

## **TOPOLOGICAL MAGNONS: CASES OF MN<sub>5</sub>GE<sub>3</sub> & CRXTE<sub>3</sub> (X=SI,GE)** Samir Lounis

Solid-state quantum theory



## Acknowledgments

## Experiment: Mn<sub>5</sub>Ge<sub>3</sub>



Karin Schmalzl Jörg Persson Frédéric Bourdarot **Thomas Brückel** 

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## Experiment: CrXTe<sub>3</sub>



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Lichuan Zhang Flaviano J. dos Santos

Theory: CrXTe<sub>3</sub>



Yuriy Mokrousov Stefan Blügel





HORIZON 2020



EPFL











Nicola Marzari Stefan Blügel



UNIVERSITÄT

D U I S B U R G E S S E N

JÜLICH

Forschungszentrum





PSI

### From topological spintronics to topological magnonics







Bosons carrying spin & heat No charge  $\rightarrow$  No Joule heating

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### From topological spintronics to topological magnonics



From topological spintronics to topological magnonics

#### Topology in electronic band structure

Quantum Hall effect

Topology in magnon band structure



## On the search for materials with Dirac magnons

Topological Spin Excitations in Honeycomb Ferromagnet  ${
m CrI}_3$ 

Lebing Chen, Jae-Ho Chung, Bin Gao, Tong Chen, Matthew B. Stone, Alexander I. Kolesnikov, Qingzhen Huang, and Pengcheng Dai

Phys. Rev. X 8, 041028 – Published 14 November 2018









Dirac Magnons, Nodal Lines, and Nodal Plane in Elemental Gadolinium

A. Scheie, Pontus Laurell, P. A. McClarty, G. E. Granroth, M. B. Stone, R. Moessner, and S. E. Nagler Phys. Rev. Lett. **128**, 097201 – Published 2 March 2022



### Common thread: hexagonal lattices



2-spin vector chirality









2-spin vector chirality

#### Holstein-Primakoff transformation from spins to bosons

 $\mathbf{K}'$  $\mathbf{K}$ b) 6 ferromagnetic honeycomb lattice E/JS $\Delta_{\rm so} = 6\sqrt{3}DS$ with zigzag edge 0  $2\pi$  $2\pi$  $4\pi$  $k_r$ 3a3a

. ...

Active component of DMI Component // magnetization of the FM Mook et al. PRB 90, 024412 '14

Kim et al. PRL 117, 227201 '16

a

### Magnon Hall Effect

# **Observation of the Magnon Hall Effect**

Y. Onose,<sup>1,2</sup>\* T. Ideue,<sup>1</sup> H. Katsura,<sup>3</sup> Y. Shiomi,<sup>1,4</sup> N. Nagaosa,<sup>1,4</sup> Y. Tokura<sup>1,2,4</sup>

Science 329, 297 (2010)

 $Lu_2V_2O_7$ 



Theoretical Prediction of a Rotating Magnon Wave Packet in Ferromagnets

Ryo Matsumoto<sup>1</sup> and Shuichi Murakami<sup>1,2,\*</sup>



2-spin vector chirality

#### Holstein-Primakoff transformation from spins to bosons

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## Why to explore $Mn_5Ge_3$ ?

The spatial distribution of magnetisation density in  $Mn_5Ge_3$ 

To cite this article: J B Forsyth and P J Brown 1990 J. Phys.: Condens. Matter 2 2713

$$Mn_1 \sim 2 \mu_B$$
  $Mn_2 \sim 3 \mu_B$   $T_C \sim 300 K$ 



### Ferromagnetic and centrosymmetric? DMI induced physics not interesting?

Dias et al. Nat. Commun. 14, 7321 (2023)

## INS Probe magnons in centrosymmetric ferromagnetic Mn<sub>5</sub>Ge<sub>3</sub>







### Constant-E or constant-q scans





Nikolaos Biniskos



**Manuel dos Santos Dias** 



Flaviano J. dos Santos

## INS Probe magnons in centrosymmetric ferromagnetic Mn<sub>5</sub>Ge<sub>3</sub>









Nikolaos Biniskos



Manuel dos Santos Dias



Flaviano J. dos Santos

 $Mn_1$  form a honeycomb lattice  $Mn_2$  form a hexagonal lattice



Interesting magnonic physics at K-point?

## INS Probe magnons in centrosymmetric ferromagnetic Mn<sub>5</sub>Ge<sub>3</sub>









Nikolaos Biniskos



Manuel dos Santos Dias



Flaviano J. dos Santos

Linear Magnetization Dependence of the Intrinsic Anomalous Hall Effect

Changgan Zeng, Yugui Yao, Qian Niu, and Hanno H. Weitering Phys. Rev. Lett. **96**, 037204 – Published 25 January 2006

► Also large Anomalous Nernst Effect:

Kraft et al, J Appl Phys **128**, 033905 (2020)



# Theoretical tools / Method development / A hierarchy of methods



#### A hierarchy of methods (flavor) JuKKR Tight-binding for AC-transport Interfacing Superconductivity & Magnetism Periodic systems Ultrafast dynamics: Interaction with laser **KKRimp** Supercells Semi-infinite Landau-Lifshitz-SWISS code Disorder Gilbert equation Order (N) Magnons (LLG) to **Complex spin-textures** explore Superconductivity EELS magnetic states KKRnano Isolated defects 🕖 spirit **KKRsusc Real-space S**AiiDA Dynamical response Many-body / correlations Large periodic systems ~thousands of atoms CT-QMC / ED / Transport





[meV]	type	APL 09	This work
<b>J</b> <sub>1</sub>	Mn <sub>1</sub> -Mn <sub>1</sub>	29.1	30.9 / 31.6
<b>J</b> <sub>2</sub>	Mn <sub>1</sub> -Mn <sub>2</sub>	8.0	8.6 / 7.8
<b>J</b> <sub>3</sub>	Mn <sub>2</sub> -Mn <sub>2</sub>	-2.0	-1.3 / -0.2
<b>J</b> 4	Mn <sub>2</sub> -Mn <sub>2</sub>	6.9	6.8 / 6.1
<b>J</b> <sub>5</sub>	Mn <sub>1</sub> -Mn <sub>1</sub>	-1.4	-3.9 / -2.5
<b>J</b> <sub>6</sub>	Mn <sub>2</sub> -Mn <sub>2</sub>	9.4	10.0 / 9.9

 $\mathcal{H} = K \sum_{i} (S_i^z)^2 - \sum_{i,j} J_{ij} \, \mathbf{S}_i \cdot \mathbf{S}_j$ 

APL09: Slipukhina et al. APL 94, 192505 (2009) Dias et al. Nat. Commun. **14**, 7321 (2023)

## DFT calculations for Mn<sub>5</sub>Ge<sub>3</sub>



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<b>J</b> <sub>1</sub>	Mn <sub>1</sub> -Mn <sub>1</sub>	29.1	30.9 / 31.6	
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J <sub>4</sub>	Mn <sub>2</sub> -Mn <sub>2</sub>	6.9	6.8 / 6.1	
<b>J</b> 5	Mn <sub>1</sub> -Mn <sub>1</sub>	-1.4	-3.9 / -2.5	
<b>J</b> <sub>6</sub>	Mn <sub>2</sub> -Mn <sub>2</sub>	9.4	10.0 / 9.9	

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Dias et al. Nat. Commun. 14, 7321 (2023)

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DMI // c		DI	MI	//	С
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*K* ~ 0.1 meV / Mn

$$\mathcal{H} = K \sum_{i} (S_{i}^{z})^{2} - \sum_{i,j} J_{ij} \mathbf{S}_{i} \cdot \mathbf{S}_{j}$$
$$- \sum_{i,j} \mathbf{D}_{ij} \cdot (\mathbf{S}_{i} \times \mathbf{S}_{j})$$

## DFT calculations for Mn<sub>5</sub>Ge<sub>3</sub>

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<b>D</b> <sub>2</sub>	Mn <sub>1</sub> -Mn <sub>2</sub>	—	0.6	
<b>D</b> <sub>3</sub>	Mn <sub>2</sub> -Mn <sub>2</sub>	—	0.5	
DMI //	С	<i>K</i> ~ 0.1 meV / Mn		

$$\begin{aligned} \mathcal{H} &= K \sum_{i} (S_{i}^{z})^{2} - \sum_{i,j} J_{ij} \, \mathbf{S}_{i} \cdot \mathbf{S}_{j} \\ &- \sum_{i,j} \mathbf{D}_{ij} \cdot (\mathbf{S}_{i} \times \mathbf{S}_{j}) \end{aligned}$$



Dias et al. Nat. Commun. 14, 7321 (2023)

## Dzyaloshinskii-Moriya interactions

Dzyaloshinskii, Sov Phys JETP **5**, 1259-1272 (1957)

Moriya, Phys Rev **120**, 2-13 (1960)

$$\mathcal{E} = \int \mathrm{d}\mathbf{r} \ \mathcal{D}_{\alpha} \cdot \left(\mathbf{m}(\mathbf{r}) \times \frac{\partial \mathbf{m}}{\partial r^{\alpha}}\right)$$

micromagnetic

$$\mathcal{E} = \sum_{i,j} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$
  
atomistic

Connection between the two pictures:

$$\mathcal{D}_{\alpha} = \frac{1}{N} \sum_{i,j} \mathbf{D}_{ij} \left( R_{j}^{\alpha} - R_{i}^{\alpha} \right)$$

Inversion symmetry:  $\mathbf{O} \quad \mathcal{D}_{\alpha} = \mathbf{O}$  always

 $D_{ii} = 0$  iff bond has inversion centre  $\bigcirc$ 

## INS measurements on Mn<sub>5</sub>Ge<sub>3</sub>



Dias et al. Nat. Commun. 14, 7321 (2023)

## Comparing experiment with theory



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## The case of CrXTe<sub>3</sub> van der Waals heterostructures



K = 0.01 or 0.02 meV (out of plane)

## Conclusions

- Gap at K point due to Dzyaloshinskii-Moriya interactions
- Mn<sub>5</sub>Ge<sub>3</sub>: gap can be closed by rotating magnetization from *c* to *a*-axis
- Mn<sub>5</sub>Ge<sub>3</sub>: topological magnons at K point due to DMI in 3D ferromagnet
- CrSiTe<sub>3</sub> & CrGeTe<sub>3</sub>: Tunability of topological gap

## Perspectives

- Mn<sub>5</sub>Ge<sub>3</sub>: Modify magnon gap by C doping and thin films towards magnonics
  - Explore other 3D ferromagnets with hexagonal crystal structures
- CrXTe<sub>3</sub>: Explore various X (C, Ge, Pb, and Ga) to tune/control topological magnons

Nat. Commun. 14, 7321 (2023)

Science Adv. 7, eabi7532 (2021)

## Conclusions

- Gap at K point due to Dzyaloshinskii-Moriya interactions
- Mn<sub>5</sub>Ge<sub>3</sub>: gap can be closed by rotating magnetization from *c* to *a*-axis
- Mn<sub>5</sub>Ge<sub>3</sub>: topological magnons at K point due to DW in 3D ferromagnet
- CrSiTe<sub>3</sub> & CrGeTe<sub>3</sub>: Tunability of topological na

## **Perspectives**

- Mn<sub>5</sub>Ge<sub>3</sub>: Modify magnon gap by C doping and thin films towards magnonics
- Explore other 3D ferromagnets with hexagonal crystal structures
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Nat. Commun. 14, 7321 (2023)

Science Adv. 7, eabi7532 (2021)

### WHY CHOSE HEISENBERG-DMI MODEL?



- □ Kitaev angle  $\theta$  are: 57.28° for CrSiTe<sub>3</sub> and 62.26° for CrGeTe<sub>3</sub>, larger than 54.74°.
- □ The fitted Kitaev value is large; large anisotropy energy is needed to ensure the FM ground state.
- □ The magnetic anisotropy is quite small from experimental observation.



### **REFERENCE FROM OTHER WORK**

PRL 124, 087205 (2020)



**Contradicts with Heisenberg-Kitaev model** 

# How different are the different structures?

#### Table 1 | Magnetic exchange interactions in Mn<sub>5</sub>Ge<sub>3</sub> from DFT

		Ref. 29		Experimental structure <sup>24</sup>		DFT structure	
	Туре	Distance (Å)	Value (meV)	Distance (Å)	Value (meV)	Distance (Å)	Value (meV)
J <sub>1</sub>	Mn1-Mn1	2.526	29.1	2.527	30.87	2.485	31.59
J <sub>2</sub>	Mn1-Mn2	3.068	8.0	3.065	8.65	3.021	7.82
J <sub>3</sub>	Mn2-Mn2	2.974	-2.0	2.983	-1.27	3.013	-0.21
J <sub>4</sub>	Mn2-Mn2	3.055	6.9	3.058	6.84	3.033	6.10
J <sub>5</sub>	Mn1-Mn1	4.148	-1.4	4.148	-3.86	4.112	-2.52
J <sub>6</sub>	Mn2-Mn2	4.263	9.4	4.271	9.97	4.276	9.86
<b>D</b> <sub>2</sub>	Mn1-Mn2	-	-	3.065	0.57	3.021	0.59
<b>D</b> <sub>3</sub>	Mn2-Mn2	-	-	2.983	0.50	3.013	0.45

We compare our results using the experimental crystal structure<sup>24</sup> with those of ref. 29, and to our results using the theoretically optimized crystal structure. Positive (negative) values characterize FM (AFM) coupling. The corresponding pairs are indicated in Fig. 1b. The calculated magnetic interactions are long-ranged and only the first few values are given in the table. The listed values are significant to the displayed decimal precision.

# **Comparing experiment with theory**



# **Constructing the simplified model**



# Surface magnons from a simplified model



# **Simulated INS spectra**

