Topological Protectorates of Fermi Surfaces

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Collaborations

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Zoology of Topological Materials



M. G. Vergniory et al., Nature **586** 480 (2020) Y. Xu et al., Nature 586 **702** (2020) P. Narang et al., Nat. Mat. AOP (2020)

Zoology of Topological Materials



the ideal Weyl metal wish list

- single pair of Weyl points
- located at EF (or very close)
- far separated in k-space
- no topologically trivial bands

M. G. Vergniory et al., Nature **586** 480 (2020) Y. Xu et al., Nature 586 **702** (2020) P. Narang et al., Nat. Mat. AOP (2020)



Topological Fermions in Transition Metal Silicides

Multi-fold degeneracies in chiral crystals



Topological Fermions in Transition Metal Silicides



Topological Fermions in Transition Metal Silicides



Peizhe Tang et al., PRL 119 206402 (2017)

ARPES of chiral fermions and long Fermi arcs in CoSi





Sanchez et al., Nature **597** 500 (2019) Zhicheng Rao et al., Nature **597** 496 (2019) ΓΓ ΜΜ Γ Μ



Quantum Oscillations in CoSi



Huan Wang et al., PRB **102** 115129 (2020) D.S. Wu et al., Chin. Phys. Lett. **36** 077102 (2019) Xitong Xu et al., PRB **100** 045104 (2019)

Maximal Chern numbers in PdGa



Schröter et al., Science **369** 179 (2020)



Band sticking in SG198



Single-Weyl point & Nodal planes in PtGa



J.-Z. Ma et al., Nat. Comms. **12** 3994 (2021) Z.-M. Yu et al., PRB **100** 041118 (2019)



non-symmorphic crystals

Table 1 | Some non-symmorphic groups and their ranks,colloquial structure names and representative materials.

d	Name	Examples	Space group	S
2	Shastry-Sutherland	SrCu ₂ (BO ₃) ₂	p4g	2
3	hcp	Be, Mg, Zn	P6 ₃ /mmc	2
3	Diamond	C, Si	FdĪm	2
3	Pyrochlore	Dy ₂ Ti ₂ O ₇ (spin ice)	FdĪm	2
3	-	α -SiO ₂ , GeO ₂	P3 ₁ 21	3
3	-	CrSi ₂	P6 ₂ 22	3
3	-	$Pr_2Si_2O_7, La_2Si_2O_7$	P4 ₁	4
3	Hex. perovskite	CsCuCl ₃	P6 ₁	6

Topological Nodal Surfaces in Acoustic Crystals











Wave vector

 A_5

 A_1

Max

Yihao Yang et al., Nat. Comms. **10** 5185 (2019) Meng Chiao et al., Sci. Adv. **6** eeav2360 (2020)

Quantum Oscillations in Metals

Electron beam in a magnetic field





Physik LK 14 - e/m - Bestimmung / Fadenstrahlrohr (Benno Köhler)



http://www.uranmaschine.de/43200.Fadenstrahlrohr/Fadenstrahlrohr_Aufnahme_11_hires.jpg

Semi-classical electron motion & Landau quantisation



S. Hunklinger (textbook on solid state physics)

Key information contained in quantum oscillations



S. R. Julian, Solid-State Sciences 180, 137 (2015)



Effects of finite temperature

Magnetic Breakdown



Topological Protectorates in CoSi



DFT band structure of CoSi with SOC

Band index	Γ	Μ	R	NP
1	+1	-	-	-1
2	-1	-2	-	+1
3	+3	-	-	-13
4	+1	+2	-4	+13
5	-1	-	-	-5
6	-3	+2	0	+5
7	-3	-	-	-1
8	-1	-2	+4	+1



Generic tight-binding model of SG198



Electronic band structure & fermion-doubling theorem in CoSi

R

-5





SdH Oscillations - Remarks on sample quality



Effect of SOC and NPs on Shubnikov - de Haas branches



scenario proposed by

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 $\tilde{5}$

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D.S. Wu et al., Chin. Phys. Lett. 36 077102 (2019) Xitong Xu et al., PRB 100 045104 (2019)



(a2) no SOC, no NPs



(a3) no SOC, with NPs





Effect of SOC and NPs on Shubnikov - de Haas branches



Huan Wang et al., PRB 102 115129 (2020)



Topological Protectorates in MnSi



Weak Itinerant (Ferro)magnetism in MnSi



Spin Fluctuation Theory

$$T_c = 2.387 c M_0^{3/2} \frac{(\hbar \gamma)^{1/4}}{k_{\rm B}}$$

Property	Experiment	Present model
$\chi^{-1}(T)$	Linear ^(c)	Linear ^(c,d)
$T_c \lesssim T \lesssim 10 T_c$ $T_c(K)$	29.5(5)	31
$P_{\rm eff}/p_0^{(e)}$	5.5(4)	4.7

Lonzarich JMMM **45**, 43 (1984) Lonzarich, Taileffer. J. Phys. Cond. Matter **18**, 4339 (1985)

Landau Quasiparticles

We conclude that a reasonable case exists for describing the quasiparticles in MnSi as magnetic polarons with masses moderately enhanced by a factor of about five above the conventional band calculated masses. The polarisation cloud associated with these polarons is the spin density within the conduction electron sea itself.

Lonzarich JMMM 76, 1 (1988)

Magnetic Phase Diagram of MnSi



Calculated Hall-Effects in Mn_{1-x}Fe_xSi

Fermi surface of MnSi



cf Jeong, Pickett, PRB **70**, 075114 (2004) Wilde, et al., Nature **594**, 374 (2021) DFT calculation (FLEUR, Jülich)

- virtual crystal approximation
- coherent potential approximation

intrinsic anomalous Hall conductivity from Berry curvature

$$\sigma_z = \frac{e^2 \hbar}{4\pi^3} \operatorname{Im} \int_{\mathrm{BZ}} d\mathbf{k} \sum_{n,m}^{o,e} \frac{\langle \psi_{n\mathbf{k}} | v_x | \psi_{m\mathbf{k}} \rangle \langle \psi_{m\mathbf{k}} | v_y | \psi_{n\mathbf{k}} \rangle}{(e_{m\mathbf{k}} - e_{n\mathbf{k}})^2}$$

cf Zhang et al. PRL 106 117202 (2011)

topological Hall resistivity from OHE in emergent magnetic field

$$\sigma_{\mathbf{xy}}^{\mathrm{OHE},s}(B^{\mathbf{z}}) = -\frac{e^{3}B^{\mathbf{z}}}{VN} \sum_{\mathbf{k}n} \tau_{s}^{2} \,\delta(E_{F} - \varepsilon_{\mathbf{k}ns}) \times \\ \times \left[(v_{\mathbf{k}ns}^{\mathbf{x}})^{2} m_{\mathbf{k}ns}^{\mathbf{yy}} - v_{\mathbf{k}ns}^{\mathbf{x}} v_{\mathbf{k}ns}^{\mathbf{y}} m_{\mathbf{k}ns}^{\mathbf{xy}} \right] \\ \rho_{\mathbf{yx}}^{\mathrm{top}}(B^{\mathrm{eff}}) = \frac{\sigma_{\mathbf{xy}}^{\mathrm{OHE},\uparrow}(B^{\mathrm{eff}}) - \sigma_{\mathbf{xy}}^{\mathrm{OHE},\downarrow}(B^{\mathrm{eff}})}{(\sigma_{\mathbf{xx}}^{\uparrow} + \sigma_{\mathbf{xx}}^{\downarrow})^{2}}$$

cf Freimuth et al. PRB 88 214409 (2013)



anomalous and topological Hall effect: large quantitative variation & change of sign

Franz, et al. PRL **112** 186601 (2014) Bauer, et al. PRB **82** 064404 (2010)

see also Chapman et al. PRB 88 214406 (2013)

Comparison of Experiment with Calculation in Mn_{1-x}Fe_xSi



origin of doping-dependence:

(1) consider paramagnetic MnSi(2) doping induced reduction of DOS(3) decrease and change of sign of OHE

Magnetic screw rotations, time-reversal symmetry & magnetic space groups







Assignment of dHvA branches & orbits to calculated Fermi surjace

Branch	Orbit	$f_{exp.}[kT]$	fpred.[kT]	$m^*[m_e]$	$m_b \left[m_e ight]$	$\frac{m^*}{m_b}$	φ [deg]
α	1Γ	0.007	0.068 🗸	0.4±0.1	0.1	4	82.5
β	9ΓR(1)	0.054	- 🗸	0.8±0.1	0.6	1.4	82.5
γ	9ΓR(2)	0.070	- 🗸	2.7±0.3	1.9	1.4	82.5
δ	9ΓR(3)	0.082	- 🗸	2.3±0.6	1.9	1.2	82.5
ϵ	9ΓR(4)	0.095	- >	2.0 ± 0.5	_	-	82.5
ζ	9FR(5)	0.110	- _	2.4 ± 0.4	-	_	82.5
η	9FR(6)	0.141	- \	2.5±0.5	_	_	82.5
μ	9ΓR(7)	0.130	- _	_	1.9	-	152.5
θ	9FR10R(1)	0.225	- \	3.5 ± 0.6	_	_	82.5
ι	9FR10R(2)	0.248	- _	5.4 ± 0.6	_	-	82.5
ĩ	9FR10R(3))	0.290	- _	5.4 ± 0.6	~ 2.0	~ 2.7	82.5
κ_1	2Γ	0.488 \(0.523)	0.369 🗸	6.3 ± 0.6	1.1	6.0	82.5 (106)
<i>к</i> ₂	2ΓY(1)	0.566 \((0.564)	0.371 🗸	6.2±0.1	1.1	5.9	82.5 (106)
К3	2ΓY(2)	0.641	0.411	6.5 ± 0.5	1.2	5.6	106
$2\kappa_1$	$2\kappa_1$	1.065	$2f_{\kappa_1}$	14.2±0.8	2m ₆₁	_	82.5
2 κ ₂	$2\kappa_2$	1.120	$2f_{\kappa_2}$	14.0 ± 0.6	2m	-	82.5
3 <i>κ</i> ₂	$3\kappa_2$	1.610	3f,,,	16±6	3m,	-	82.5
ξ_1	5ΓY(1)	2.459 / (2.576)	2.532 🗡	10.3 ± 0.1	2.0	5.4	82.5 (165)
ξ_2	5ΓY(2)	2.653	_	_	_	_	165
ø'	7U8Ù	2.658	2.765 /	10.0 ± 0.3	2.0	5.0	82.5
π	6ГҮ	2.701 /	2.822 /	11.1±0.3	2.0	5.6	82.5
ρ	ЗГ	2.786	2.891→	10.9 ± 0.4	1.5	7.1	82.5
ρ'	3Г4Г(1)	2.833	2.934→	-	1.5	-	82.5
σ	3Г4Г(2)	2.879	2.976→	11.2 ± 0.4	1.5	7.5	82.5
σ'	3Г4Г(3)	2.918	3.021→	_	-	_	82.5
τ	3Г4Г(4)	2.966	3.019→	10.2 ± 0.4	1.5	6.8	82.5
υ	3Г4Г(5)	3.034 🗸	3.061 🗸	8.7±0.3	1.5	5.9	82.5
υ'	3Г4Г(6)	3.105	3.231→	_	-	_	82.5
φ	3Г4Г(7)	3.229	3.453→	13.2±0.4	_	_	82.5
X'	3Г4Г(8)	3.350	3.583→	_	-	_	82.5
ψ	3Г4Г(9)	3.450	3.715→	11.6 ± 0.6	-	_	82.5
ω	3Г4Г(10)	3.485 /	3.626→	11.6±0.6	-	_	82.5
A	3Г4Г(11)	3.671	3.931→	13.6 ± 0.1	-	_	82.5
В	3Г4Г(12)	3.717	4.017→	13.7 ± 0.3	-	_	82.5
Γ'	3Г4Г(13)	3.840	4.323 /	_	3.2	_	82.5
Δ	3Г4Г(14)	3.940	4.366→	14±1	3.2	4.4	82.5
Ε	3Г4Г(15)	4.040	4.409→	17±4	3.2	5.5	82.5
Ζ	3Г4Г(16)	4.120	4.451→	15±3	3.2	4.7	82.5
H	4Γ [`]	4.180	4.493→	16±5	3.1	5.1	82.5
Θ	7ΓY(1)	4.350	4.569	15±5	4.0	3.8	82.5
$2\xi_1$	$2\xi_1$	4.920	2f., 🔪	24±5	2m.,	_	82.5
ĸ	7ΓY(2)	5.304	5.179	_	4.2	_	85
Λ	7Y (5.304	5.481	_	3.4	_	85
M_1	5U6U	6.715\(6.634)	6.627	15.1±0.2	~2.8	5.4	82.5 (175)
M_2	5U6U	6.587			_	_	175
	8ГҮ	_	6.610 \.	_	4.0	_	_



Key properties of Fermi surface sheets



Extremal orbits and spectroscop







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Momentum dependence of screw-rotation eigenvalues



Berry curvature on a FS in a tight-binding model









Topological surface states on a (010) surface in SG 19.27



^{4.8} [t]	201	17.8 [t	lo er			ith sym	26.67	29.100 Optor	$a^{31.124}$	dal ^{33,145}
36.1 13/	ayı	1 63 (t	ic sh	Jawe Gr	acaquis vv	19.11.1104 .7 3 y 1 1	1931 CE [0] Y		JC 🛛 .186 🖽	
113.268		114.27	'6	169.114 [t]	170.118 [t]	173.130 [t]	178.156 [t]	179.162 [t]	182.180 [t] 185.198
186.204	4.8 [t]	198.10	17.8 [t]	212.60 [T] [t]	213,64 [T] 19.26 [T]	20.32 [t]	26.67	29.100	31.124	33.145
4.0 [4]	36.173	11 54	76.8 [t]	78.20 [t]	90.96 [t]	91.104 [t]	92.112 [T]	94.128 [T]	95.136 [t]	96.144 [T]
4.9 [l]	113.268	311.34	114.276	14.79169.114 [t]	17. HV7001,118 [t]	191.739.1133D [t]	11798.11966.44	179.¥62/[t]]	182.1 90 . [t]	185.19820.00
26.69	186.204	29.101	198.10[I] 29.10 2 12.60 [1]	31.1235.64[1]	31.126	33.146	33.147	36.174	36.175
51.294	1 0 [+]	51.296	11 54	52.310	52.311 17.10 [t]	53.327 18.18.[t]	53.328	54.342	54.344 20 34 [t]	26.68
55.358	4.9 [l]	56.369	20 101	56.3704.79	57.382 ^{10 [1]}	57.383 ^[1]	57.384	¹⁹ 58.897	^{20.34} 58.398	^{20.00} 59.409
59.410	20.09 51 20/	60.422	51 206	$60.423^{9.102}_{52.310}$	60.424	61.436	62.446	54 342	54 344	^{55,357} 63.463
63.464	55 358	64.475	56 369	64.476 _{6 370}	90.98 [1]	90.995[1]	92,114 [T]	58,92,115 [T]	94.130 [T]	59.409 94.131 [t]
96.146 [1	r] _{59,410}	96.147	60.000	113.268 423	113 ₆ 27 <u>1</u> 5[t]	114.237	_f 1 <u>f</u> 4279 [t]	62,127.390	62.44 ¹ 27.393	63.463 128.402
128.405	63.464	129.41	464.475	129.467.476	130 96268 [t]	130. 4 891	<u>9</u> 29,51486	92.135.489	94.13 b301498	94.131 [1]β6.501
137.510	96.146	[11]37.51	3 96.147 [T] 138.5223.269	1381 525 271 [t]	169412157[t]	1117402799tj[t]	1271. 739 0131 [t]	127.3936.147	128.402 78.157 [t]
178.158	[t]28.405	5179.16	31/19.414	179.1 64 9 <mark>.1</mark> 17	1821 89:142 6	18201829[t]	113854899	135.889200	136.4 98 6.205	136.501 86.206
193.258	137.510	⁾ 193.25	9137.513	194.268 ^{8.522}	194. ¹ 289 ⁵²⁵	169.115 [t]	170.119 [t]	173.131 [t]	176.147	178.157 [t]
	178.158	8 [t]	179.163 [1	t] 179.164 [t]	182.181 [t]	182.182 [t]	185.199	185.200	186.205	186.206
3.5 [t]	193.258	3.6 [t]	193.259	4.10 [t] ^{194.268}	194.269 16.4 [t]	16.5 [t]	16.6 [T]	17.11 [t]	17.13 [t]	17.14 [T]
17.15 [T]	3 5 [t]	18.20		18.21 [T] _{0 [t]}	18.22 [T]	18,24 [4]	19,28,[T]	17 19.29 [t]	17 13 0.36 [t]	17 14 [2 1.42 [t]
21.44 [t]	17.15	-25.61	18.20 [t]	25.64 _{18.21} [T]	25.65 22 [T]	26 7 3 _{4 [t]}	199274T1	19 29 .76	20.36 ² [7].82	21.42 [t] 27.85
27.86	21.44 [t	, 28.94	25.61	28.9525.64	28.926.65	28881	2897204	26.278.105	27.8229.109	27.85 30.118
30.119	27.86	30.120	28.94	30.12 2 8.95	31.1228896	31281. 29	2391.11023.3	29 32 5139	29.10332.142	30.118 32.143
33.149	30.119	33.150	30.120	33.15 4 0.122	34. PØ 1 ¹²⁸	3\$.4.6 2 9	341964	32.399169	32.1495.171	^{32.143} 36.178
37.184	33.149	37,186	33.150	75.4 [f] ^{3.154}	75.8 ³⁴ 1 ¹⁶¹	784197	3/47.166 [t]	35. 76 918 [t]	^{35.17} /8.23 [t]	^{36.178} 81.36 [t]
81 38 [t]	37.184	89 92 1	37.186	89 93 [f]. ⁴ [t]	89 92 15 6 [t]		77,16,[1]	⁷⁷ .18 [tho [T]	78.23 ^[1] 110 [T]	81.36 [t] 92 116 [T]
02 117 [+	81.38 [t	00.02	89.92 [t]	89.93 [t]	89.94 [T]	90.100 [T]	90.102 [t]	91.109 [T]	91.110 [T]	92.116 [T] 96 148 [T]
06 1 40 [+	92.117	[t]	93.124 [t]	93.1291.125 [T]	^{93.} 93.126 [T]	³ 94.132 [1]	94.134 [t] ¹	95.141'[†]	95.142 [T] +2 [1]	96.148 [1]
96.149 [[96.149	[t]99.168	99.168	99.1799.170	1001069176	1960.178	101!1884	101.486180	102.192	102.194 02.194
103.200	103.200	103.20	2103.202	104.200	10410410	1405-246	1052488	106.224	106.226	111.256 11.256
111.257	111.257	111.25	8111.258	112.2 64 2.264	11212065265	111212226666	1111332272	113.234274	114.28104.280	114.282 14.282
115.288	115.288	115.29	0115.290	116.2966.296	116.1298298	1 117.7380044	111773906	118.882312	118.3148.314	168.112 [b]B.112 [t]
171.124	[t] ^{71.124}	悼2.12	28 ¹ [72.128 [1	^{t]} 177.154 ⁷ [t] ⁵⁴ [t]	180 ^{,1} 892 ¹ 76 ² [t]	18847788	4831990	¹⁸⁴ 846196	^{195.3} 105.3 [T]	^{207.43} 207.43 [T]
208.47 [1	rj^{208.47}	215.73	215.73	218.84 ^{218.84}						

Table listing all magnetic SGs with symmetry-enforced NPs. The list is grouped into three blocks: 32 SGs with time-reversal symmetry (describing non-magnetic materials), 94 SGs without time-reversal symmetry (describing ferro- or ferrimagnets), and 129 SGs with a symmetry that combines time-reversal symmetry with a translation (describing antiferromagnets). For the NPs to have non-zero topological charge, the SG must be chiral (labelled by '[**T**]'). The 33 SGs labelled by '[**T**]' have NPs whose topological charge is enforced to be non-zero by symmetry, as discussed in Supplementary Note 3.

