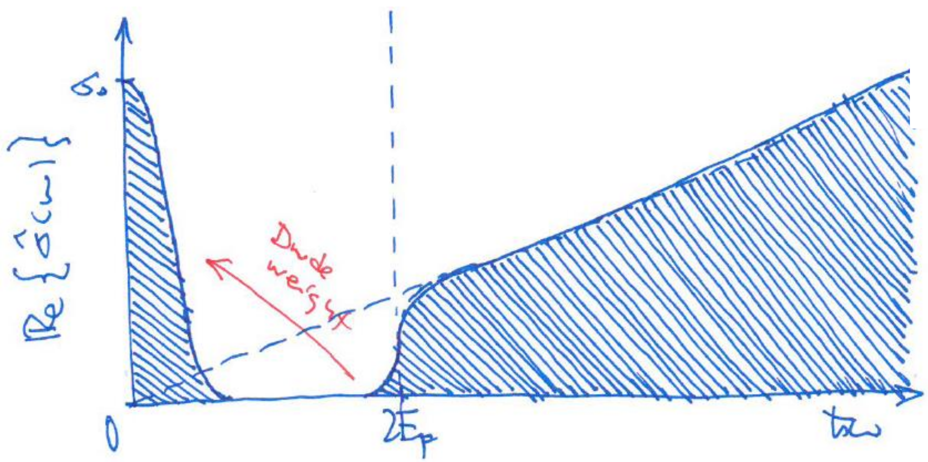
(Joint) density of states:



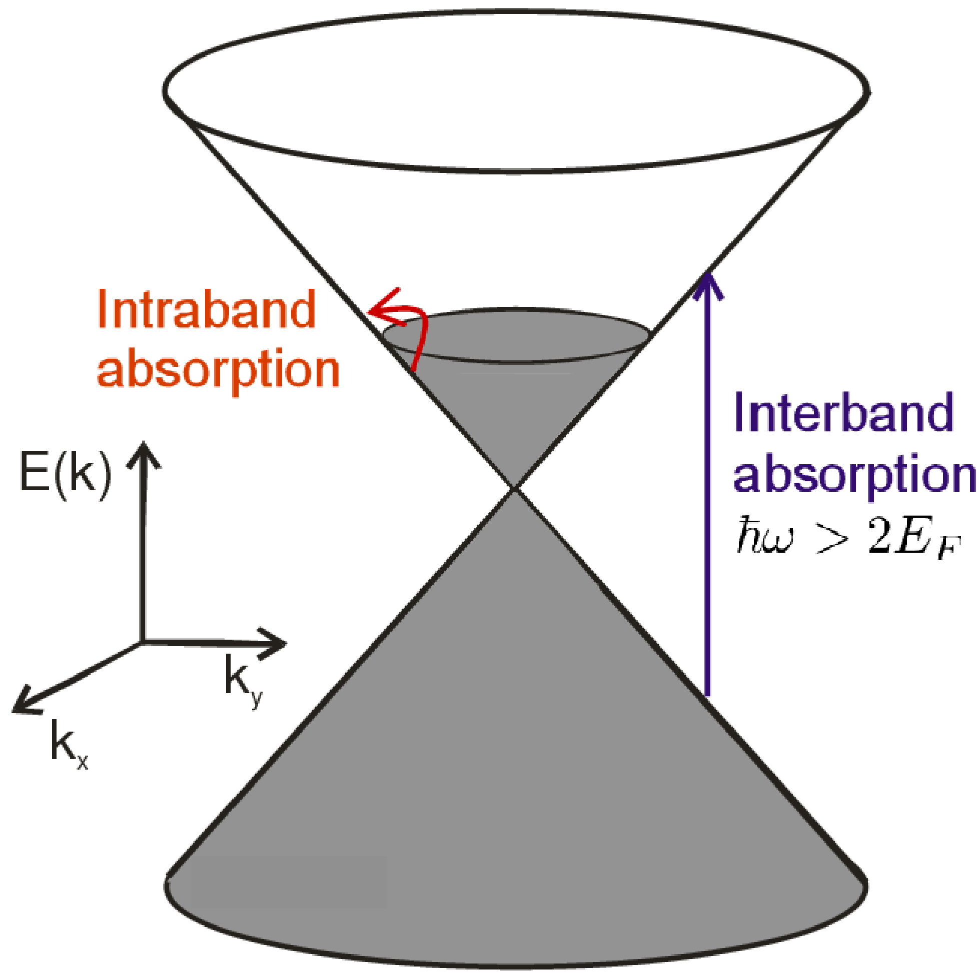


Optical conductivity:





Optical response of electrons in conical bands



[1]st order, electric-dipole excitations considered only

Optics of topological materials – second and higher order effects

nature materials

REVIEW ARTICLE

https://doi.org/10.1038/s41563-021-00992-7

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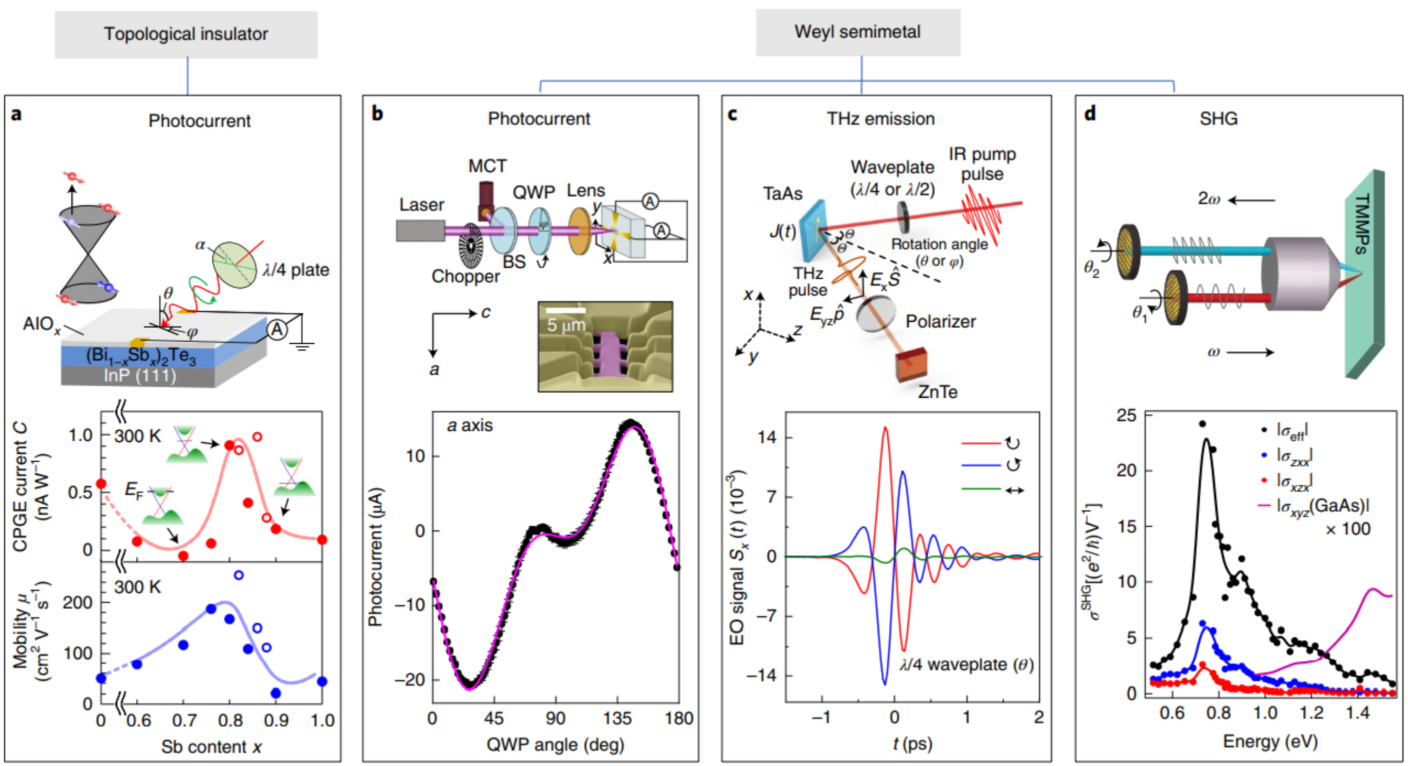
Topology and geometry under the nonlinear electromagnetic spotlight

Qiong Ma[1,2], Adolfo G. Grushin[3] and Kenneth S. Burch[2]

NATURE MATERIALS | VOL 20 | DECEMBER 2021 | 1601-1614

Current non-linearities

$$\vec{J} = \overleftrightarrow{\sigma}^{(1)} \cdot \vec{E} + \boxed{\vec{E} \cdot \overleftrightarrow{\sigma}^{(2)} \cdot \vec{E} + \dots}$$



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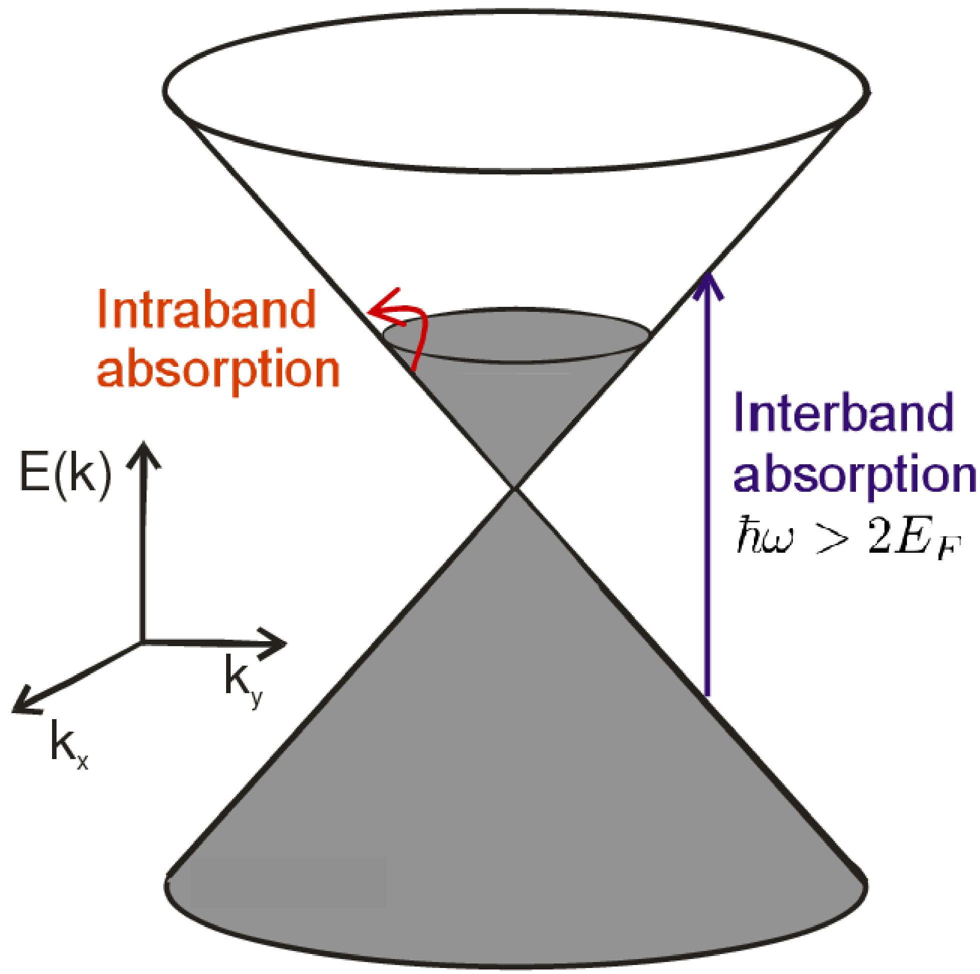
Optical response of electrons in conical bands

Magnetic field?



1st order, electric-dipole excitations considered only

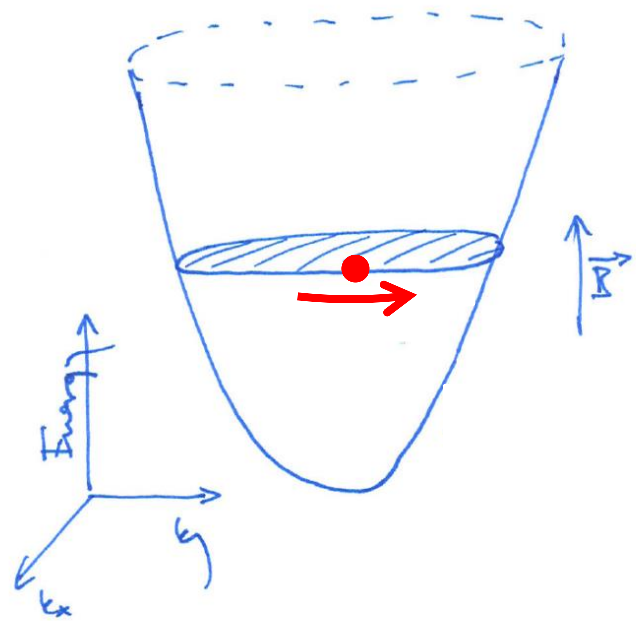
Cyclotron resonance

Charged particle in magnetic field:

$$\frac{d\mathbf{p}}{dt} = e[\mathbf{v} \times \mathbf{B}]$$

Cyclotron motion at the frequency:

$$\omega_c = \frac{eB}{m}$$



Cyclotron resonance = resonant absorption of light at the cyclotron frequency

Cyclotron resonance in solid-state physics

Letters to the Editor

PUBLICATION of brief reports of important discoveries in physics may be secured by addressing them to this department. The closing date for this department is five weeks prior to the date of issue. No proof will be sent to the authors. The Board of Editors does not hold itself responsible for the opinions expressed by the correspondents. Communications should not exceed 600 words in length and should be submitted in duplicate.

Observation of Cyclotron Resonance in Germanium Crystals*

G. Dresselhaus, A. F. Kip, and C. Kittel
Department of Physics, University of California, Berkeley, California
(Received September 8, 1953)

WE have observed cyclotron or diamagnetic resonance in n- and p-type germanium crystals at 4°K at a frequency of 9050 Mc/sec. In cyclotron resonance absorption the conduction electrons or holes are curved in spiral orbits by the application of a static magnetic field; resonant absorption of energy from an rf electric field perpendicular to the static magnetic field occurs when the frequency of the electric field is equal to the frequency of rotation of the particle. This is the principle of the cyclotron an the simple magnetron. The angular rotation frequency in a crystal is

$$\omega_L = (eH)/(m^*c), \qquad (1)$$

where m^* is the appropriate effective mass; thus the experiment determines the effective mass directly. Cyclotron resonance should not be confused with electron spin resonance. Cyclotron resonance arises from an electric dipole transition, whereas spin resonance arises from a magnetic dipole transition: the transition probabilities for the former are larger by a factor of the order of 10^{10} under the conditions of our experiment.

Germanium = the first solid-state system in which cyclotron resonance was observed

G. Dresselhaus, A. F. Kip, and C. Kittel Phys. Rev. 92, 827 (1953)

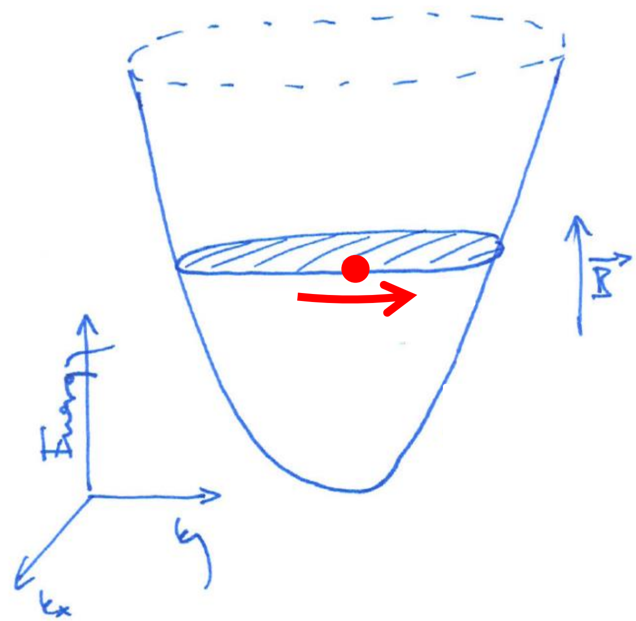
More than the estimate of the effective mass, important observation for the concept of quasi-particles in condensed matter physics

see, e.g., M. L. Cohen, AIP Conference Proceedings 772, 3 (2005)

Cyclotron resonance

Charged particle in magnetic field:

$$\frac{d\mathbf{p}}{dt} = e[\mathbf{v} \times \mathbf{B}]$$



Cyclotron motion at the frequency:

$$\omega_c = \frac{eB}{m}$$

Cyclotron resonance = resonant absorption of light at the cyclotron frequency

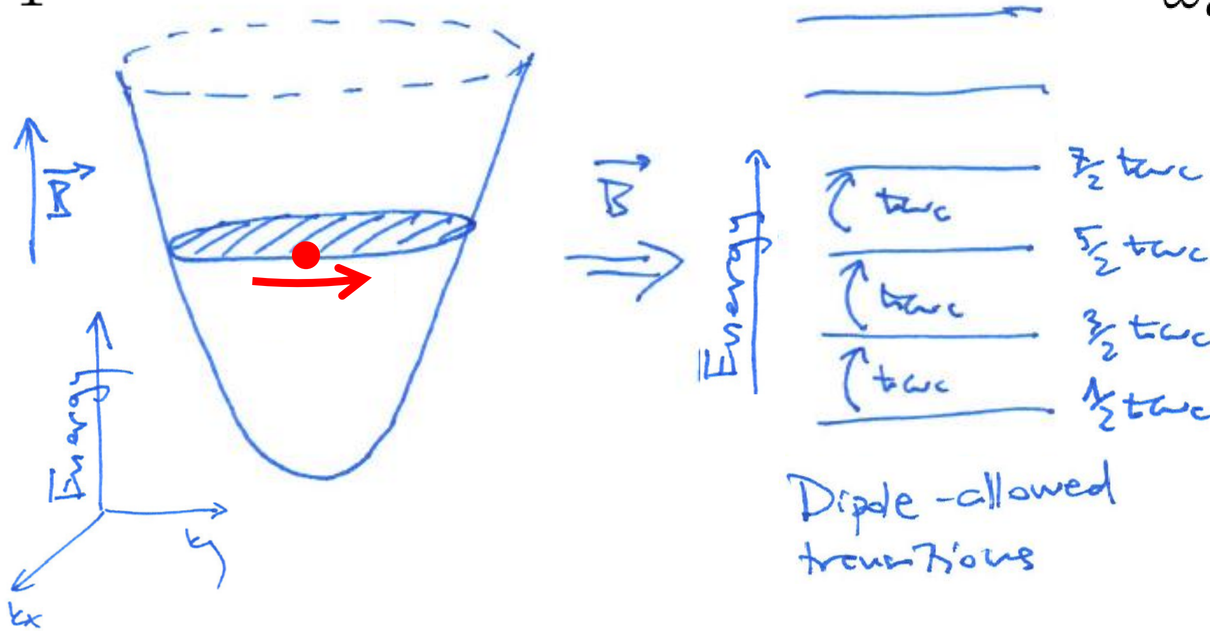
Cyclotron resonance (quantum description)

Classical regime:

$\omega_c \tau \sim 1$

Quantum regime:

$\omega_c \tau \gg 1$



Landau levels (parabolic band):

$$E_n = \hbar\omega_c(n + 1/2)$$

$$\omega_c = eB/m$$

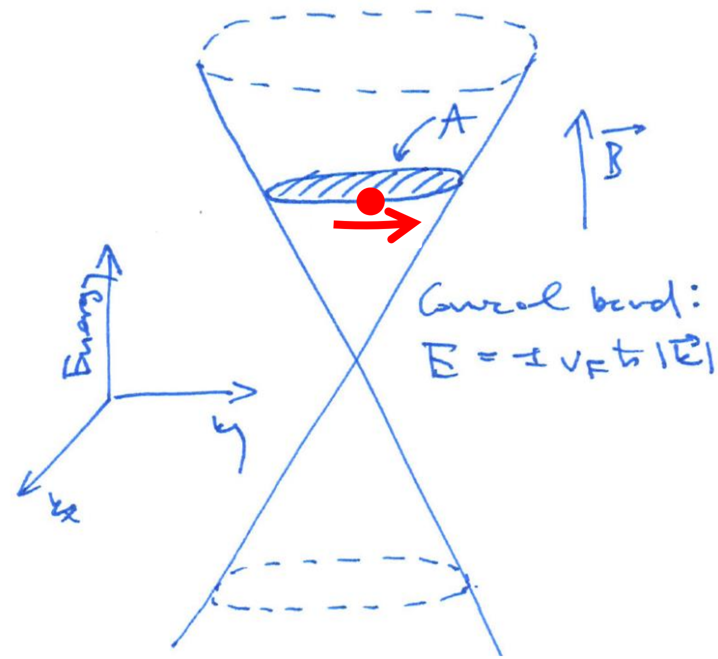
Single-particle mass, no electron-electron interaction effects…

W. Kohn, Phys. Rev. 123, 1242 (1961)

Cyclotron motion of massless electrons (classical description)

Charged particle in magnetic field:

$$\frac{d\mathbf{p}}{dt} = e[\mathbf{v} \times \mathbf{B}]$$



Cyclotron motion at the frequency:

$$\omega_c = \frac{eB}{\underbrace{E/v^2}}$$

Linear in B

Cyclotron mass (energy dependent)

"Effective" effective mass of massless particles, i.e., Einstein energy-mass relation $E = mv^2$

Cyclotron motion of massless electrons (classical description)

Charged particle in magnetic field:

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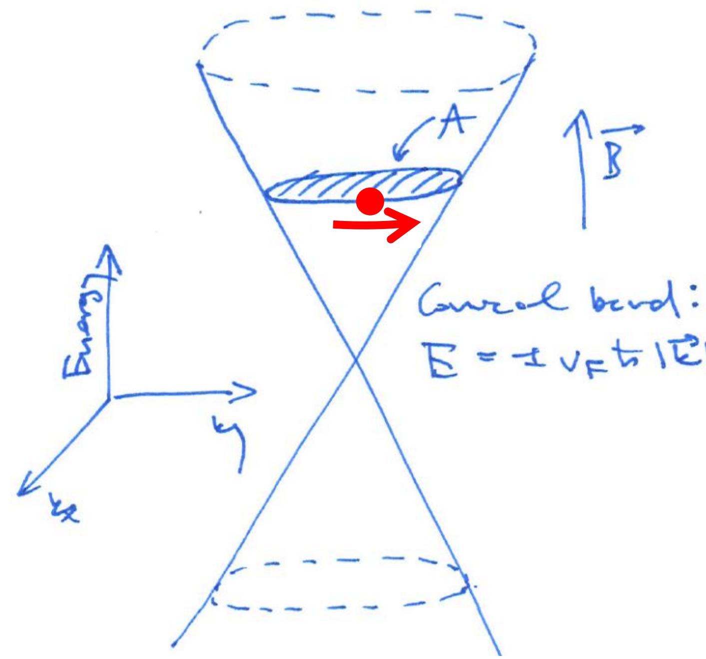


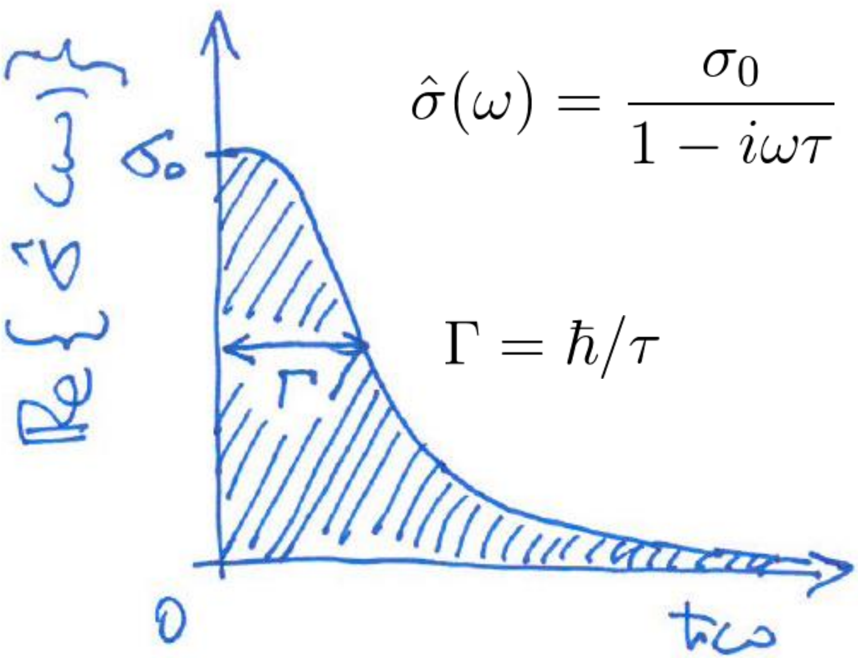
"Effective" effective mass of massless particles, i.e., Einstein energy-mass relation $E = mv^2$

General definition of cyclotron mass: $$m = \frac{\hbar^2}{2\pi}\frac{\partial A}{\partial \varepsilon}$$

see, e.g., Ashcroft & Mermin

Conical bands: Absorption of light on free carriers

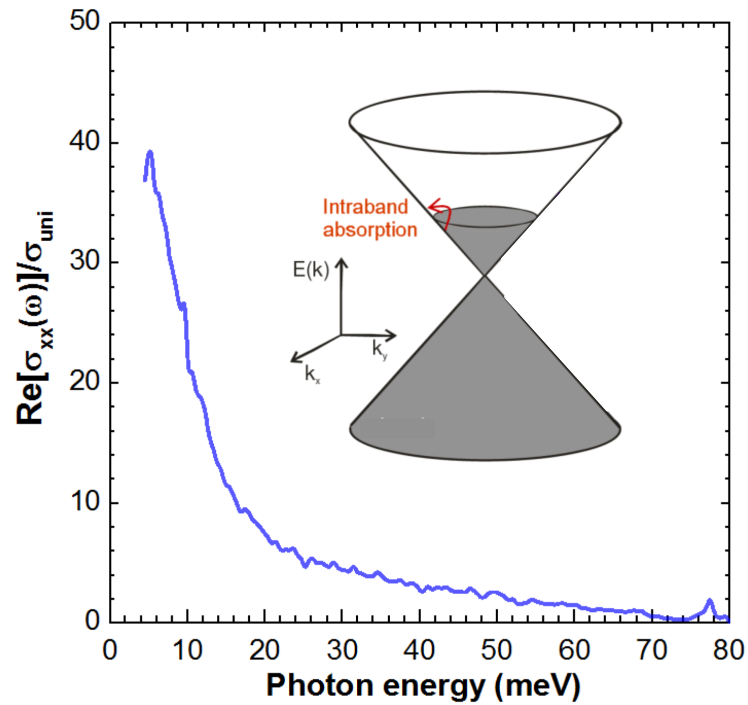
Classical Drude model for optical conductivity



$$\hat{\sigma}(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

$$\Gamma = \hbar/\tau$$

Free-carrier absorption in epitaxial graphene on SiC



dc conductivity

$$\sigma_0 = \frac{e\tau n}{m} \propto \boxed{\frac{n}{m}}$$

Drude (optical) weight

Cyclotron motion of massless electrons (classical description)

Charged particle in magnetic field:

$$\frac{d\mathbf{p}}{dt} = e[\mathbf{v} \times \mathbf{B}]$$

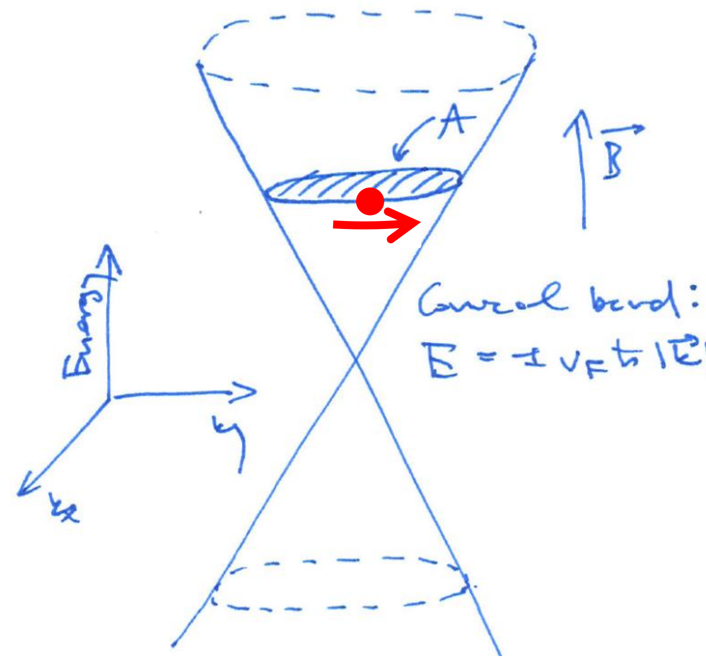
Cyclotron motion at the frequency:

$$\omega_c = \frac{eB}{\underbrace{E/v^2}}$$

Linear in B

Cyclotron mass (energy dependent)

"Effective" effective mass of massless particles, i.e., Einstein energy-mass relation $E = mv^2$

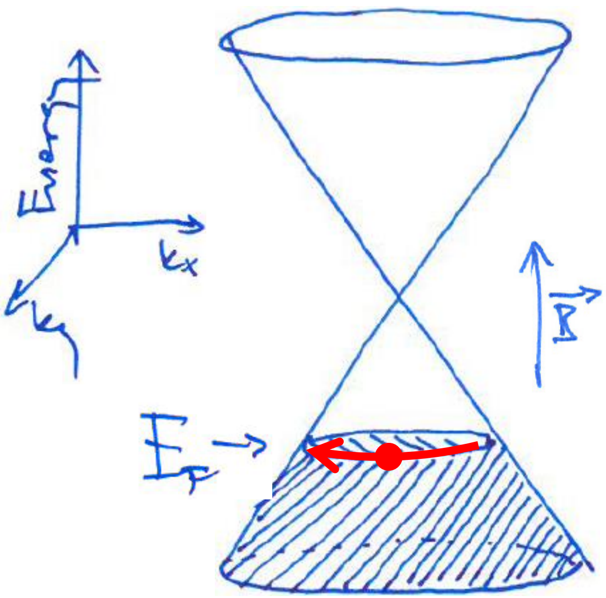


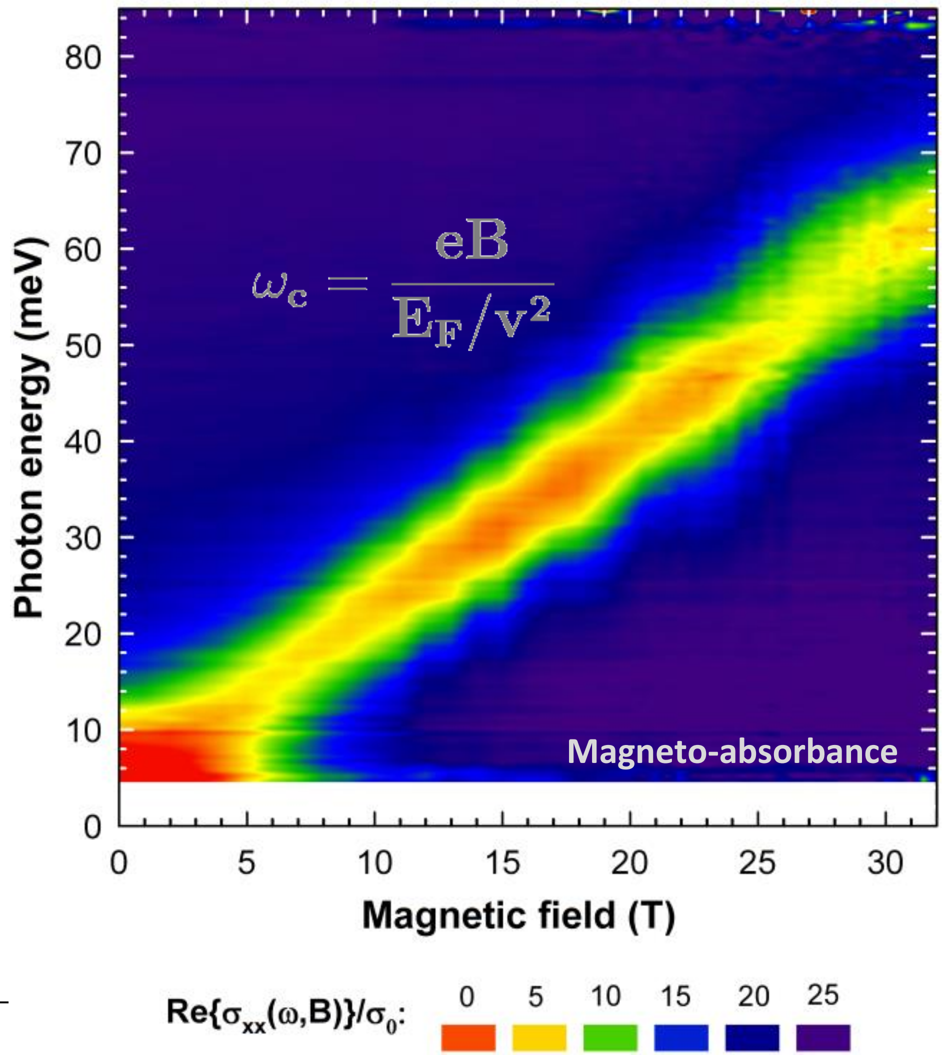
General definition of cyclotron mass: $m = \frac{\hbar^2}{2\pi} \frac{\partial A}{\partial \varepsilon}$

see, e.g., Ashcroft & Mermin

Cyclotron resonance in graphene

Quasi-free-standing graphene on SiC
in classical regime $\omega_c \tau = \mu . B \sim 1$

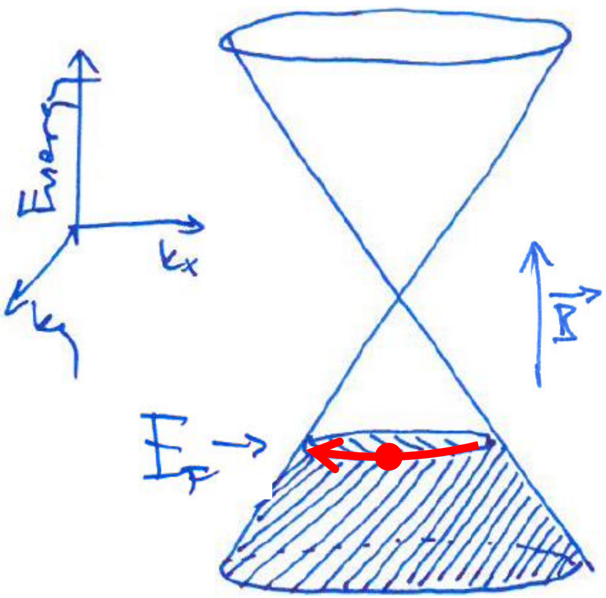


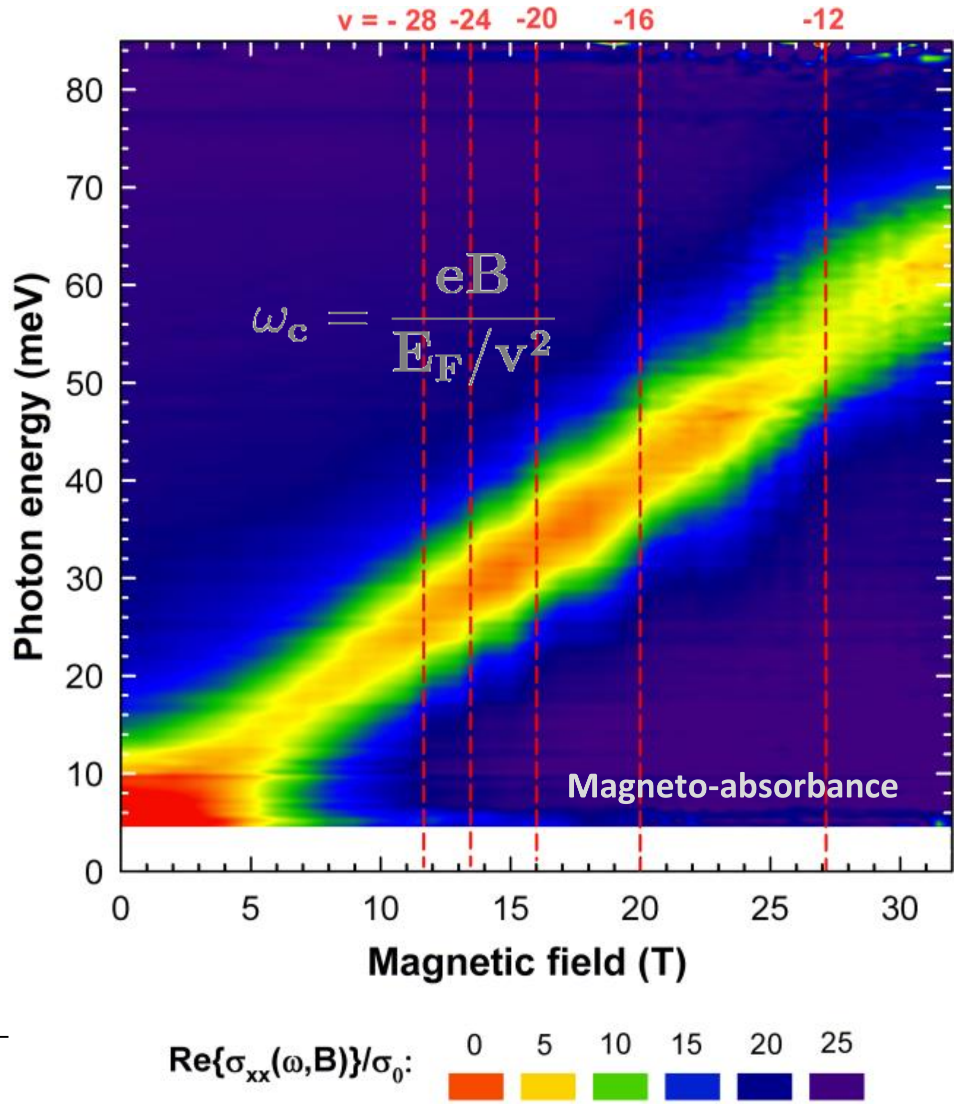


MO et al., New J. Phys. 14, 095008 (2012)
A. M. Witowski et al., Phys. Rev. B 82, 165305 (2010)

Cyclotron resonance in graphene

Quasi-free-standing graphene on SiC in classical regime $\omega_c \tau = \mu . B \sim 1$





MO et al., New J. Phys. 14, 095008 (2012)
A. M. Witowski et al., Phys. Rev. B 82, 165305 (2010)

Cyclotron resonance in graphene

Landau levels:

$$E_n = \pm v_F \sqrt{2e\hbar|Bn|}$$

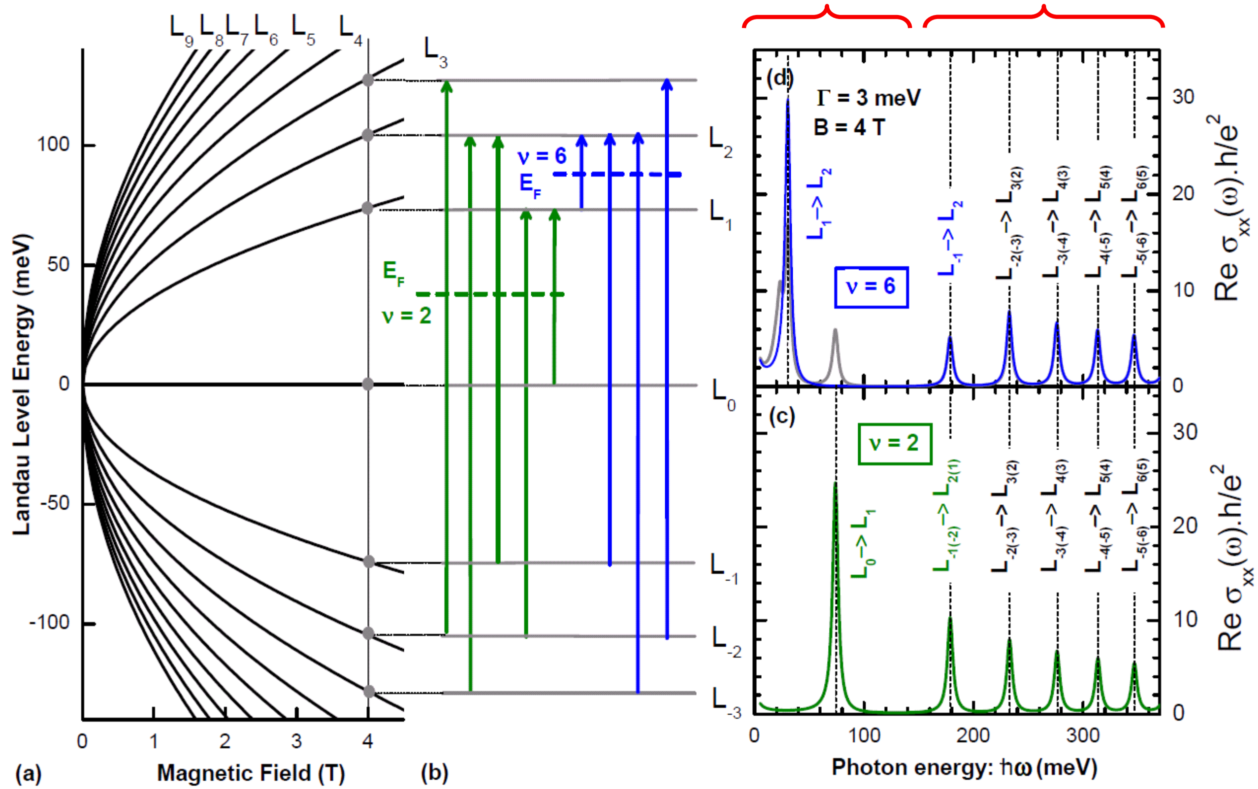
Quantum regime

$$\omega_c \tau = \mu . B \gg 1$$

Selection rules: $n \rightarrow n \pm 1$

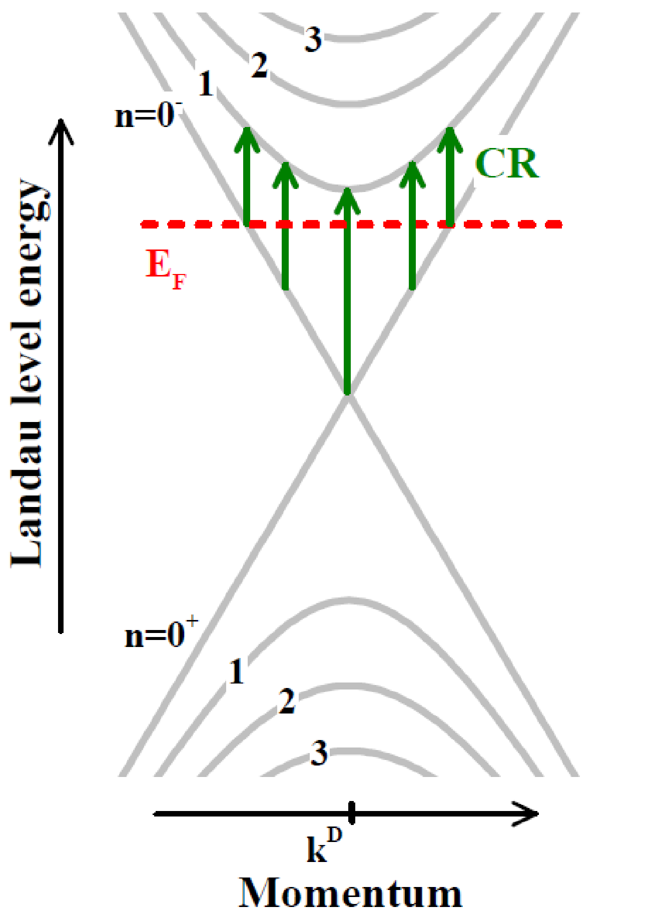
Cyclotron resonance

Interband excitations



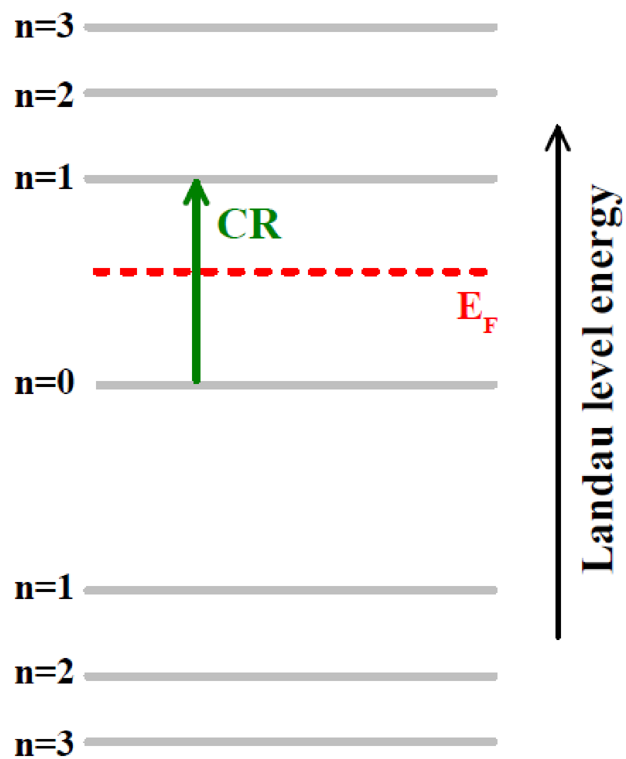
Dirac electrons – Landau level spectrum

3D Dirac electrons



$$E_n = \pm v\sqrt{2e\hbar Bn + \hbar^2 k^2}$$

2D Dirac electrons

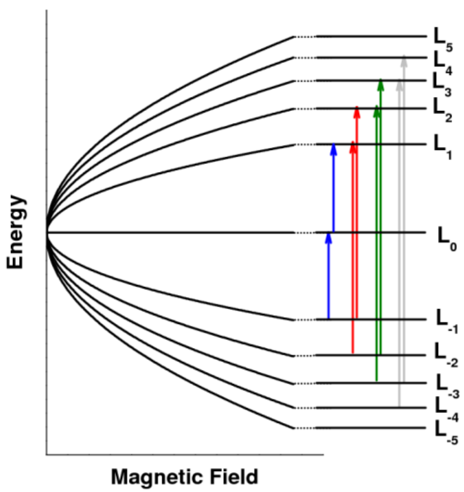


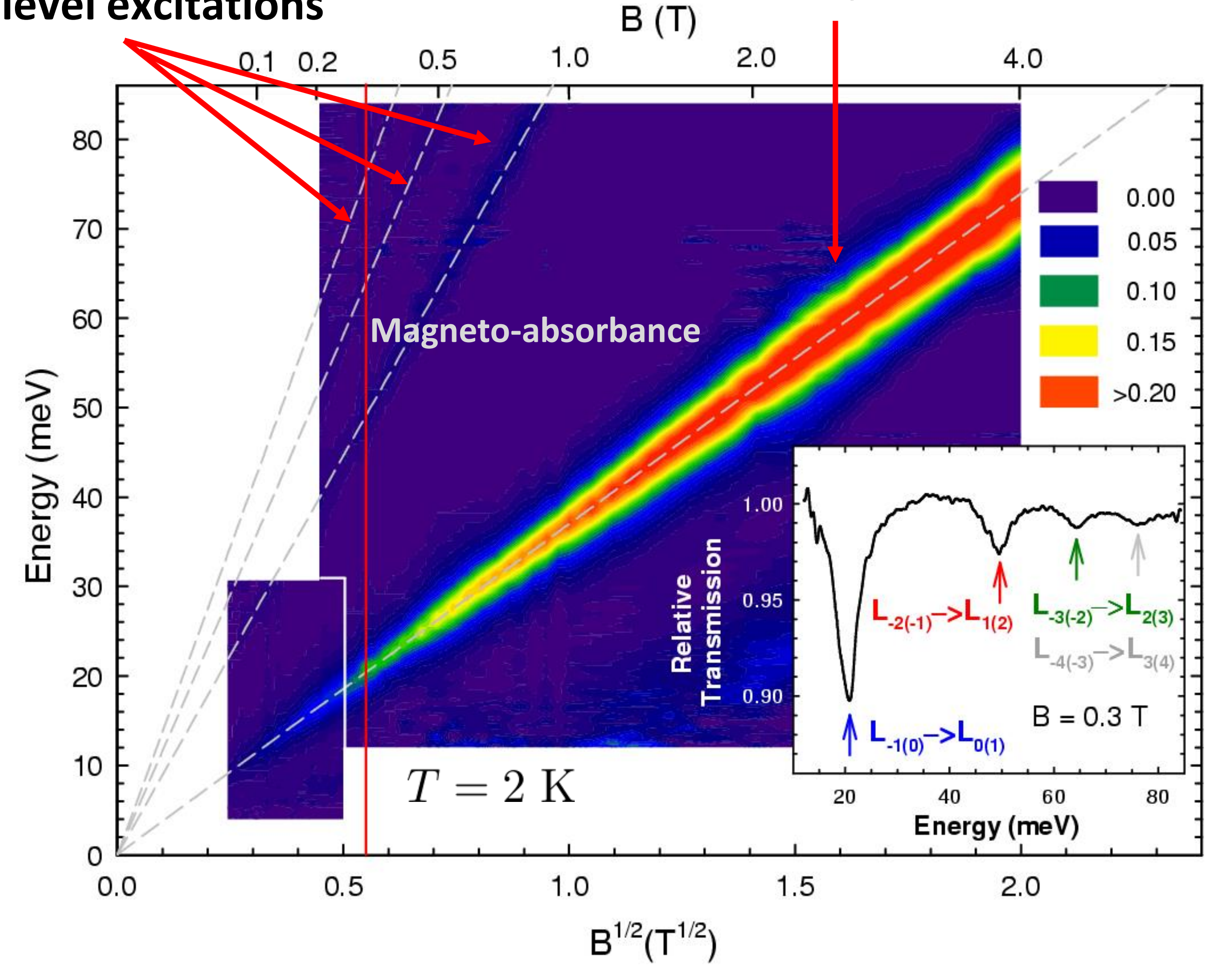
$$E_n = \pm v\sqrt{2e\hbar Bn}$$

Cyclotron resonance in graphene

Interband inter-Landau level excitations

Cyclotron resonance





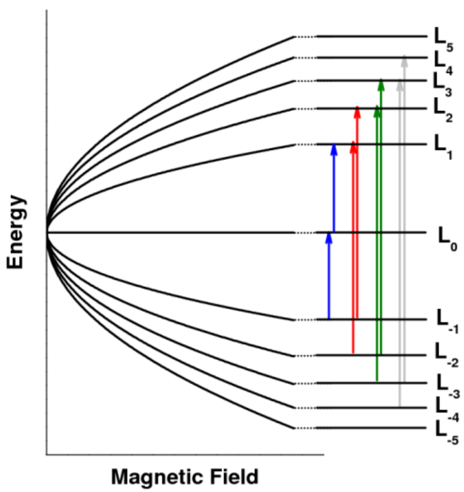
Multilayer epitaxial graphene on SiC
in quantum regime $\omega_c \tau = \mu . B \gg 1$

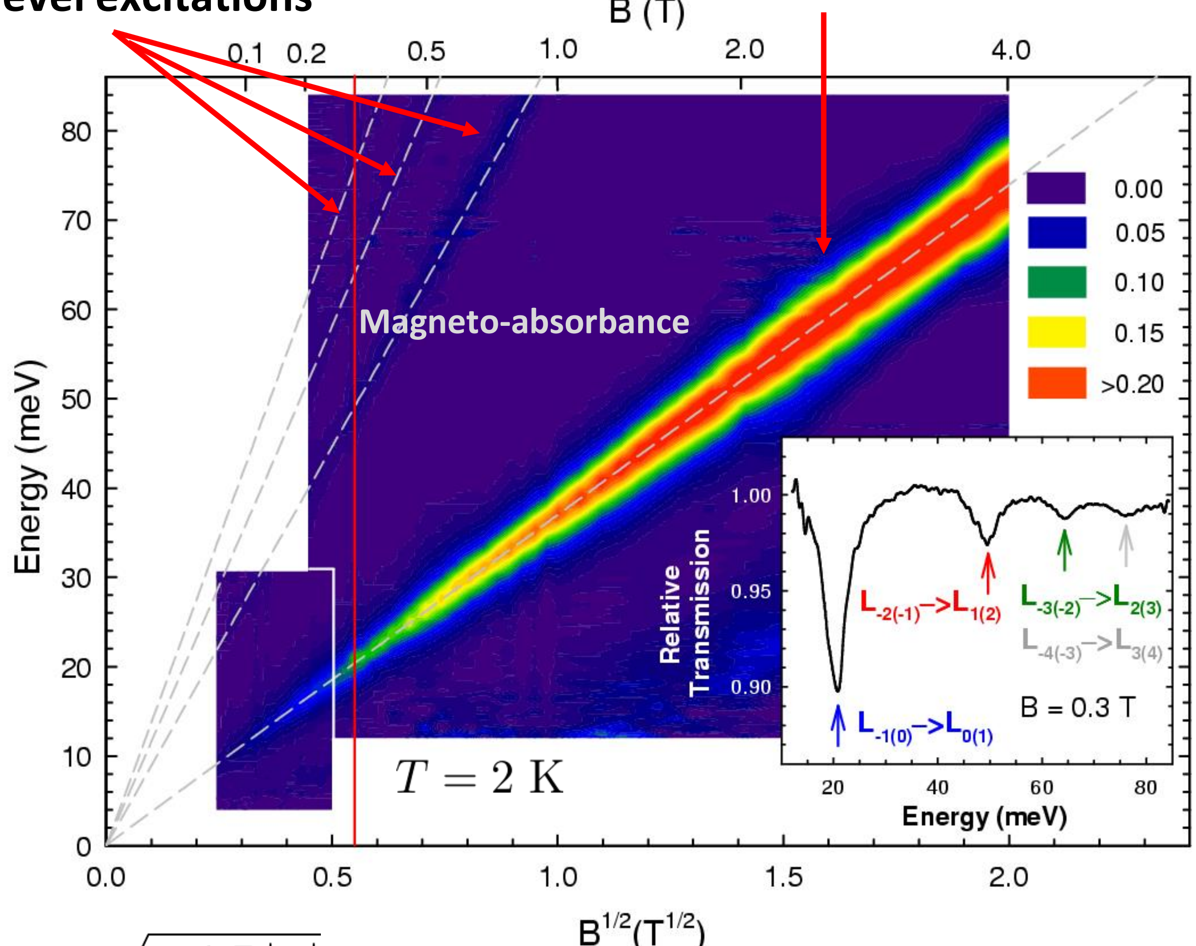
MO et al., Phys. Rev. Lett. 101, 267601 (2008)

Cyclotron resonance in graphene

Interband inter-Landau level excitations

Cyclotron resonance





Energy spectrum: $E_n = \pm v\sqrt{2e\hbar B|n|}$

Velocity parameter: $v = 1.02 \times 10^6 \text{ m/s}$

MO et al., Phys. Rev. Lett. 101, 267601 (2008)

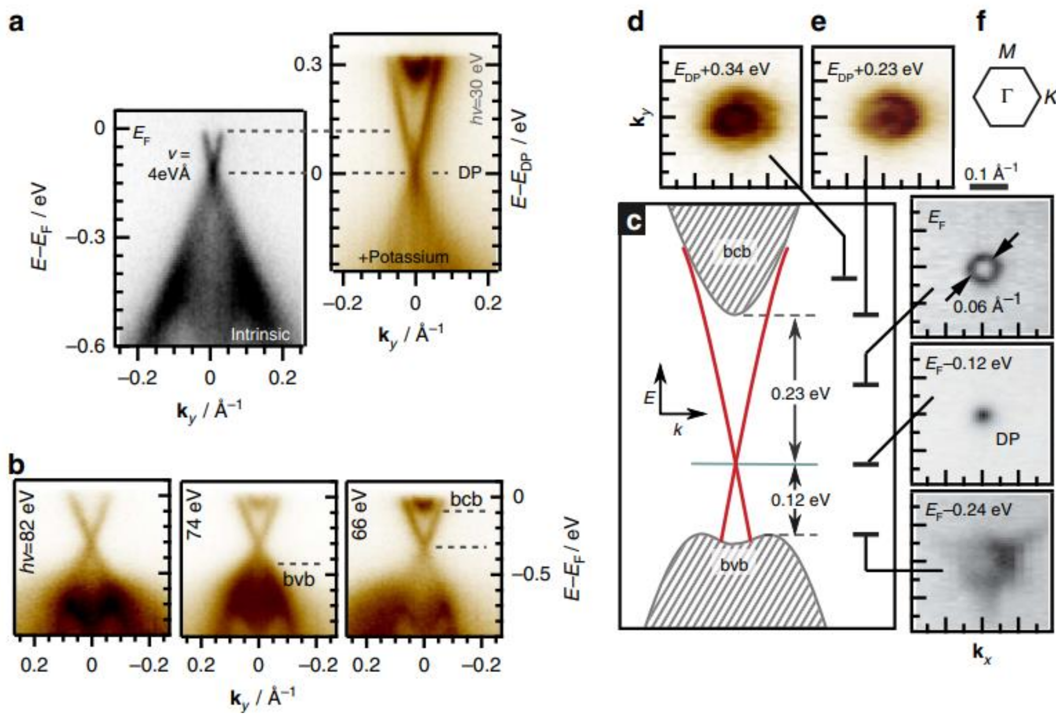
Disorder, energy gap (?), departure from linearity

Sn-doped $BiSbTe_2S$ – 3D topological insulator

Similar to tedradymite family
(Bi_2Se_3, Bi_2Te_3...)

Energy band gap ~300 meV
(STM & ARPES)

Insulating in bulk (Sn-doping)

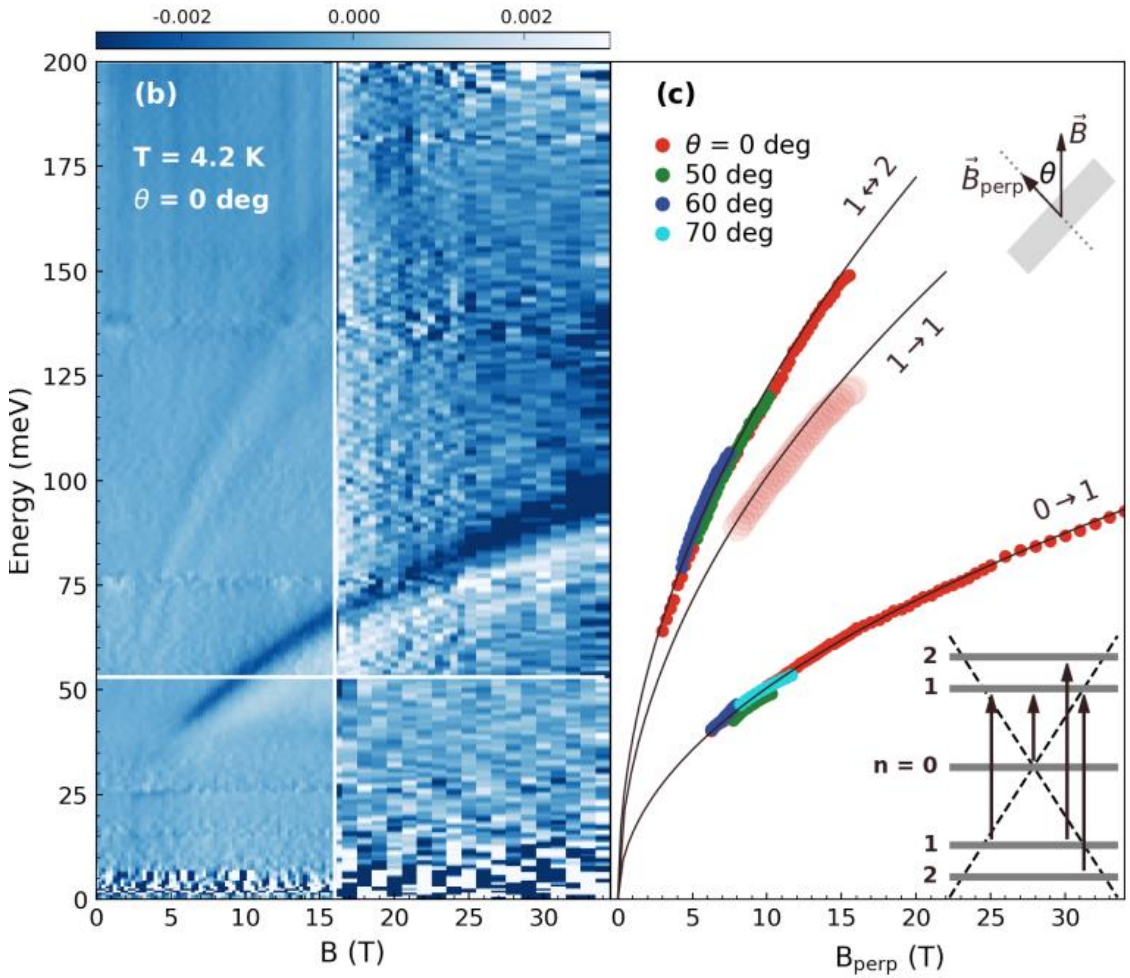


S. K. Kushwaha et al., Nature Comm. 7, 11456 (2016)

Sn-doped $BiSbTe_2S$ – 3D topological insulator

Landau level spectroscopy of surface electrons

Magneto-reflectivity (B-derivative):



I. Mohelsky et al., unpublished (2024)

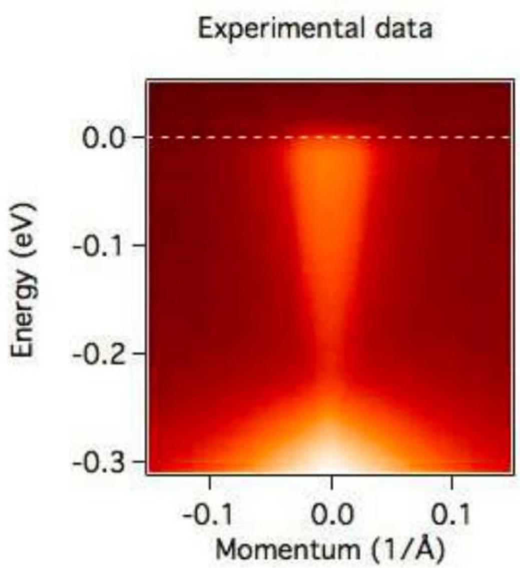
3D Dirac semimetal Cd_3As_2

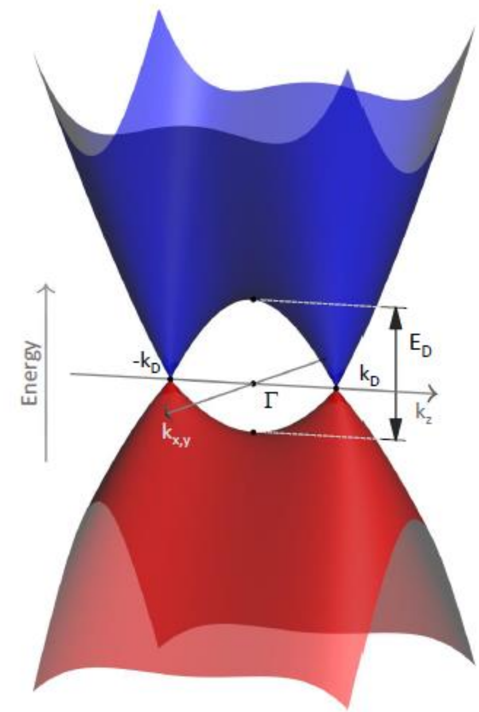
nature materials
LETTERS
PUBLISHED ONLINE: 25 MAY 2014 | DOI: 10.1038/NMAT3990

A stable three-dimensional topological Dirac semimetal Cd_3As_2

Z. K. Liu[1†], J. Jiang[2,3†], B. Zhou[2,4†], Z. J. Wang[5†], Y. Zhang[1,4], H. M. Weng[5], D. Prabhakaran[2], S-K. Mo[4], H. Peng[2], P. Dudin[6], T. Kim[6], M. Hoesch[6], Z. Fang[5], X. Dai[5], Z. X. Shen[1], D. L. Feng[3], Z. Hussain[4] and Y. L. Chen[1,2,4,6★]

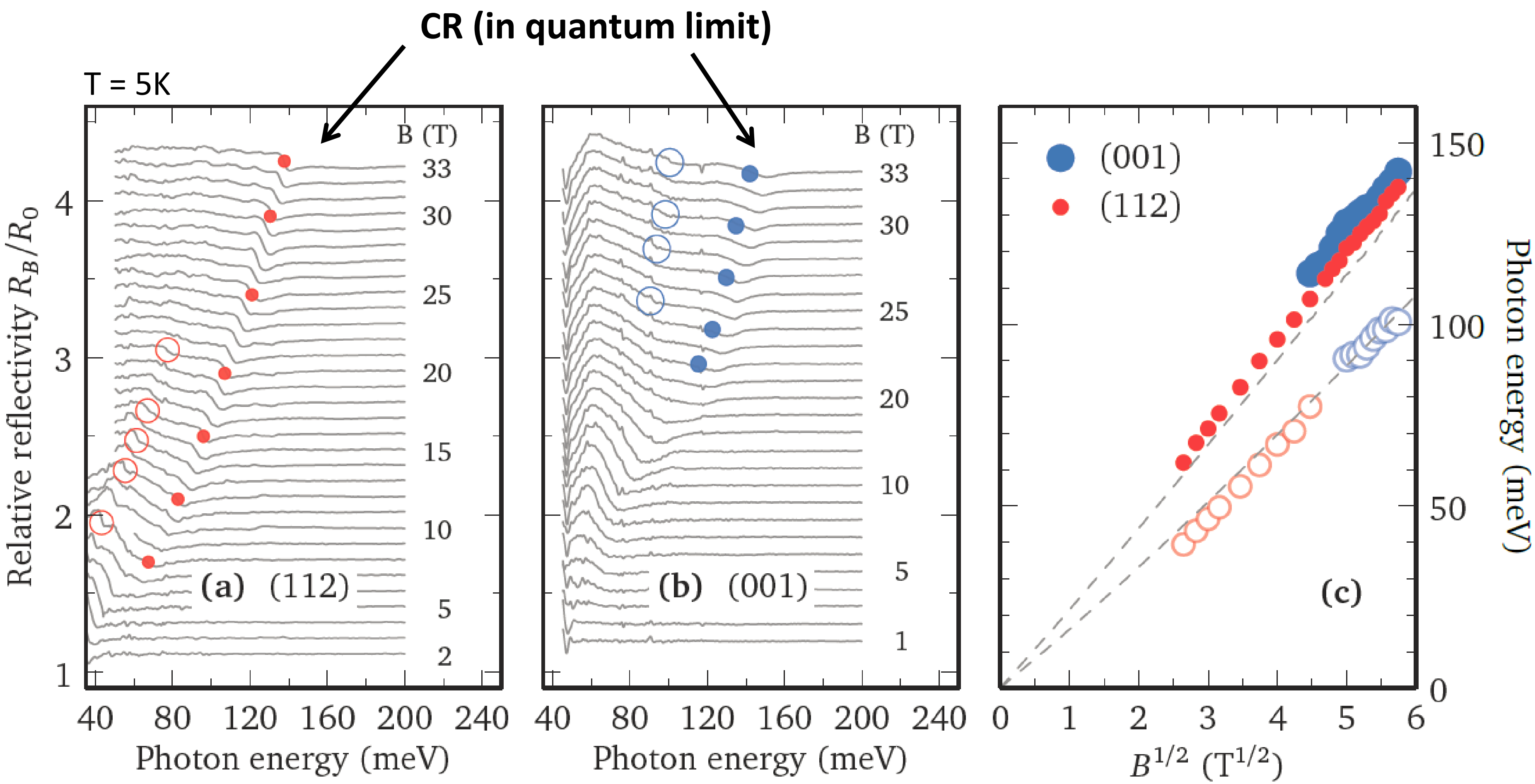
ARPES:





Z. K. Liu et al., Nature Mater. 13, 677 (2014)
S. Borisenko et al., Phys. Rev. Lett. 113, 027603 (2014)
M. Neupane et al., Nature Comm. 5, 3786 (2014)

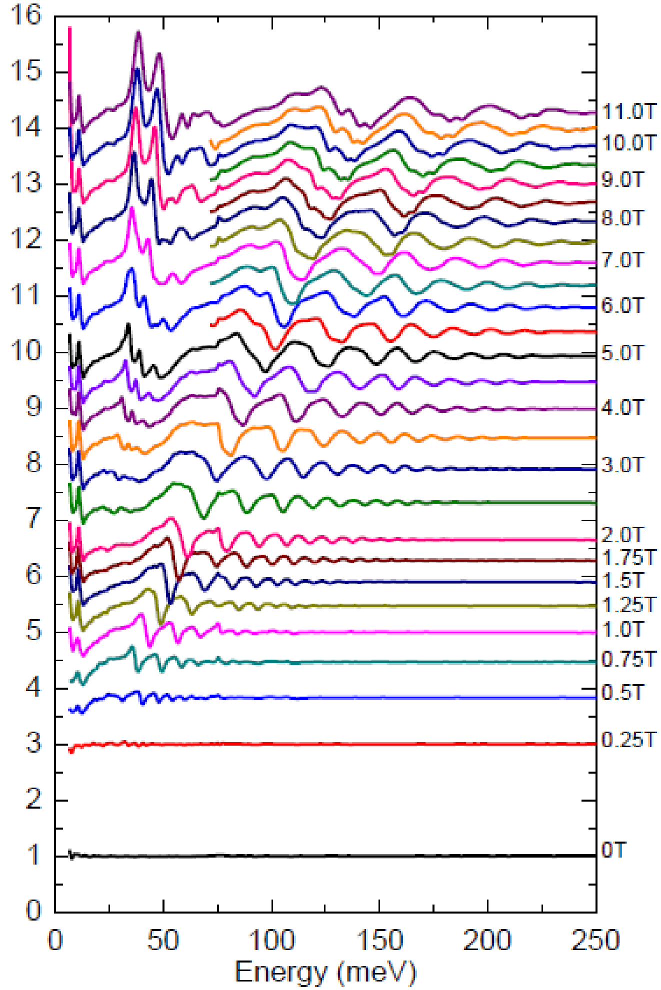
Cd_3As_2 – High-field magneto-reflectivity

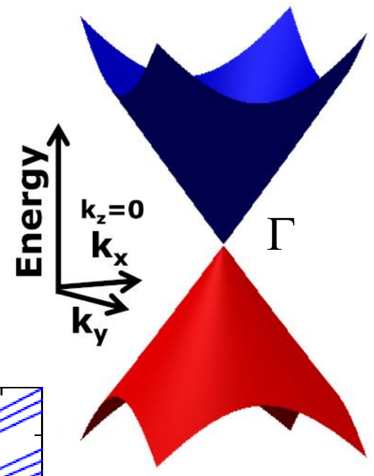


A. Akrap et al., Phys. Rev. Lett. 117, 136401 (2016)
see I. Crassee et al. Phys. Rev. Mater. 2, 120302 (2018) for review

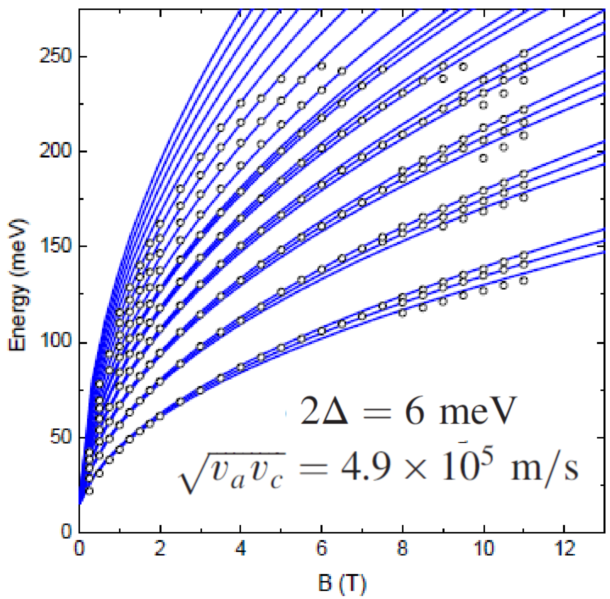
Landau level spectroscopy of 3D Dirac electrons in $ZrTe_5$

Magneto-transmission:





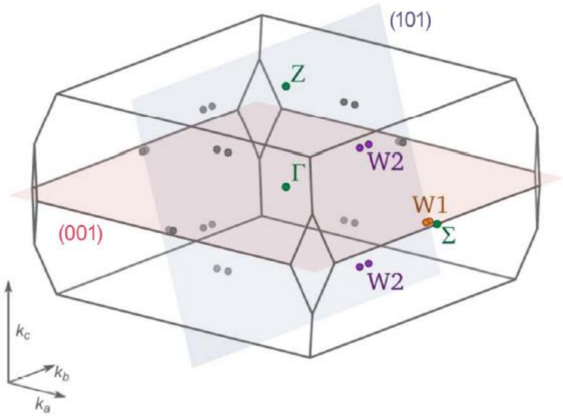
Fan chart:



Energy gap (STI versus WTI), velocity parameter, Zeeman splitting (g factors)…

E. Martino et al., Phys. Rev. Lett. 122, 217402 (2019)

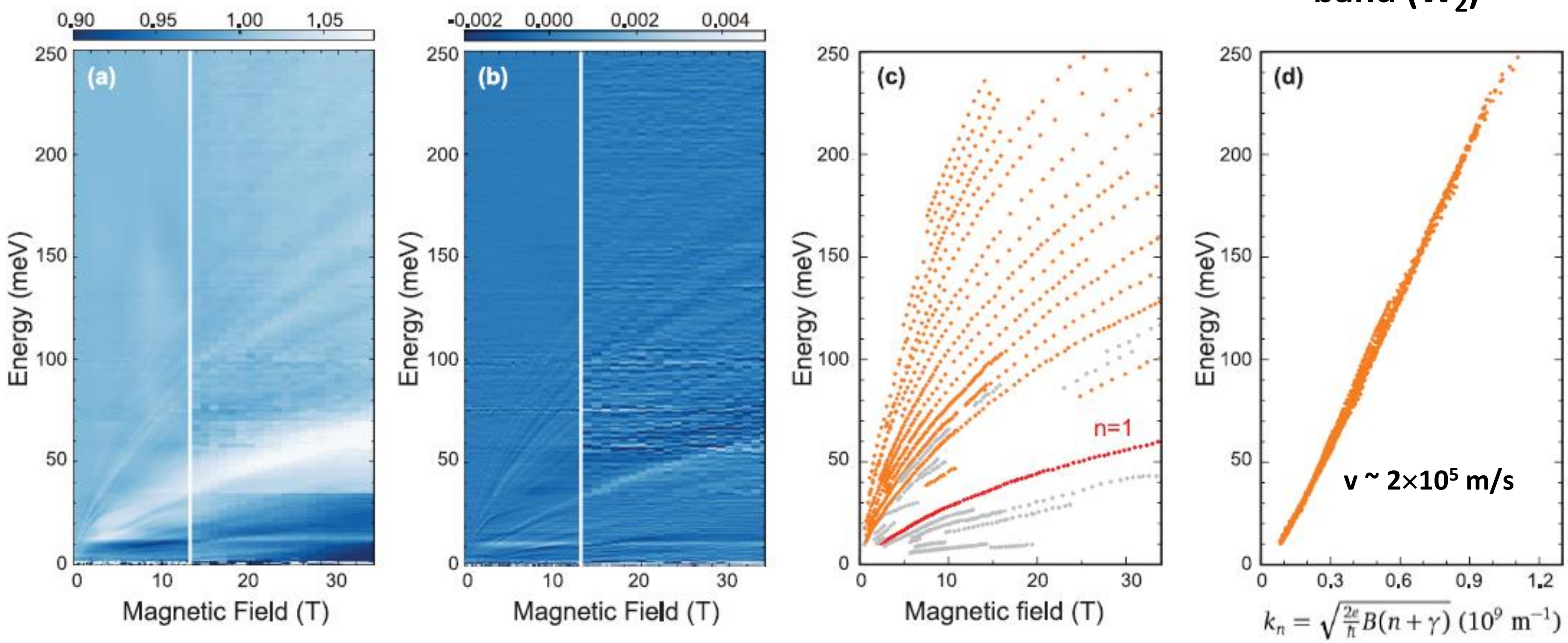
see also, Z. G. Chen et al. , PNAS 114, 816 (2017)
R. Y. Chen et al., Phys. Rev. Lett. 115, 176404 (2015)
Y. Jiang et al., Phys. Rev. Lett. 125, 046403 (2020)



Landau level spectroscopy of 3D Weyl semimetals: TaAs

Relative reflectivity R_B/R_0, its derivative + fan chart

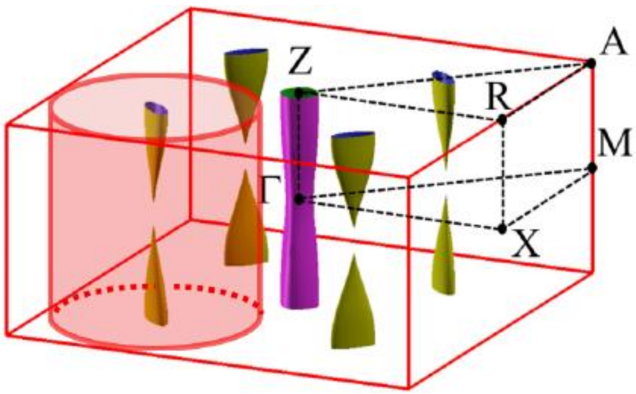
Reconstructed conical band (W_2)



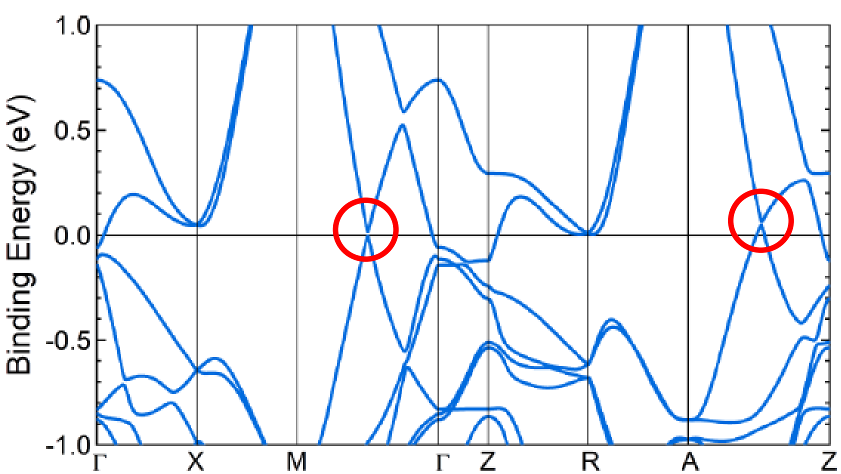
D. Santos-Cottin et al., Phys. Rev. B 105, L081114 (2022)

Landau level spectroscopy of $BaNiS_2$ nodal line semimetal

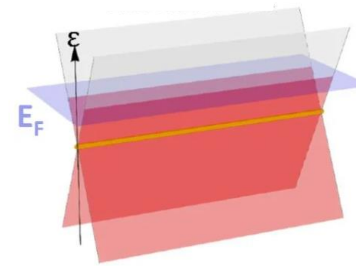
Square-lattice system with weakly dispersing nodal lines:



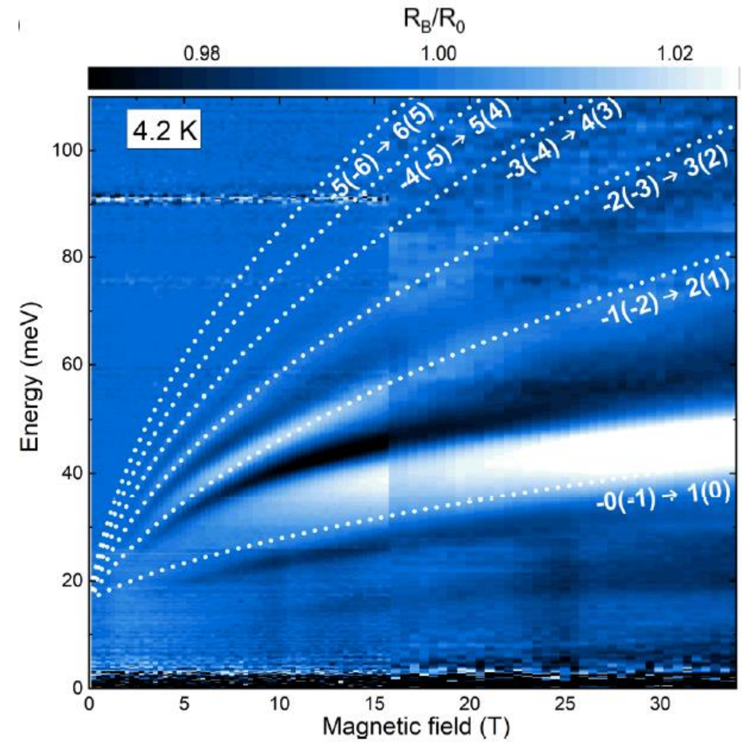
DFT:



Graphene-like dispersion (weakly gapped) in a 3D solid

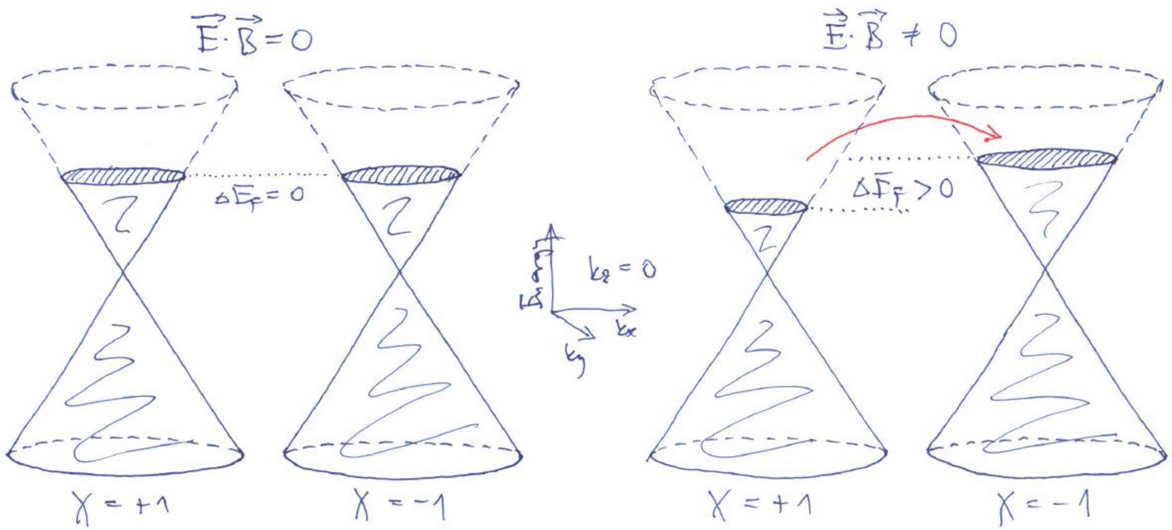


Magneto-reflectivity:



D. Santos-Cottin et al., Phys. Rev. B 104, L201115 (2021)

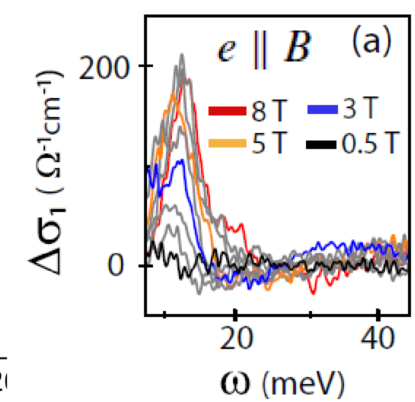
Optical detection of chiral anomaly in Weyl semimetals?



S. L. Adler, Phys. Rev. 177, 2426 (1969)

Chiral-anomaly-induced changes in Drude weight or in interband absorption (dc or ac regime of electric field)

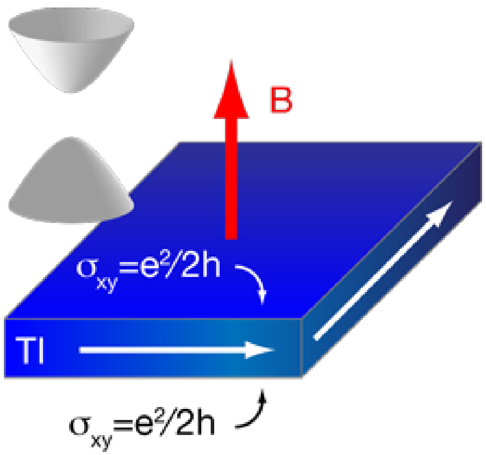
D. T. Son and B. Z. Spivak, Phys. Rev. B 88, 104412 (2013)
E. C. Ashby and J. P. Carbotte, Phys. Rev. B 89, 245121 (2014)

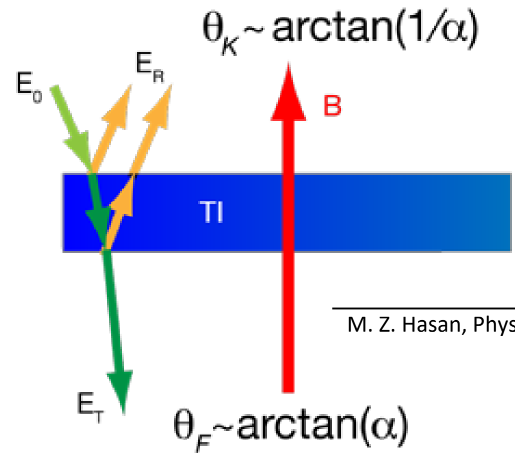


A. L. Levy et al., Phys. Rev. B 101, 125102 (2

Universal optical effects in topological insulators

Thin layer of a topological insulator:





M. Z. Hasan, Physics 3, 62 (2010)

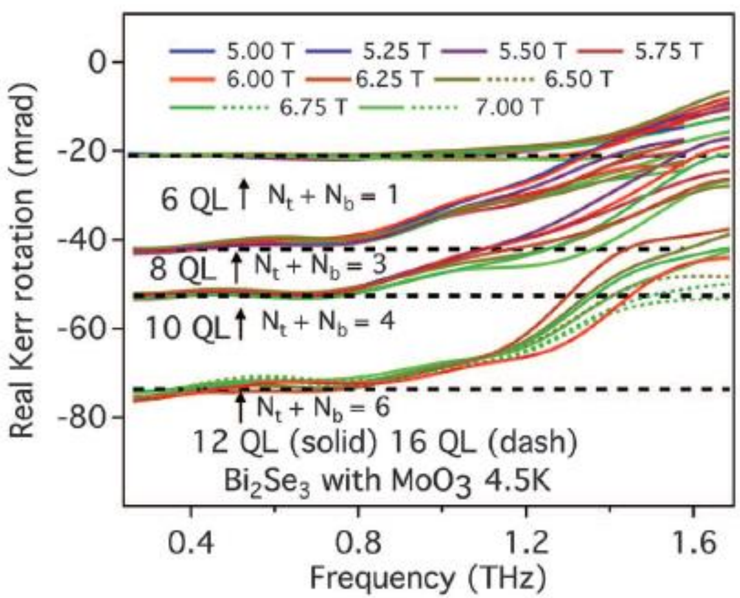
Universal Faraday and Kerr rotations (determined by fine structure constant α only) predicted for topological insulators with broken TR-symmetry

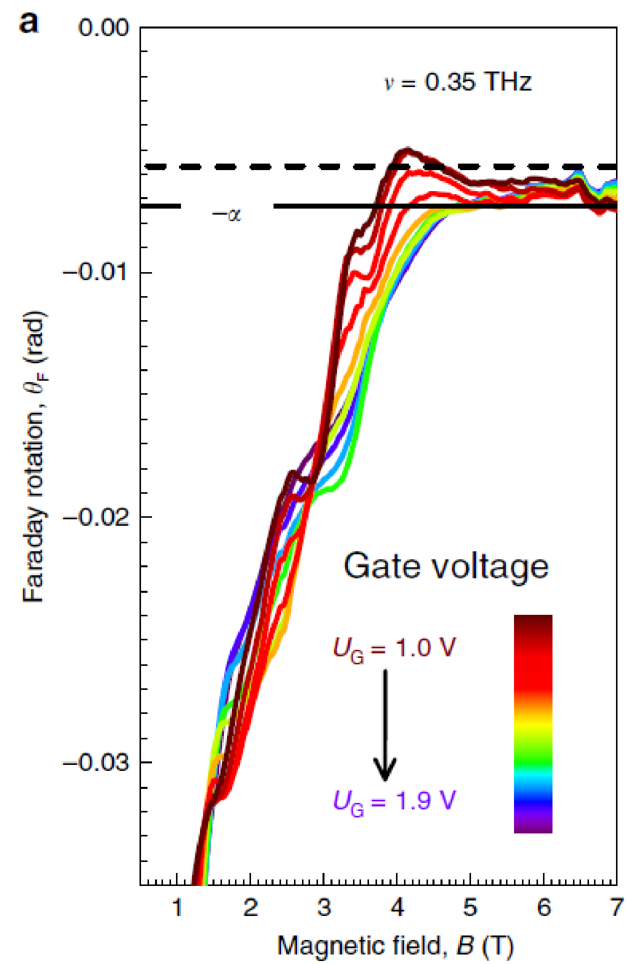
W.-K. Tse and A. H. MacDonald, Phys. Rev. Lett. 105, 057401 (2010)
J. Maciejko et al., Phys. Rev. Lett. 105, 166803 (2010)

Universal magneto-optical effects in topological insulators

Universal Faraday rotation on strained HgTe films (TI regime):

Universal Kerr rotation on thin layers of Bi_2Se_3:

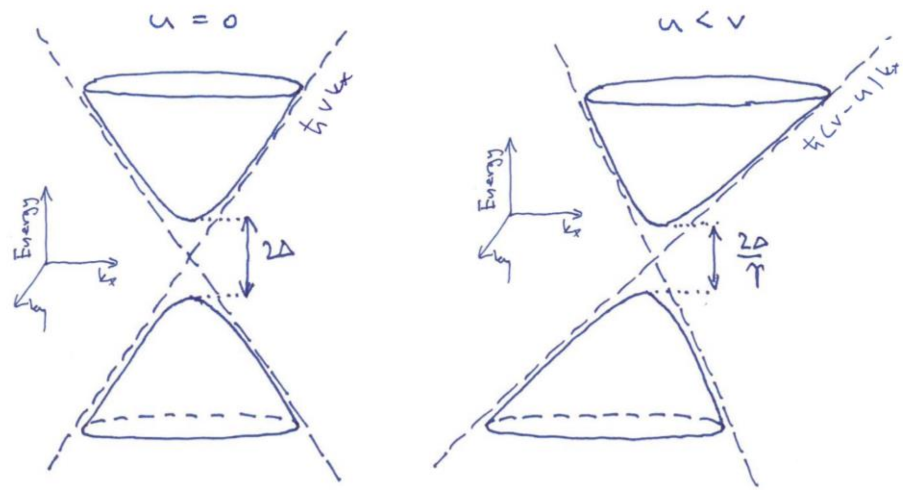




L. Wu et al., Science 354, 1124 (2016)

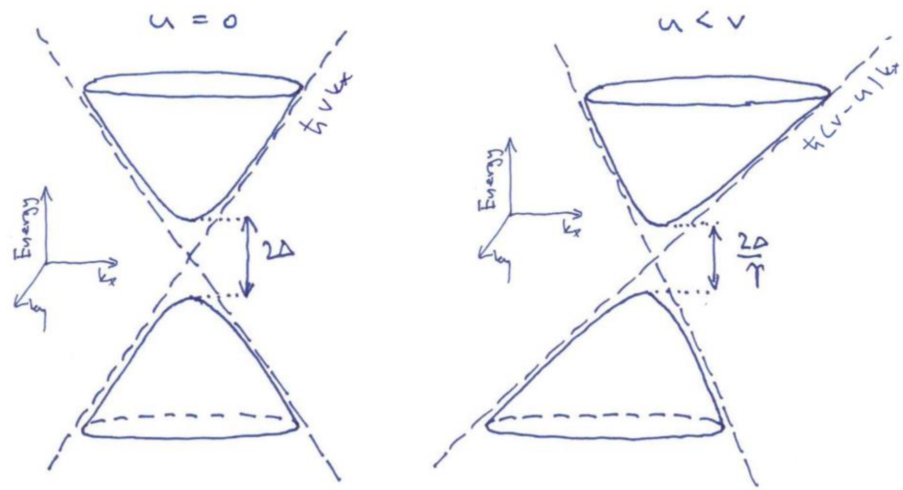
V. Dziom et al. Nat. Commun. 8, 15197 (2017)

Electronic states in gapped & tilted conical band



Gapped & tilted-conical band = indirect-gap semiconductor

Electronic states in gapped & tilted conical band



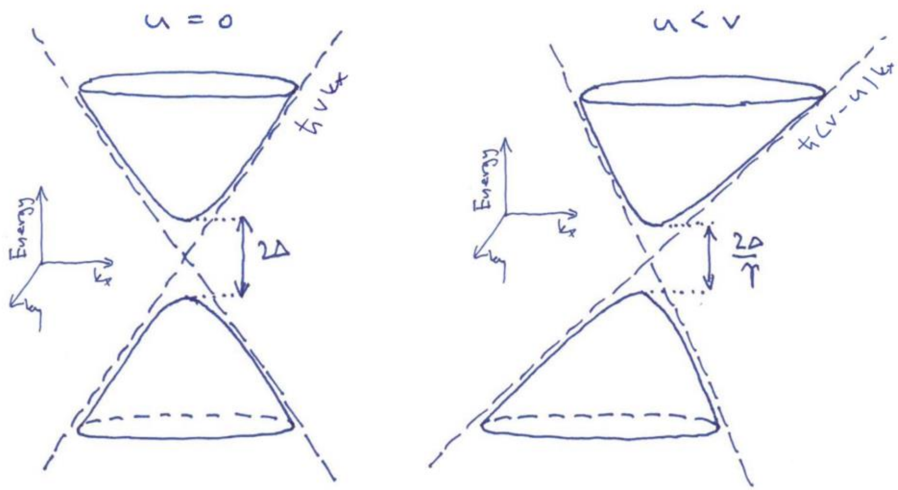
Gapped & tilted-conical band = indirect-gap semiconductor

or

System with massive Dirac electrons in a moving reference frame (velocity u)

see, e.g., M. O. Goerbig et al. Phys. Rev. B 78, 045415 (2008)
or V. Lukose et al. Phys. Rev. Lett. 98, 116802 (2008)
cf. also A. G. Aronov, G. E. Pikus, Sov. Phys.– JETP 24, 339 (1967)

Electronic states in gapped & tilted conical band



Gapped & tilted-conical band = indirect-gap semiconductor

or

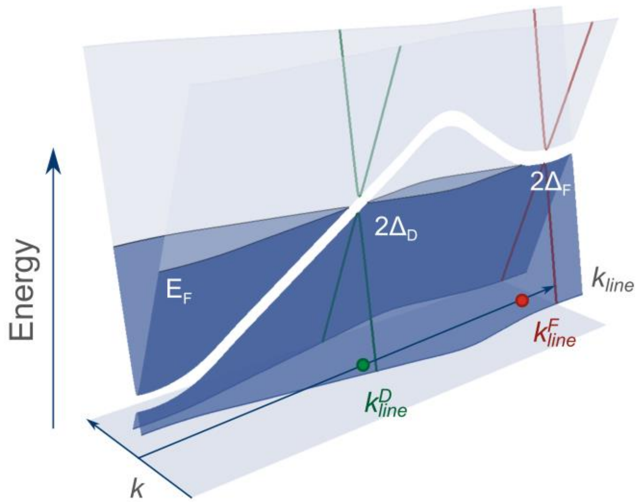
System with massive Dirac electrons in a moving reference frame (velocity u)

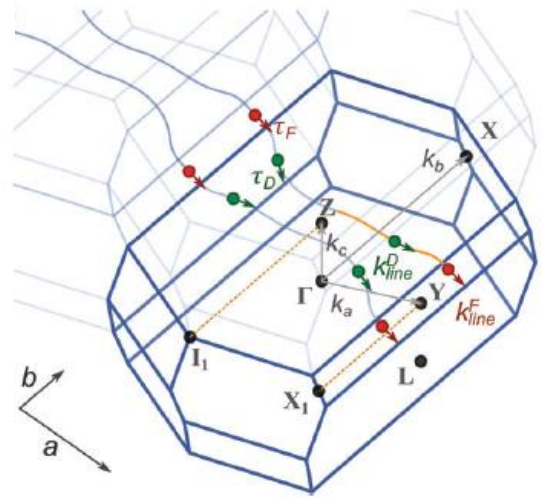
Lorentz-boost-driven renormalization of the energy spectrum

$$2\Delta \rightarrow \frac{2\Delta}{\gamma} \qquad \gamma = \frac{1}{\sqrt{1-\beta^2}} \qquad \beta = \frac{u}{v}$$

NbAs$_2$ Dirac nodal-line semimetal – band structure

Weakly gapped dispersive nodal line in NbAs$_2$:

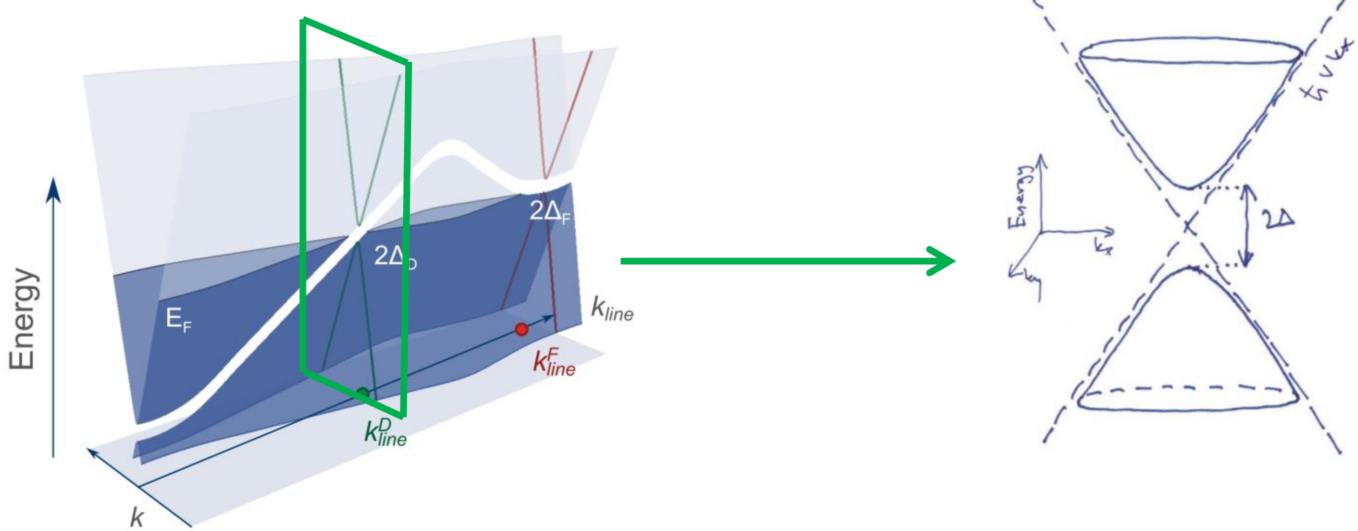




Y. Shao et al., PNAS 116, 1167 (2019)

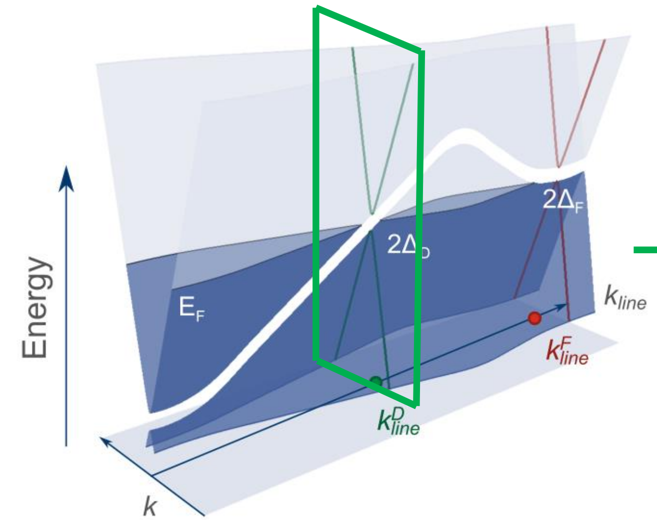
$NbAs_2$ Dirac nodal-line semimetal – band structure

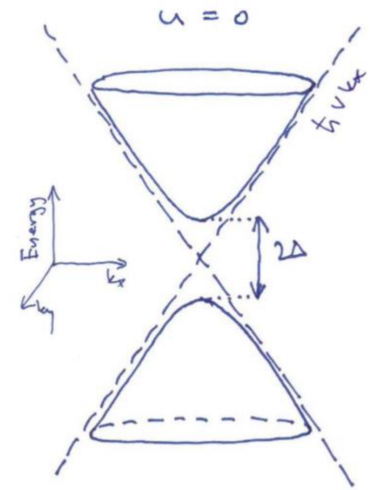
Weakly gapped dispersive nodal line in $NbAs_2$:

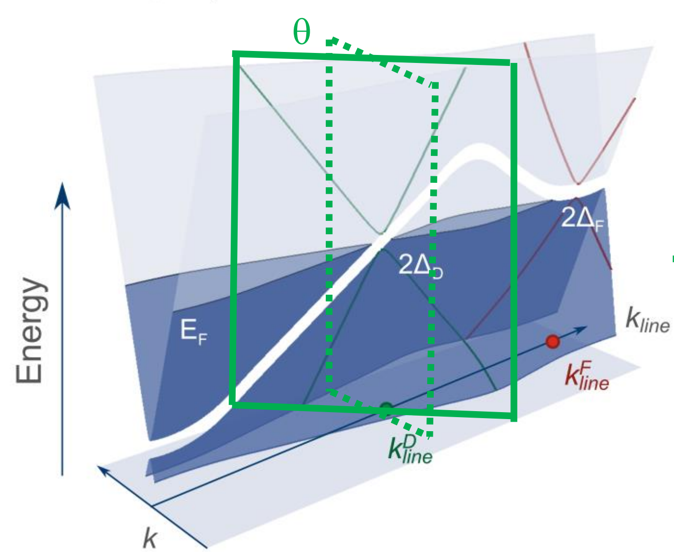


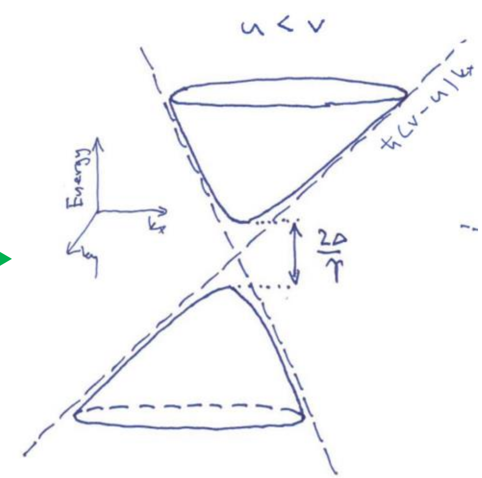
$NbAs_2$ Dirac nodal-line semimetal – band structure

Weakly gapped dispersive nodal line in $NbAs_2$:



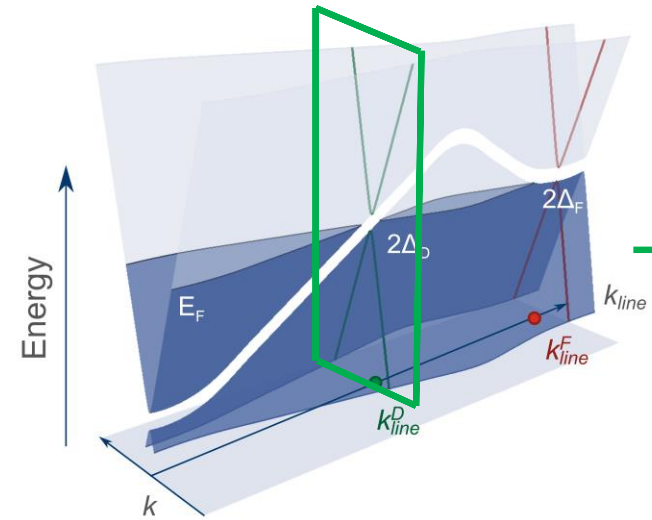


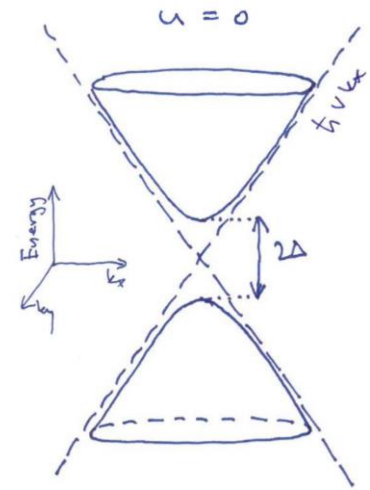


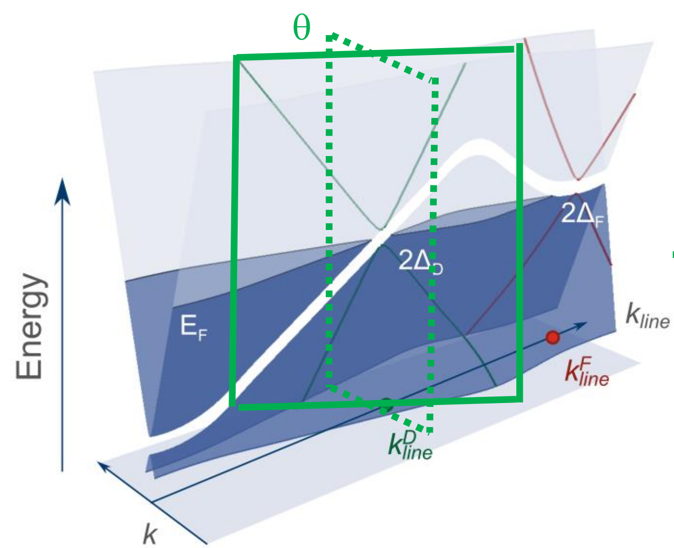


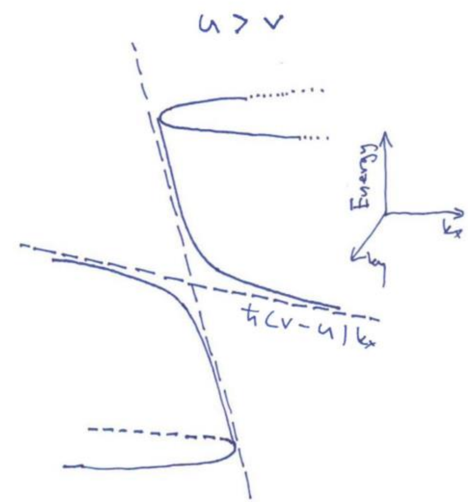
NbAs$_2$ Dirac nodal-line semimetal – band structure

Weakly gapped dispersive nodal line in NbAs$_2$:

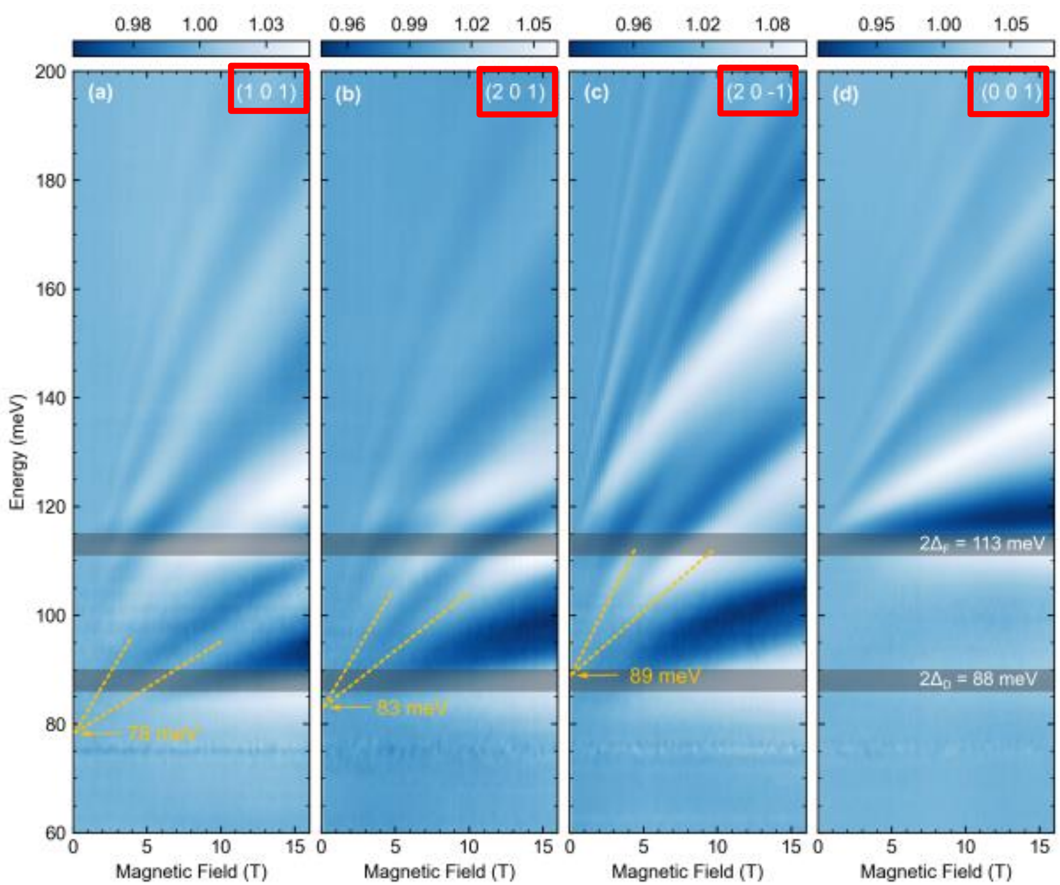




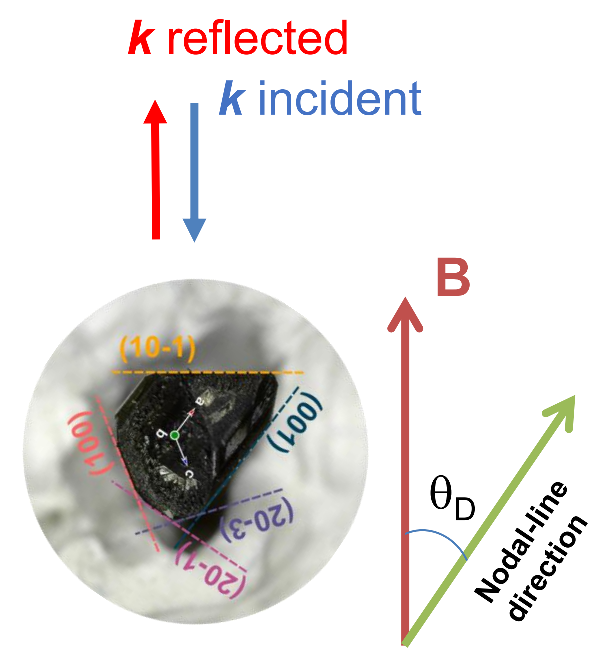




Landau level spectroscopy of $NbAs_2$



Magneto-reflectivity, Faraday configuration, different crystal facets



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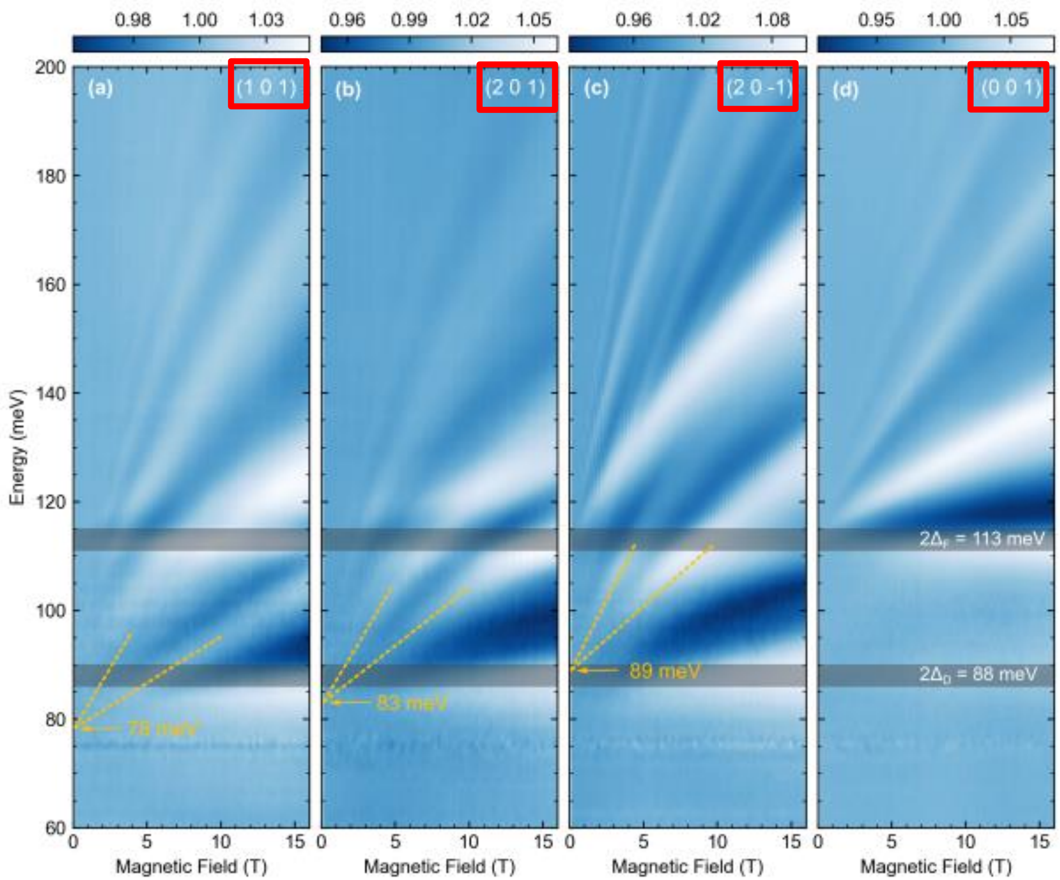
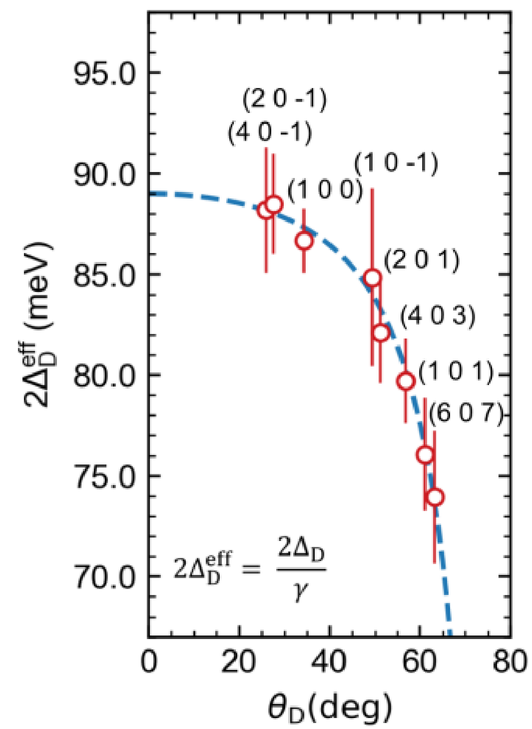
Landau level spectroscopy of $NbAs_2$



Optical band gap renormalized via Lorentz boost

Optical band gap for $NbAs_2$ crystal with various orientation with respect to B:



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Conclusions/Summary

Topological materials ≅ solids with conical bands in bulk or on the surface (…band crossing instead of avoided crossing)

Optical and magneto-optical spectroscopy (in the THz and infrared) is a well-suited experimental method to explore topological materials

Band structure parameters – masses, velocities, gaps; carrier density; scattering mechanisms, relaxation times/mobilities; phenomena due to electron-phonon or electron-electron interaction; appealing “universal” and QED effects