

# Topology, non-collinear spin structures and Skyrmions in Heusler compounds



**Claudia Felser** 

## Co-workers in Dresden and elsewhere





Andrei Bernevig, Princeton, CNR Rao, Bangalore, India Uli Zeitler, et al. HFML - EMFL, Nijmegen; J. Wosnitza et al., HFML Rossendorf Yulin Chen et al., Oxford; Günter Reiss, Bielfeld S.C.Zhang et al. and A. Kapitulnik, Stanford S. S. P. Parkin et al., IBM Almaden, MPI Halle





# Particles – Universe – Condensed matter

### uantum field theory – Berry curvature

**Dirac** Cd<sub>3</sub>As<sub>2</sub> Guido Kreiner



**Higgs** YMnO<sub>3</sub> Lichtenberg Spaldin



**Weyl** TaAs Vicky Süss, Marcus Schmidt

Majorana YPtBi Chandra Shekhar







# Family of quantum Hall effects



2016



Klaus von Klitzing 1998

Horst Ludwig Störmer and Daniel Tsui **2010** 

David Thouless, Duncan Haldane und Michael Kosterlitz

Andre Geim and Konstantin Novoselov



### Anomalous – Hall effect

REVIEWS OF MODERN PHYSICS, VOLUME 82, APRIL-JUNE 2010

#### Anomalous Hall effect

#### Naoto Nagaosa

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Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

(Published 13 May 2010)

The anomalous Hall effect (AHE) occurs in solids with broken time-reversal symmetry, typically i ferromagnetic phase, as a consequence of spin-orbit coupling. Experimental and theoretical studies the AHE are reviewed, focusing on recent developments that have provided a more compl framework for understanding this subtle phenomenon and have, in many instances, replacontroversy by clarity. Synergy between experimental and theoretical works, both playing a crue role, has been at the heart of these advances. On the theoretical front, the adoption of the Berry-ph concepts has established a link between the AHE and the topological nature of the Hall currents. the experimental front, new experimental studies of the AHE in transition metals, transition-me oxides, spinels, pyrochlores, and metallic dilute magnetic semiconductors have established system; trends. These two developments, in concert with first-principles electronic structure calculatic strongly favor the dominance of an intrinsic Berry-phase-related AHE mechanism in meta ferromagnets with moderate conductivity. The intrinsic AHE can be expressed in terms of Berry-phase curvatures and it is therefore an intrinsic quantum-mechanical property of a perf crystal. An extrinsic mechanism, skew scattering from disorder, tends to dominate the AHE in hig conductive ferromagnets. The full modern semiclassical treatment of the AHE is reviewed wh incorporates an anomalous contribution to wave-packet group velocity due to momentum-space Be curvatures and correctly combines the roles of intrinsic and extrinsic (skew-scattering and side-jur scattering-related mechanisms. In addition, more rigorous quantum-mechanical treatments based

Intrinisic Hall

- Berry curvature
- Magnetisation?

### **Extrinsic Hall**

- Skew scattering
- Side jumps



#### Anomalous Nernst and Hall effects in magnetized platinum and palladium

G. Y.  $\operatorname{Guo}^{1, 2, *}$  Q.  $\operatorname{Niu}^{3, 4}$  and N. Nagaosa<sup>5, 6</sup>



## Heusler compounds



**1 + 2 + 5 = 8** 



## Predicting new compounds



# multifunctional topologic insulators

### Magnetism and heavy fermion-like behavior in the RBiPt series

P. C. Canfield, J. D. Thompson, W. P. Beyermann, A. Lacerda, M. F. Hundley, E. Peterson, and Z. Fisk Los Alamos National Laboratory, Los Alamos, New Mexico 87545

Pt

H. R. Ott ETH, Zurich, Switzerland

J. Appl. Phys. 70 (10), 15 November 1991

### Multifunctional properties

- RE: Y, La, Lu, Er, ... superconductivity RE: Gd, Tb, Sm Magnetism and TI
  - Antiferromagnetism with GdPtBi
- RE: Ce
  - complex behaviour of the Fermi surface
- RE: Yb Kondo insulator and TI
  - YbPtBi is a super heavy fermion with the highest γ value



$10 + 3 (+f^n) +$	5 = 18
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## ARPES of LnPtBi

















# Weyl Semimetals Breaking symmtery - TaAs



# Weyl semimetals





3D topological Weyl semimetals - breaking time reversal symmetry – in transport measurement we should see:

1. Intrinsic anomalous Hall effect



2. Chiral anomaly  

$$\partial_{\mu} j^{\mu}_{\chi} = -\chi \frac{e^{3}}{4\pi^{2}\hbar^{2}} \boldsymbol{E} \cdot \boldsymbol{B}$$

$$\sigma_a = \frac{e^3 v_f^3}{4\pi^2 \hbar \mu^2 c} B^2,$$

S. L. Adler, Phys. Rev. 177, 2426 (1969) J. S. Bell and R. Jackiw, Nuovo Cim. A60, 47 (1969) AA Zyuzin, AA Burkov - Physical Review B (2012) AA Burkov, L Balents, PRL 107 12720 (2012)





# Weyl semimetals in non-centro NbP



NbP is a topological Weyl semimetal

NbP, NbAs, TaP, TaAs

- with massless relativistic electrons
- extremely large magnetoresistance of 850,000% at 1.85 K, 9T (250% at room temperature)
- an ultrahigh carrier mobility of 5\*10<sup>6</sup> cm<sup>2</sup> / V s

Shekhar, et al. , Nature Physics 11 (2015) 645, Frank Arnold, et al. Nature Communication 7 (2016) 11615 Weng, et al. Phys. Rev. X 5, 11029 (2015) Huang . et al. preprint arXiv:1501.00755



### NbP and the Fermi surface





d

NbP microribbon

Ti/Pt

00

80

60

40

20

0

-5

0

10

5

15

# **Chiral Anomaly**



of the chiral anomaly the, NMR survives up

to room temperature



# **Gravitational Anomaly**





- Landsteiner, et al. Gravitational anomaly and transport phenomena. Phys. Rev. Lett. 107, 021601 (2011). URL
- Jensen, et al. Thermodynamics, gravitational anomalies and cones. Journal of High Energy Physics 2013, 88 (2013).
- Lucas, A., Davison, R. A. & Sachdev, S. Hydrodynamic theory of thermoelectric transport and negative magnetoresistance in weyl semimetals. PNAS 113, 9463–9468 (2016).

A positive longitudinal magnetothermoelectric conductance (PMTC) in the Weyl semimetal NbP for collinear temperature gradients and magnetic fields that vanishes in the ultra quantum limit.

Johannes Gooth et al. Experimental signatures of the gravitational anomaly in the Weyl semimetal NbP, preprint arXiv:1703.10682



# NbP, TaP, TaAs

Increasing spin orbit coupling increases – heavier elements Distance between the Weyl points increases







# WP<sub>2</sub> protected Weyl







Prediction: G. Autès, et al.; Phys. Rev. Lett. 117 (2016) 066402 Extremely high magnetoresistance and conductivity in the type-II Weyl semimetal WP2, Nitesh, et al.; arXiv:1703.04527



# WP<sub>2</sub> protected Weyl







Prediction: G. Autès, et al.; Phys. Rev. Lett. 117 (2016) 066402 Extremely high magnetoresistance and conductivity in the type-II Weyl semimetal WP2, Nitesh, et al.; arXiv:1703.04527



Magnetotransport in a novel Weyl WP<sub>2</sub>



Prediction: G. Autès, et al.; Phys. Rev. Lett. 117 (2016) 066402 Extremely high magnetoresistance and conductivity in the type-II Weyl semimetal WP2, Nitesh, et al.; arXiv:1703.04527



# Weyl Semimetals Magnetically induced

# multifunctional topologic insulators

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 $10 + 3 (+f^n) + 5 = 18$ 





# Weyl GdPtBi in a magnetic field





# Chiral Anomaly – neg. quadratic MR



Claudia Felser and Binghai Yan, Nature Materials 15 (2016) 1149

M. Hirschberger et al. Nature Mat. online, arXiv:1602.07219, (2016).



# GdPtBi – Anomalous Hall Effect





In Ferromagnets an AHE scales with the magnetic moment Antiferromagnets show no AHE A Hall angle of 0.2 is exceptional high



## Chiral Anomaly – neg. quadratic MR



Claudia Felser and Binghai Yan, Nature Materials 15 (2016) 1149

C. Shekhar et al., arXiv:1604.01641, (2016). M. Hirschberger et al. Nature Mat. online, arXiv:1602.07219, (2016).



# Magnetic Weyl Semimetals



# Materials: ... to half metallic ferromagnets



Kübler *et al.*, PRB **28**, 1745 (1983) de Groot RA, et al. PRL **50** 2024 (1983) Galanakis *et al.*, PRB **66**, 012406 (2002)

Example: Co<sub>2</sub>MnSi

- magic valence electron number: 24
- valence electrons = 24 + magnetic moments  $Co_2MnSi: 2 \times 9 + 7 + 4 = 29$  Ms =  $5\mu_B$





## Weyl semimetals in Heusler compounds

WХ



WΚ





-1

-2

Х



# AHE in half metallic ferromagnets

PHYSICAL REVIEW B 85, 012405 (2012)

#### Berry curvature and the anomalous Hall effect in Heusler compounds



Jürgen Kübler<sup>1,\*</sup> and Claudia Felser<sup>2</sup>

Compound <sup>a</sup>	$N_V$	<i>a</i> (nm)	$M^{exp}$	$M^{calc}$	$\sigma_{xy}$	P (%)
Co <sub>2</sub> VGa	26	0.5779	1.92	1.953	66	65
Co <sub>2</sub> CrAl	27	0.5727	1.7	2.998	438	100
Co <sub>2</sub> VSn	27	0.5960	1.21	1.778	-1489	35
Co <sub>2</sub> MnAl	28	0.5749	4.04	4.045	1800	75
Rh <sub>2</sub> MnAl	28	0.6022		4.066	1500	94
Mn <sub>2</sub> PtSn <sup>b</sup>	28	0.4509 (1.3477)		6.66	1108	91
Co <sub>2</sub> MnSn	29	0.5984	5.08	5.00	118	82
Co <sub>2</sub> MnSi	29	0.5645	4.90	4.98	228	100

The AHE depends only on the Berry curvature in Heusler compounds and not on the magnetic moment



FIG. 4. (Color online) Band structure near the Fermi edge of  $Co_2VSn$ . Majority-spin electron states appear in red, minority-spin states in black. Note the Dirac cone at the  $\Gamma$  point at about -0.22 eV.

Kübler, Felser, PRB 85 (2012) 012405 Vidal et al Appl.Phys.Lett. 99 (2011) 132509 Kübler, Felser, EPL 114 (2016) 47005.



Giant AHE in Co<sub>2</sub>MnAl

 $\sigma_{xy} = 1800 \text{ S/cm}$  calc.  $\sigma_{xy} \approx 2000 \text{ S/cm}$  meas.



Kübler, Felser, PRB 85 (2012) 012405 Vidal et al.; APL 99 (2011) 132509 Kübler, Felser, EPL 114 (2016) 47005.



#### Weyl points are the origin for a large Berry phase and a Giant AHE



## Spin gapless semiconductor Mn<sub>2</sub>CoAl



Wang PRL **100**, 156404 (2008) Ouardi et al., PRL 110 (2013) 100401

# Magnetic Heusler compounds with and without inversion

 $Co_2MnAl$ L2<sub>1</sub> space group 225 (Fm $\overline{3}$ m) Mn<sub>2</sub>CoAl X space group 216 (F43m)









# From Gap to Weyl





# Weyl or Spingapless





# From Gap to Weyl





 $F_z(k_x,k_y,0)$ 





### More semiconductors





# MnP and CuMnAs



First-principles calculations of the magnetic and electronic structures of MnP under pressure

Yuanji Xu<sup>1</sup>, Min Liu<sup>1,2</sup>, Ping Zheng<sup>1</sup>, Xiangrong Chen<sup>2</sup>, Jin-guang Cheng<sup>1</sup>, Jianlin Luo<sup>1,3,4</sup>, Wenhui Xie<sup>5</sup> and Yi-feng Yang<sup>1,3,4,\*</sup>



# Structural distortion



Non-collinear magnetism **Topological Hall effect Skyrmions** 

compensated ferrim. ...

### Phase transitions

- Magn. shape memory ٠
- Magnetocalorics CDW ٠
- **Multiferroics** •

Permanent magnets Antiferromagnets: Mn<sub>3</sub>Ge Ferromagnets: Fe<sub>3</sub>Sn Anomalous Hall effect Spin reorientation transition?



# Hexagonal Antiferromagnet





EPL, **108** (2014) 67001 doi: 10.1209/0295-5075/108/67001 December 2014

www.epljournal.org

### Non-collinear antiferromagnets and the anomalous Hall effect

J.  $\mathrm{K\ddot{U}BLER^1}$  and C.  $\mathrm{FeLSER^2}$ 

PRL 112, 017205 (2014)	PHYSICAL	REVIEW	LETTERS	week ending 10 JANUARY 2014
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#### Anomalous Hall Effect Arising from Noncollinear Antiferromagnetism

Hua Chen, Qian Niu, and A. H. MacDonald



Chen, Niu, and MacDonald, Phys. Rev. Lett., 112 (2014) 017205 Kübler and Felser EPL 108 (2014) 67001



# Non-collinear AFM in metallic Mn<sub>3</sub>Ge





# Non-collinear AFM Mn<sub>3</sub>Ge/Mn<sub>3</sub>Sn



doi:10.1038/nature15723



Large anomalous Hall effect in a non-collinear antiferromagnet at room temperature

Satoru Nakatsuji<sup>1,2</sup>, Naoki Kiyohara<sup>1</sup> & Tomoya Higo<sup>1</sup>



Nayak et al. preprint: arXiv:1511.03128, Science Advances 2 (2016) e1501870 Kiyohara, Nakatsuji, preprint: arXiv:1511.04619,

Nakatsuji, Kiyohara, & Higo, Nature, doi:10.1038/nature15723



## Fermiarcs in the Weyl AFM





# $Mn_3Ir - no AHE$





# Application Spin Hall Effect







Yan Sun et al., Physical Review Letter 117 (2016) 146401





### Anomalous Hall effect





# **Topological Metals**



## Rewriting the text book: Au





# Rewriting the text book: Au



Cs<sup>+</sup>Au<sup>-</sup>

K



## MoP better than Copper





## Fermi surfaces



 $2.7 \times 10^{22} cm^{-3}$ 





Chandra Shekhar et al. arXiv:1703.03736



Charge carriers are mainly from the open Fermi surface

Experimental measurement is around  $3.2 \times 10^{22} \, cm^{-3}$  at 2K

Experiment and calculation have the same order of magnitude



### **Quantum Oscillations**





# Skyrmions Real space Berry curvature



# Mn-Pt-Sn – non collinear





# Real space topology - Skyrmions





# Mn<sub>1.4</sub>Pt<sub>0.9</sub>Pt<sub>0.1</sub>Sn: Anti-Skyrmions





# Tunability of Heusler compounds

- Tuning the band gap
- Tuning spin orbit coupling
  - Trivial and topological Heusler
- Adding spins
  - half metals, magnetic semiconductors
  - Weyl semimetals
- Localized and delocalized spins
- Tuning the magnetic sublattices
  - ferro to ferri: Compensated ferrimagnets
  - Centro and non-centro symmetric Weyl
  - Adding anisotropy
  - lattice distortion via van Hove and Jahn Teller
- In and out of plane magnetization
- Non collinear spin structures and frustration
  - Dzyaloshinskii-Moriya
  - Berry phase in antiferromagnets
  - Skyrmions





# Summary

Is there a relation between reciprocal and real space Berry curvature

Many materials proposed, only a few made

- More Weyl and Dirac semimetals
- More new Fermions
- High quality single crystals, defect free or with defects
- Topological insulators in oxides, correlated systems
- Generalization of the concept Magnetic Fermions Thin films Superconductors – Majorana Chemical reactions Phase transitions

New properties

- Thermal (magneto) transport
- (Magneto) optical properties ...
- Devices

### Applications

- Electronics
- Chemistry (Catalysis) ...





# Single Crystals available

BaCr2As2	AlPt	MoSe2-xTex	Ag2Se	YPtBi	YbMnBi2
BaCrFeAs2	GdAs	MoTe2-xSex	lrO2	NdPtBi	Ni2Mn1.4In0.6
	CoSi	MoTe2 (T´/2H)	OsO2	GdPtBi	YFe4Ge2
CaPd3O4			ReO2	YbPtBi	
SrPd3O4	MoP	PtTe2	WP2	ScPdBi	Mn1.4PtSn
BaBiO3	WP	PtSe2	MoP2	YPdBi	
		PdTe2		ErPdBi	CuMnSb
Bi2Te2Se	TaP	PdSe2	VAI3	GdAuPb	CuMnAs
Bi2Te3	NbP	OsTe2	Mn3Ge	TmAuPb	
Bi2Se3	NbAs	RhTe2	Mn3lr	AuSmPb	Co2Ti0.5V0.5Sn
BiSbTe2S	TaAs	TaTe2	Mn3Rh	AuPrPb	Co2VAl0.5Si0.5
BiTel	NbP-Mo	NbTe7	Mn3Pt	AuNdPb	Co2Ti0.5V0.5Si
BiTeBr	NbP-Cr	WSe2	) n	V .5 St	Mn2CoGa
BiTeCl	TaP-Mo	HfTe5		uLusn	Co2MnGa
	TaAsP	MoTe2		AuYSn	Co2Al9
LaBi, LaSb		TaS2		ErAuSn	Co2MnAl
GdBi, GdSb	CrNb3S6	PdSb2		EuAuBi	Co2VGa0.5Si0.5
	V3S4	CuxWTe2			Co2TiSn
HfSiS	Cd3As2	FexWTe2		CaAgAs	Co2VGa
		WTe2			Co2V0.8Mn0.2Ga
Bi4I4	MnP	Co0.4TaS2		KMgSb	CoFeMnSi
	MnAs	Fe0.4TaS2		KMgBi	
BaSn2		,		KHgSb	
				KHgBi	
				LiZnAs	

LiZnSb