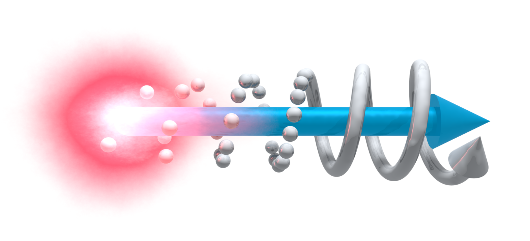
Chiral phonons for spintronics

Universität Konstanz

U. Nowak
University of Konstanz, Germany

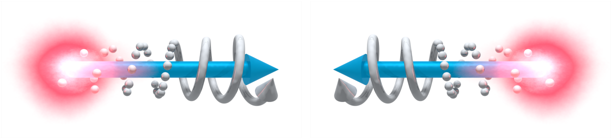
Contents:

- chiral phonons and electronic angular momentum
- modelling spin lattice dynamics



Chirality and phonons

handed chirality

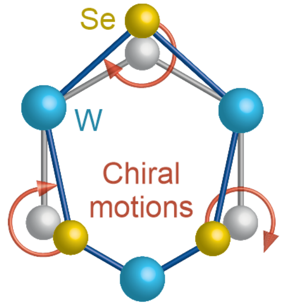


in physics: rotating and moving object

- **circularly polarized in a plane perpendicular to their propagation direction**
  Zhang et al. PRL **115**, *115502 (2015)*
  Juraschek et al., Nature Physics, perspective accepted (2025)

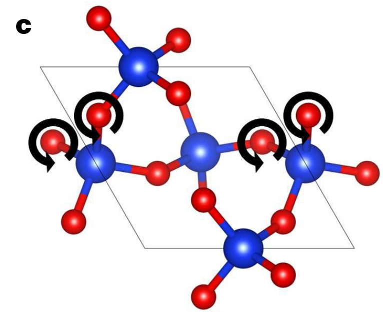
Chiral phonons

- naturally arise in non-centrosymmetric materials:



in monolayer of the dichalcogenide WSe_2

Zhu et al., Science **359**, *579 (2018)*



in the prototypical chiral material quartz

Ueda et al., Nature **618**, *946 (2023)*

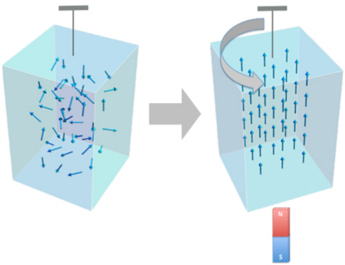
- **phonon angular momentum** leads to a variety of new effects:
  - significant chiral phonon magnetic moment — *Juraschek et al., PRR* 4, *013129 (2022)*; *Luo et al. Science* 382, *698 (2023)*
  - phonon Hall effect — *Grissonnanche et al., Nature Physics* **16**, *1108 (2020)*
  - phonon Faraday effect — *Nova et al., Nature Physics* **13**, *132 (2017)*; *Juraschek et al., PRM* **1**, *014401 (2017)*
  - phonon Zeeman effect — *Baydin et al., Phys. Rev. Lett.* **128**, *075901 (2022)*

Einstein - De Haas effect

- **magnetic moment and angular momentum are connected**

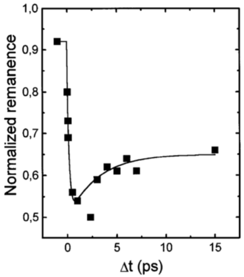
  A. Einstein and W. de Haas, KNAW proceedings, **18 I**, *691 (1915)*

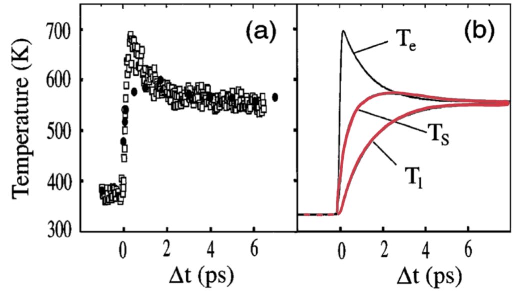
  Barnett, Phys. Rev. **6**, *239 (1915)*



Matsuo et al., Front. Phys. **3:54** *(2015)*

- **on fundamental time and length scales?**





- magnetisation can break down on a time scale of some hundred femtoseconds

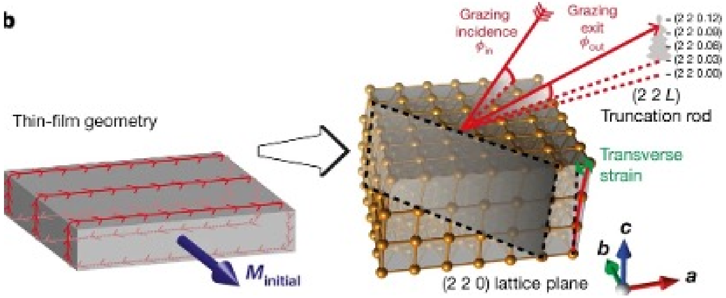
  Beaurepaire et al., PRL **76**, *4250 (1996)*

- phenomenological three-temperature model based on heat
- but: angular momentum conservation violated

Einstein - De Haas effect

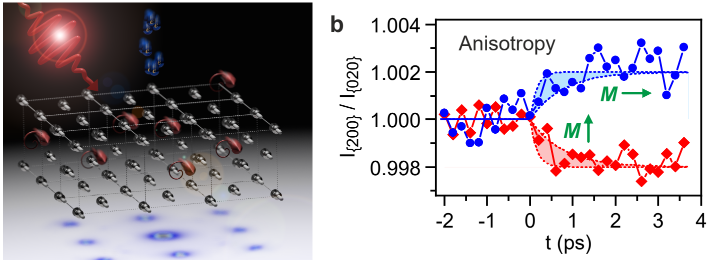
- angular momentum of phonons and the Einstein-de Haas effect
  Zhang et al., PRL **112**, *085503 (2014)*

- **Ultrafast Einstein-de Haas effect:**
  measured as transverse strain waves



Dornes et al., Nature **565**, *209 (2019)*

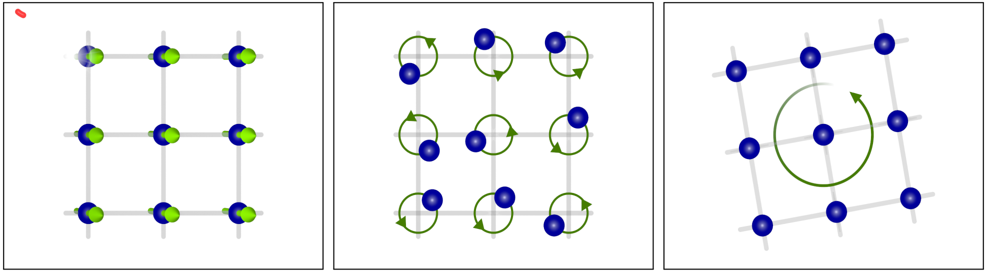
- **Ultrafast circularly polarized phonons:**
  measured via ultrafast electron diffraction



Tauchert et al., Nature **602**, *73 (2022)*

Ultrafast generation of circularly polarized phonons

How can the lattice absorb the spin angular momentum?

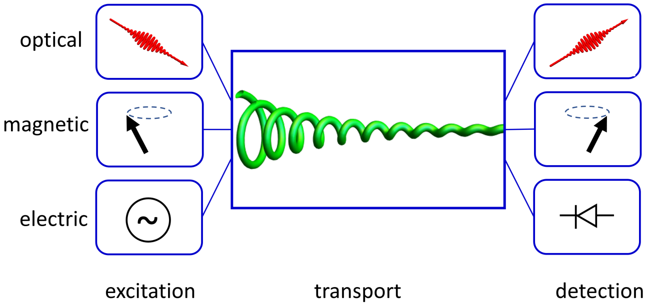


demagnetization   local atomic rotation   Einstein - de Haas

New Research Unit: ChiPS

ChiPS

Funded by German Science Foundation: **Chi**ral **P**honons for **S**pintronics



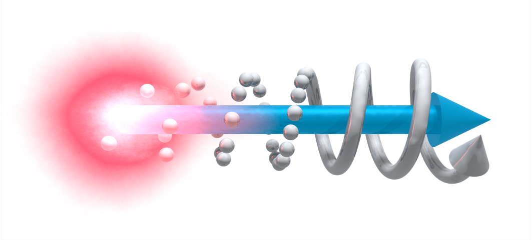
Peter Baum	Visualization of chiral phonons in space and time	Uni Konstanz
Ulrich Nowak	Modeling spin-lattice dynamics	Uni Konstanz
Manfred Albrecht	Advanced magnetic materials for chiral phonons	Uni Augsburg
Sangeeta Sharma	Ab-initio description of chiral-phonon and spin coupling	FU & MBI Berlin
Tobias Kampfrath	Ultrafast propagation and detection of chiral phonons	FU Berlin
Sebastian Goennenwein	Chiral phonon pumping	Uni Konstanz
Silvia Viola Kusminskiy	Angular momentum transduction between magnons and phonons in patterned microstructures	RWTH Aachen
Hans Huebl	Tayloring phonon angular momentum transport	WMI Garching

- fundamental **length and time scales** of chiral phonons
- mechanisms behind **creation, detection and decay** of chiral phonons
- chiral **transport phenomena**
- chiral phonon **hybridization with other excitations**
- exploit **magnon-phonon interaction** in tailored nanostructures
- assess potential of **phonon-based spintronics**

Chiral phonons for spintronics

D. Schick, L. Borysenko, T. Dannegger, U. Nowak
University of Konstanz, Germany

In collaboration with:
M. Weißenhofer, Ph. Rieger, P. Oppeneer, Uppsala University
S. Mankovsky, S. Polesya, H. Ebert, LMU München
A. Kamra, RPTU Kaiserslautern
L. Rosza, L. Szunyogh, Wigner Institute and BUTE Budapest

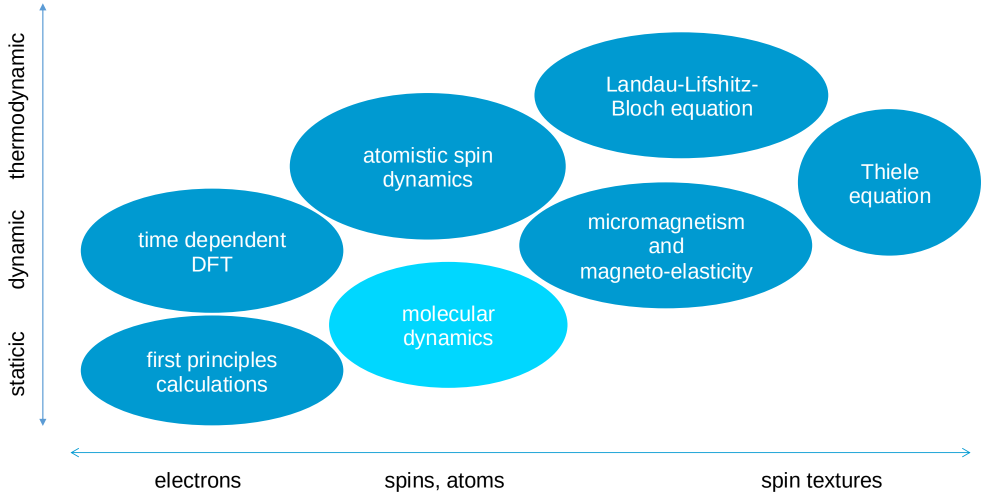


Contents:

- chiral phonons and electronic angular momentum
- **modelling spin lattice dynamics**

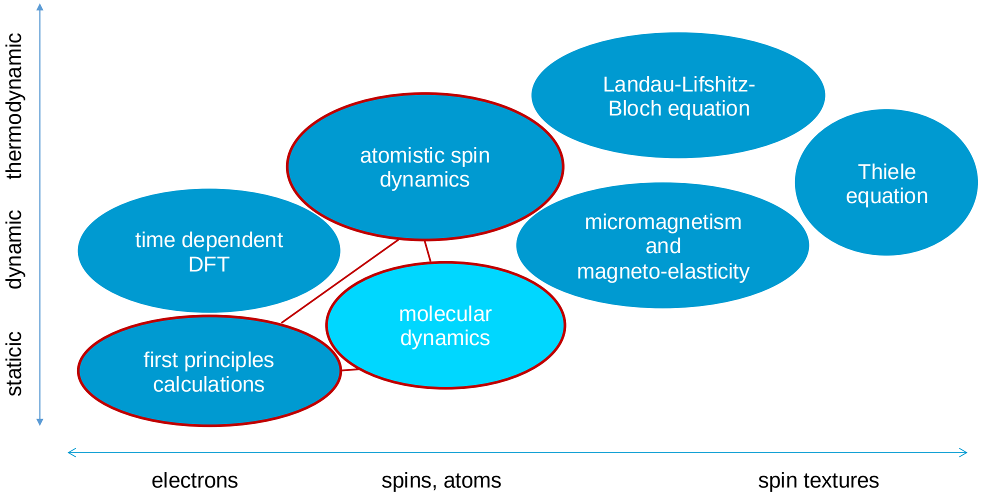
Multi-scale modelling in magnetism

- time scales from femtoseconds to years
- length scales from electronic to sample size
- temperatures from zero to above Curie temperature
- opto-magnetic effects, charge currents, laser heating



Multi-scale modelling in magnetism

- time scales from femtoseconds to years
- length scales from electronic to sample size
- temperatures from zero to above Curie temperature
- opto-magnetic effects, charge currents, laser heating



Atomistic spin model

- Hamiltonian for spins $\underline{S}_i = \underline{\mu}_i/\mu_s$ on a given lattice:

spin model including relativistic interactions

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} \boldsymbol{S}_i \mathrm{J}_{ij} \boldsymbol{S}_j - \sum_i d_i^z (S_i^z)^2 - \boldsymbol{B}\cdot\sum_i \mu_i \boldsymbol{S}_i - \sum_{i,j} \frac{\mu_0 \mu_i \mu_j}{8\pi} \frac{3(\boldsymbol{S}_i\cdot\boldsymbol{e}_{ij})(\boldsymbol{e}_{ij}\cdot\boldsymbol{S}_j) - \boldsymbol{S}_i\cdot\boldsymbol{S}_j}{r_{ij}^3}$$

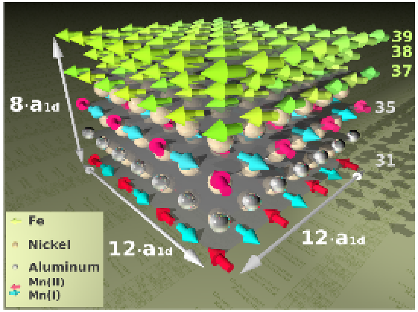
exchange anisotropy external field dipole-dipole

- **tensorial exchange interactions** J_{ij} can be decomposed in:

$$\mathcal{H}_{\mathrm{ex}} = -\frac{1}{2}\sum_{i,j} J_{ij}^{\mathrm{iso}} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \quad -\frac{1}{2}\sum_{i,j} \boldsymbol{S}_i \mathrm{J}_{ij}^{\mathrm{S}} \boldsymbol{S}_j \quad -\frac{1}{2}\sum_{i,j} \boldsymbol{D}_{ij}\cdot(\boldsymbol{S}_i \times \boldsymbol{S}_j)$$

isotropic exchange two-site anisotropy Dzyaloshynskii-Moriya

- different types of **anisotropies** ...
- **dipole-dipole interaction** leads to:
  - shape anisotropy
  - domain structures
  - large numerical effort



Yanes et al., PRB **96**, *064435 (2017)*

Spin model parameters from first principles

- exchange integrals, isotropic but **orbital resolved**

  Liechtenstein et al., JMMM ***67****, 65 (1987)*

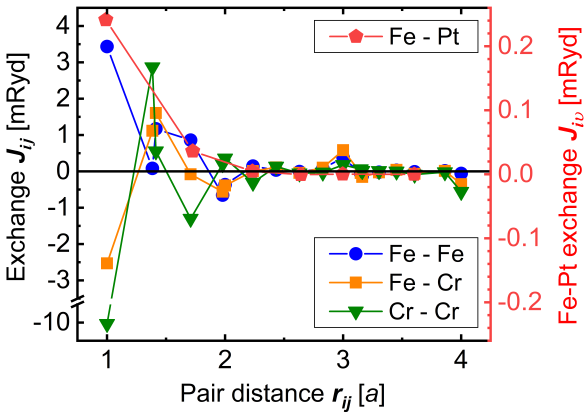
- fully **relativistic** SKKR method plus **spin cluster expansion** for layered systems and clusters

  Szunyogh et al., PRB ***83****, 024401 (2011)*

- calculations of **opto-magnetic effects** such as IFE

  Berritta et al., PRL ***117****, 137203 (2016)*

  John et al., Scientific Reports ***7****, 4114 (2017)*



Schmidt et al., PRB ***102****, 214436 (2020)*

Gd	orbital-resolved dynamics	*Frietsch et al., Nature Com.* ***6*** *8262 (2015)*
Tb	orbital-resolved dynamics	*Frietsch et al., Science Advances,* ***6****, eabb1601 (2020)*
CrPt	switching with IFE in an AFM	*Dannegger et al., Phys. Rev. B Lett.****104****, 060413 (2021)*
Hematite	altermagnet	*Dannegger et al., Phys. Rev. B* ***107****, 184426 (2023)*

Atomistic spin dynamics

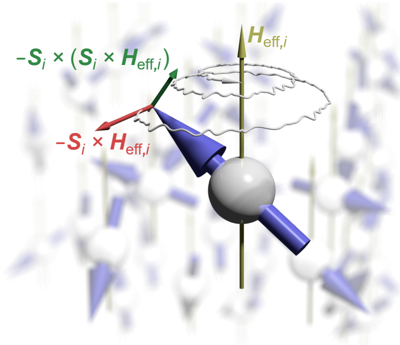
stochastic Landau-Lifshitz-Gilbert equation

$$\dot{\mathbf{S}}_i = -\frac{\gamma}{(1+\alpha^2)\mu_s}\,\mathbf{S}_i \times \mathbf{H}_i(t)$$ precession

$$-\frac{\alpha\gamma}{(1+\alpha^2)\mu_s}\,\mathbf{S}_i \times \left(\mathbf{S}_i \times \mathbf{H}_i(t)\right)$$ dissipation

with $\mathbf{H}_i(t) = -\frac{\partial \mathcal{H}}{\partial \mathbf{S}_i} + \boldsymbol{\zeta}_i(t)$ fluctuations

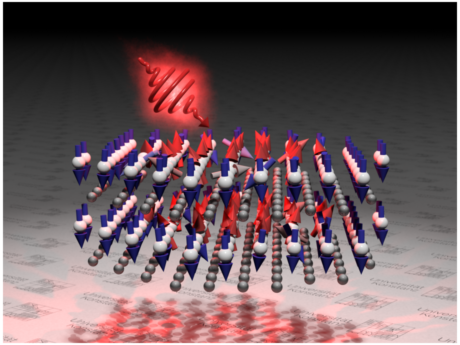
and $\langle \zeta_{i\eta}(0)\zeta_{j\vartheta}(t)\rangle = \delta_{ij}\delta_{\eta\vartheta}\delta(t)2\alpha k_{\mathrm{B}} T \mu_s/\gamma$.



- **numerical integration** for up to 10^8 spins
  Lyberatos et al., J. Phys. C **5**, *8911 (1993)*
- statistical average in the **canonical ensemble**

☺ realistic dispersion relations; non-linear prozesses; critical behavior; fluctuations

☹ electrons and phonons only as heat-bath with coupling constant α; classical approximation; large numerical effort



Spin-lattice dynamics

Hamiltonian for spin and lattice degrees of freedom

$$\mathcal{H}(\boldsymbol{S},\boldsymbol{r},\boldsymbol{p}) = \underbrace{\sum_{i,j} J(\boldsymbol{S}_i,\boldsymbol{S}_j)}_{\text{spin}} + \underbrace{\mathcal{H}_{sl}(\boldsymbol{S}_i,\boldsymbol{r}_i)}_{\text{spin-lattice}} + \underbrace{\sum_i \frac{\boldsymbol{p}_i^2}{2m_i} + \sum_{i,j} V(\boldsymbol{r}_{ij})}_{\text{lattice}}$$

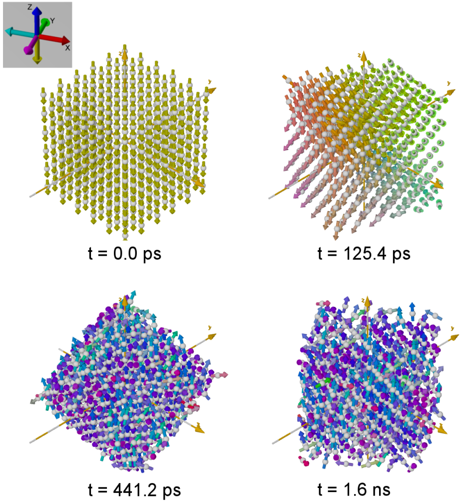
equations of motion

$$\dot{\boldsymbol{r}}_i = \frac{\partial \mathcal{H}}{\partial \boldsymbol{p}_i}, \quad \dot{\boldsymbol{p}}_i = -\frac{\partial \mathcal{H}}{\partial \boldsymbol{r}_i}, \quad \dot{\boldsymbol{S}}_i = \frac{\gamma}{\mu_s}\boldsymbol{S}_i \times \frac{\partial \mathcal{H}}{\partial \boldsymbol{S}_i}$$

Strungaru et al., PRB **103**, *024429 (2021)*

Hellsvik et al., PRB **99**, *104302 (2019)*

- **no heat bath** → microcanonic ensemble
- **open problems**:
  - calculation of spin-lattice coupling parameters from first-principles
  - correct expressions for spin-lattice coupling
  - conservation of energy, momentum, angular momentum



Aßmann et al, JMMM **469**, *217 (2019)*

Spin-lattice coupling from first principles

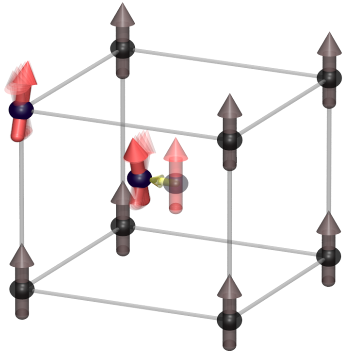
expansion of relativistic Heisenberg Hamiltonian in terms of displacements $\boldsymbol{u}_i = \boldsymbol{r}_i - \boldsymbol{r}_i^{\mathrm{eq}}$

spin-lattice Hamiltonian

$$\mathcal{H}^{\mathrm{SLC}} = \sum_{ij,\alpha\beta} J_{ij}^{\alpha\beta}(\boldsymbol{r}_k) S_i^\alpha S_j^\beta = \underbrace{\sum_{ij,\alpha\beta} J_{ij}^{\alpha\beta}(\boldsymbol{r}^{\mathrm{eq}}) S_i^\alpha S_j^\beta}_{\text{spin}-\text{spin interactions}} + \underbrace{\sum_{ijk,\alpha\beta\mu} J_{ijk}^{\alpha\beta\mu}(\boldsymbol{r}^{\mathrm{eq}}) S_i^\alpha S_j^\beta u_k^\mu}_{\text{spin}-\text{spin}-\text{lattice interactions}} + \ldots$$

spin-lattice coupling tensors $J_{ijk}^{\alpha\beta\mu}$ can be calculated via:

- super cell method
  Hellsvik et al., PRB **99**, *104302 (2019)*
- extension of Liechtenstein formula
  Mankovsky et al., PRL **129**, *067202 (2022)*
- embedded cluster method
  Lange et al., PRB **107**, *115176 (2023)*

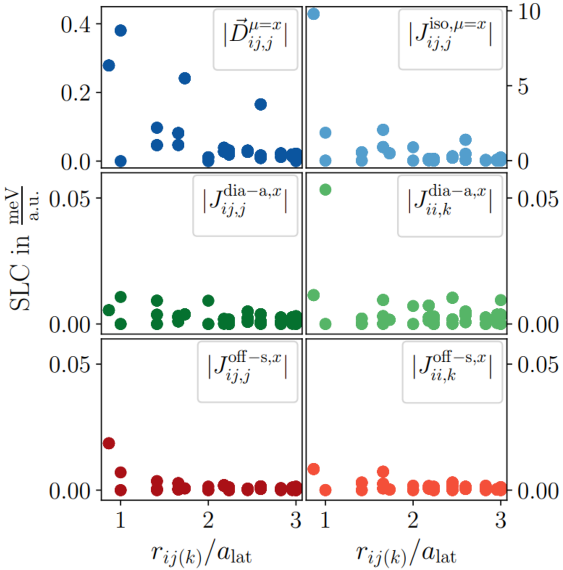


Spin-lattice coupling parameters for bcc iron from first principles

spin-lattice Hamiltonian

$$\mathcal{H}_{sl} = \sum_{i,j,\alpha,\beta} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta + \sum_{i,j,\alpha,\beta} \sum_{k,\mu} J_{ij,k}^{\alpha\beta,\mu} S_i^\alpha S_j^\beta u_k^\mu + \sum_{i,j,\alpha,\beta} \sum_{k,l,\mu,\nu} J_{ij,kl}^{\alpha\beta,\mu\nu} S_i^\alpha S_j^\beta u_k^\mu u_l^\nu$$

- example: **bcc Fe**
- fully-relativistic scheme treats changes of spin configuration and atomic positions equally
- even in inversion symmetric lattice leading term for angular momentum transfer is **DMI-type interaction**
- **beyond magneto-elastic theory**



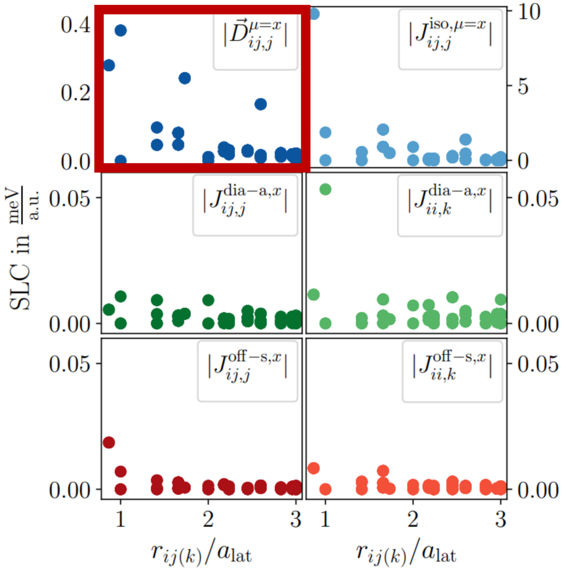
Mankovsky et al., PRL **129**, *067202 (2022)*

Spin-lattice coupling parameters for bcc iron from first principles

spin-lattice Hamiltonian

$$\mathcal{H}_{sl} = \sum_{i,j,\alpha,\beta} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta + \sum_{i,j,\alpha,\beta} \sum_{k,\mu} J_{ij,k}^{\alpha\beta,\mu} S_i^\alpha S_j^\beta u_k^\mu + \sum_{i,j,\alpha,\beta} \sum_{k,l,\mu,\nu} J_{ij,kl}^{\alpha\beta,\mu\nu} S_i^\alpha S_j^\beta u_k^\mu u_l^\nu$$

- example: **bcc Fe**
- fully-relativistic scheme treats changes of spin configuration and atomic positions equally
- even in inversion symmetric lattice leading term for angular momentum transfer is **DMI-type interaction**
- **beyond magneto-elastic theory**



Mankovsky et al., PRL ***129****, 067202 (2022)*

Towards combined spin-lattice dynamics

Full spin-lattice Hamiltonian

$$\mathcal{H} = \sum_{ij,\alpha\beta} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta + \sum_{ijk,\alpha\beta\mu} J_{ijk}^{\alpha\beta\mu} S_i^\alpha S_j^\beta u_k^\mu + \sum_i \frac{\boldsymbol{p}_i^2}{2m_i} + \sum_{ij} V(\boldsymbol{r}_{ij})$$

resulting equations of motion:

$$\dot{\boldsymbol{S}}_i = \frac{\gamma}{\mu_\mathrm{s}} \boldsymbol{S}_i \times \frac{\partial \mathcal{H}}{\partial \boldsymbol{S}_i} = -\frac{\gamma}{\mu_\mathrm{s}} \boldsymbol{S}_i \times \left(\boldsymbol{H}_i^{\mathrm{SS}} + \boldsymbol{H}_i^{\mathrm{SLC}} \right)$$

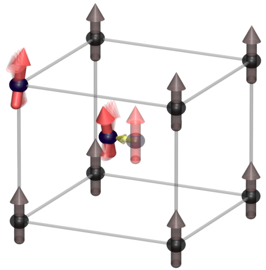
$$\dot{\boldsymbol{r}}_i = \frac{\boldsymbol{p}_i}{m_i}$$

$$\dot{\boldsymbol{p}}_i = -\frac{\partial \mathcal{H}}{\partial \boldsymbol{r}_i} = \boldsymbol{F}_i^{\mathrm{lattice}} + \boldsymbol{F}_i^{\mathrm{SLC}}$$

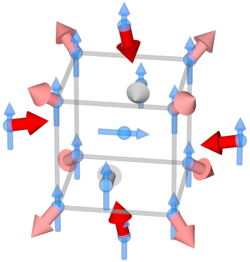
- spin lattice coupling breaks rotational symmetry

⇒ **total angular momentum not conserved!**
(see also *Melcher, PRL* **25**, *1201 (1970)* for corresponding magneto-elastic theory)

- what about the chiral phonon magnetic moment?
  $\boldsymbol{S}_i \cdot (\boldsymbol{u}_i \times \boldsymbol{p}_i)$



SLC-fields



SLC-forces

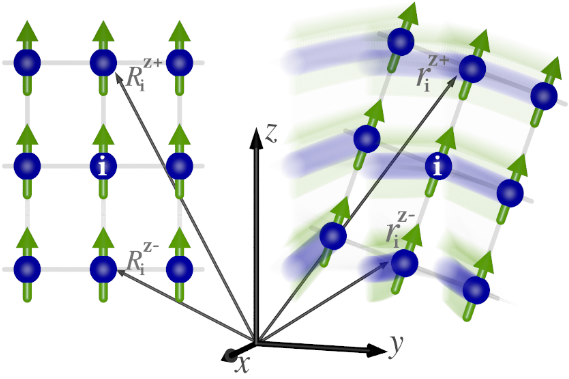
Angular momentum conserving formulation of spin-lattice dynamics

replacing components of spins and displacements with **projection onto local lattice orientation**

$$\boldsymbol{e}_i^\alpha = \frac{\boldsymbol{r}_i^{\alpha+} - \boldsymbol{r}_i^{\alpha-}}{|\boldsymbol{r}_i^{\alpha+} - \boldsymbol{r}_i^{\alpha-}|}$$

Resulting spin-lattice Hamiltonian

$$\mathcal{H} = \sum_{ij,\alpha\beta} J_{ij}^{\alpha\beta}(\boldsymbol{S}_i \cdot \boldsymbol{e}_i^\alpha)(\boldsymbol{S}_j \cdot \boldsymbol{e}_j^\beta) + \sum_{ijk,\alpha\beta\mu} J_{ijk}^{\alpha\beta\mu}(\boldsymbol{S}_i \cdot \boldsymbol{e}_i^\alpha)(\boldsymbol{S}_j \cdot \boldsymbol{e}_j^\beta)(\boldsymbol{u}_k \cdot \boldsymbol{e}_k^\mu) + \sum_i \frac{\boldsymbol{p}_i^2}{2m_i} + \sum_{ij} V(\boldsymbol{r}_{ij})$$



e.g. direction of easy axis is defined by the lattice not via the lab frame

$$d_z \sum_i (S_i^z)^2 \quad \rightarrow \quad d_z \sum_i (\boldsymbol{S}_i \cdot \boldsymbol{e}_i^z)^2$$

- this Hamiltonian is based on difference vectors and scalar products

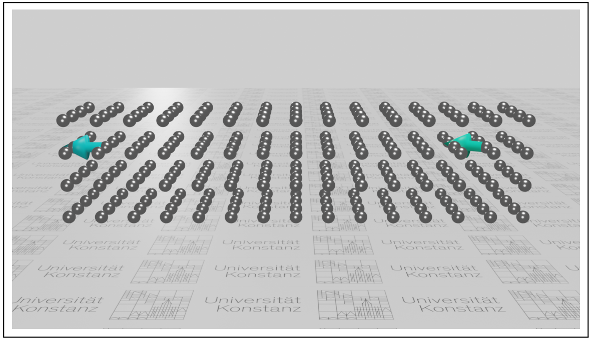
⇒ it is rotational and translational invariant

⇒ **momentum and angular momentum are conserved** in the total system!

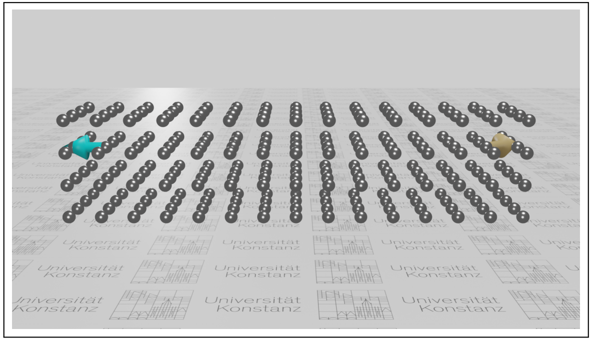
Weißenhofer et al., PRB **108***, L060404 (2023)*

Spin-spin interaction via phonons

2 parallel spins

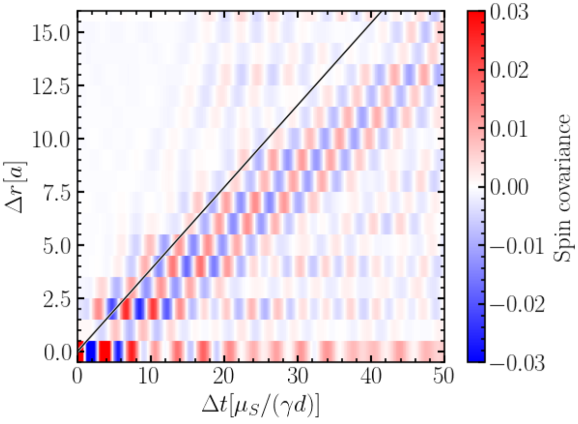


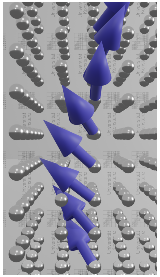
2 antiparallel spins

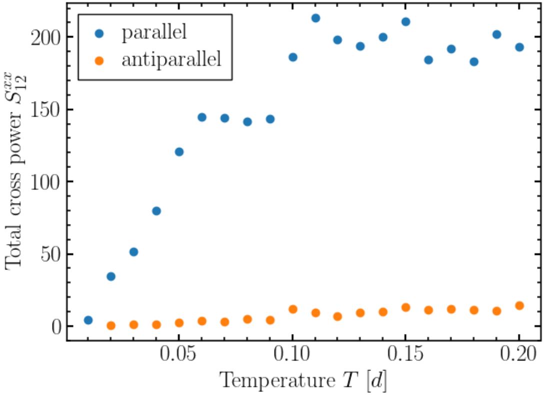


Two parallel and magnetically uncoupled spins in a phonon bath couple via exchange of angular momentum

Spin-spin interaction via phonons







correlation quantified via **cross covariance** of spin components:

$$K_{ij}^{\mu\nu}(\Delta t) = \langle S_i^{\mu}(t+\Delta t) S_j^{\nu}(t)\rangle - \langle S_i^{\mu}\rangle\langle S_j^{\nu}\rangle$$

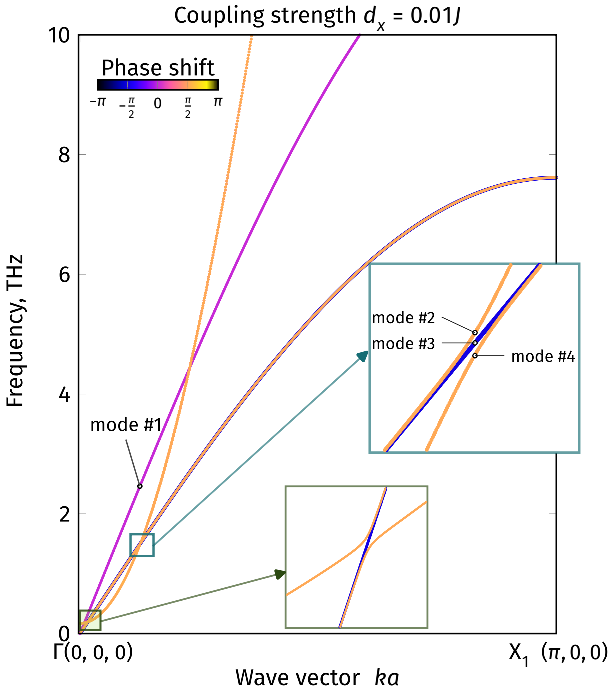
and cross power spectral density (CPSD):

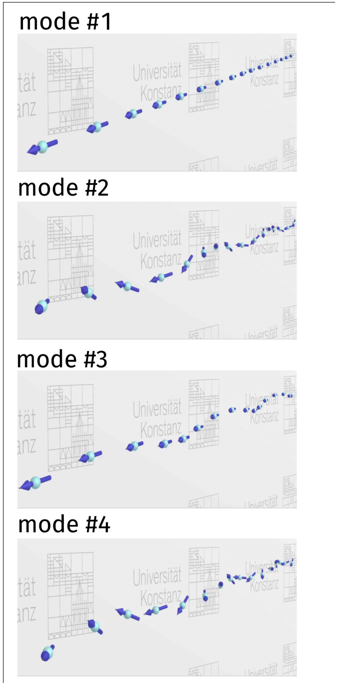
$$P_{ij}^{\mu\nu} = \int_0^{\infty} \left|\tilde{S}_{ij}^{\mu\nu}(f)\right|^2 \, \mathrm{d}f$$

Schick et al., in preparation

see also: Yokoyama, JPSJ ***93****, 123705 (2024)*

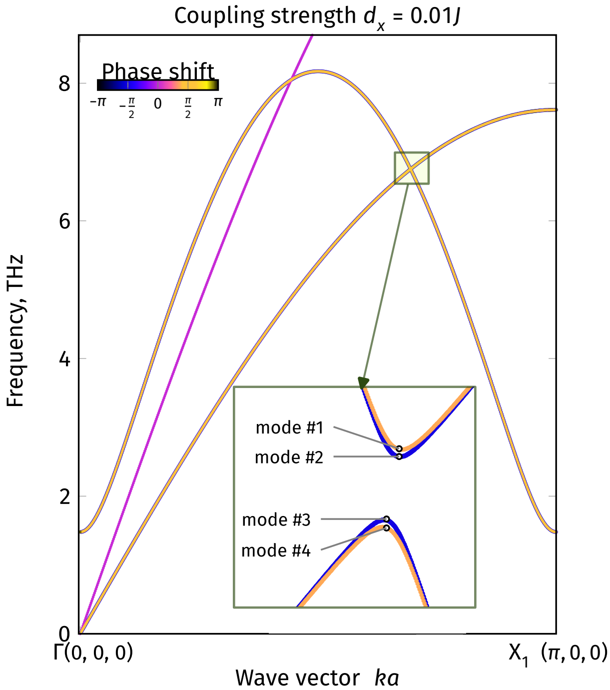
Chirality-selective magnon-phonon dispersion: ferromagnets





- **avoided crossings**, magnon polarons *(Li et al., APL Materials* **9***, 060902 (2021))* *Borysenko et al., in preparation*
- degeneracy lifted: **transverse phonons turn into chiral**, only one of the two chiral phonon modes affected

Chirality-selective magnon-phonon coupling: antiferromagnets

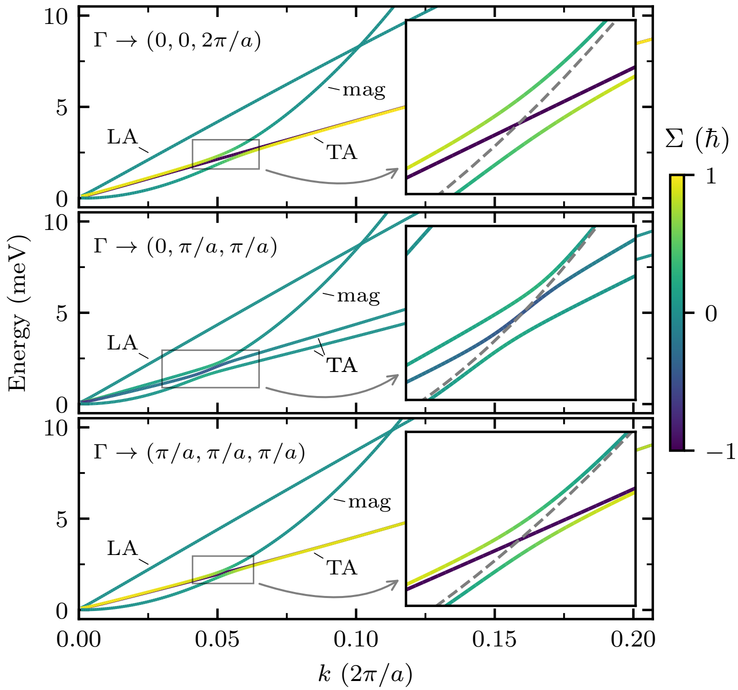


- **avoided crossings**, hybridized quasiparticles
- degeneracy lifted: **both chiral phonon modes affected**

Borysenko et al., in preparation

Chiral phonons from chirality-selective magnon-phonon coupling

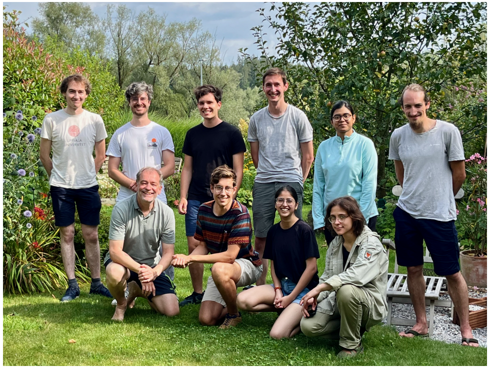
- coupled **magnon-phonon bands in bcc Fe from first principles** via Holstein-Primakoff transformation
- grey dashed lines are the bare magnon energies
- colors encode the phonon chirality
- transverse modes are degenerate for $\Gamma \to (0, 0, 2\pi/a)$ and $\Gamma \to (\pi/a, \pi/a, \pi/a)$
- degeneracy lifted: **only one of the two chiral phonon modes affected**



Weißenhofer et al., arXiv:2411.03879 (2024)

Thanks to . . .

My group in Konstanz:



T. Dannegger, L. Borysenko, H. Devda., M. Kundu, D. Schick, J. Schlegel, D. Angster, J. Beisch, F. Renner, B. Schwanewedel

Collaborations with groups of:

- in Konstanz: *P. Baum, D. Bossini, W. Belzig, S. Goennenwein, A. Leitenstorfer, M. Müller*
- *M. Aeschlimann*, Universität Kaiserslautern
- *M. Albrecht*, Universität Augsburg
- *H. Ebert*, LMU München
- *T. Kampfrath*, FU Berlin
- *A. Kamra*, University of Madrid
- *T. Kurihara*, Tokyo University
- *M. Kläui*, Universität Mainz
- *R. Mondal*, IIOT, Dhanbad
- *P. Oppeneer, M. Weißenhofer*, Uppsala University
- *L. Rózsa, L. Szunyogh, L. Udvardi*, Budapest University

Universität Konstanz

DFG Deutsche Forschungsgemeinschaft

SCCKN Scientific Compute Cluster Konstanz

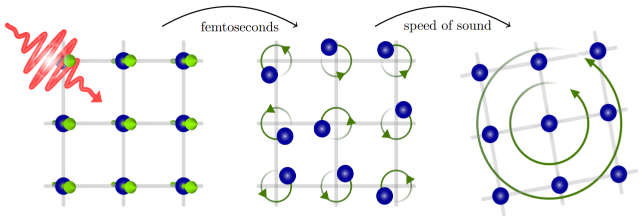
ChiPS Research Unit ChiPS

SFB 1432 Fluctuations

Schwerpunktprogramm Skyrmionics

Summary:

- **ultrafast transfer of spin angular momentum into the lattice**
  - polarized phonons absorb the spin angular momentum in Ni
  - chiral phonons for spintronics



- **modelling spin-lattice dynamics**
  - relativistic spin-lattice coupling parameters from first principles
  - rotationally invariant formulation of spin-lattice Hamiltonian
  - phonon mediated spin spin interaction
  - chirality-selective magnon-phonon coupling