Anisotropic exchange and non-collinear antiferromagnets on a noncentrosymmetric fcc structure as in the half-Heuslers

Seydou-Samba Diop [1]*, George Jackeli [2,3], Lucile Savary [1]

[1] Univ Lyon, ENS de Lyon, Univ Claude Bernard, CNRS, Laboratoire de Physique, F-69342 Lyon, France
[2] Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany
[3] Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

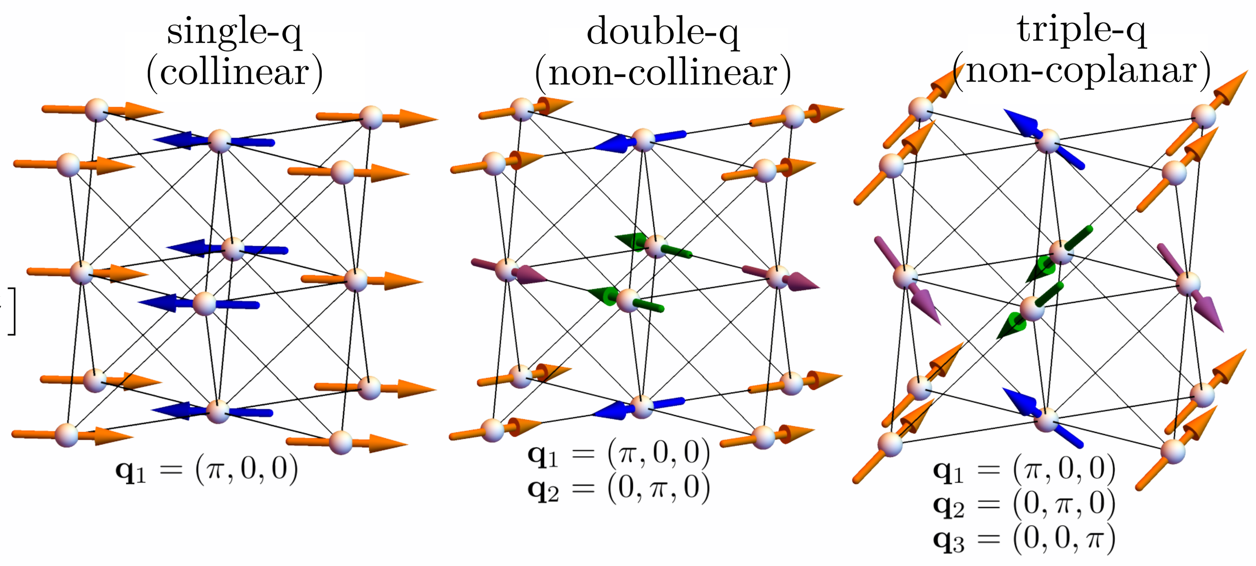
* seydou-samba.diop@ens-lyon.fr

1. Introduction

In a classical antiferromagnet, **geometrical frustration** is expected to lead to interesting ground states. On the face-centered cubic (fcc) lattice, the J_1-J_2 Heisenberg model hosts a ground state manifold where collinear orders are degenerate with non-collinear and non-coplanar orders such as **multi-q states**.

Example: type-I order
$(J_1 > 0, J_2 < 0)$

$$\mathbf{S}_i = \frac{1}{2}\sum_\ell \left[\mathbf{u}_\ell e^{i\mathbf{q}_\ell\cdot\mathbf{r}_i} + \mathbf{u}_\ell^* e^{-i\mathbf{q}_\ell\cdot\mathbf{r}_i}\right]$$



In real materials the single-q states are commonly selected, so the perspective to find a physical realisation of multi-q states is rather exciting. One may find candidates among the **half-Heusler compounds** RPtBi or RPdBi (R = rare-earth), a family of non-centrosymmetric fcc antiferromagnets with rare-earth ions carrying localized magnetic moments. Strong spin-orbit coupling will expectedly lead to **anisotropic exchange interactions**. In this work, we explored the effects of such interactions and the possible zero-temperature orders in these antiferromagnets. In particular, we clarified the role of anisotropy in the realization of non-collinear and non-coplanar states [1].

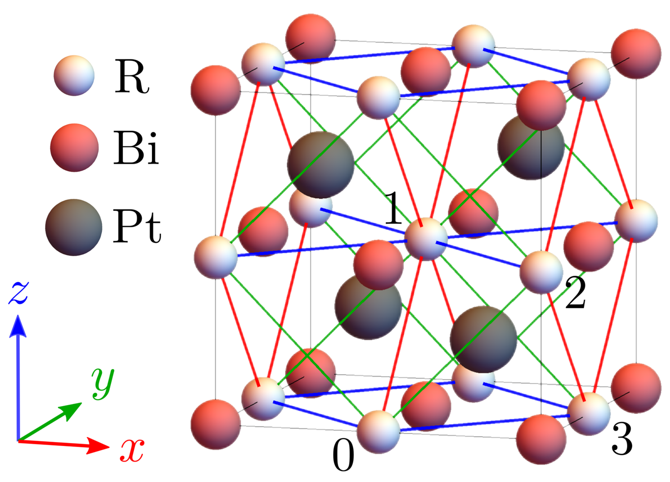
2. Symmetry-allowed anisotropic model for the half-Heusler structure

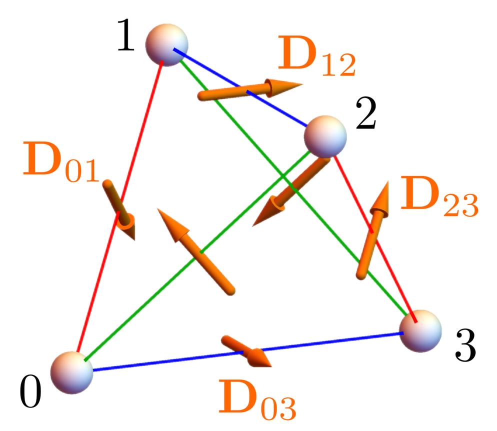
We derived the most general exchange model on fcc allowed by the symmetries of the half-Heusler compounds (space group f-43m). Besides the isotropic Heiseberg terms, 3 anisotropic interaction terms are allowed between nearest-neighbors:

$$H = \frac{1}{2}\sum_{ij} S_i^\mu A_{ij}^{\mu\nu} S_j^\nu$$

$$H = \underbrace{J_1 \sum_{\langle i,j\rangle} \mathbf{S}_i\cdot\mathbf{S}_j + J_2 \sum_{\langle\langle i,j\rangle\rangle} \mathbf{S}_i\cdot\mathbf{S}_j}_{\text{Heisenberg coupling}} + \underbrace{K \sum_{\langle i,j\rangle_\gamma} S_i^\gamma S_j^\gamma}_{\text{Kitaev coupling}}$$

$$+\underbrace{\Gamma \sum_{\langle i,j\rangle_\gamma} \xi_{ij}(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)}_{\text{“}\Gamma\text{” coupling}} + \underbrace{\sum_{\langle i,j\rangle} \mathbf{D}_{ij}\cdot(\mathbf{S}_i\times\mathbf{S}_j)}_{\text{Dzyaloshinskii-Moriya coupling}}$$

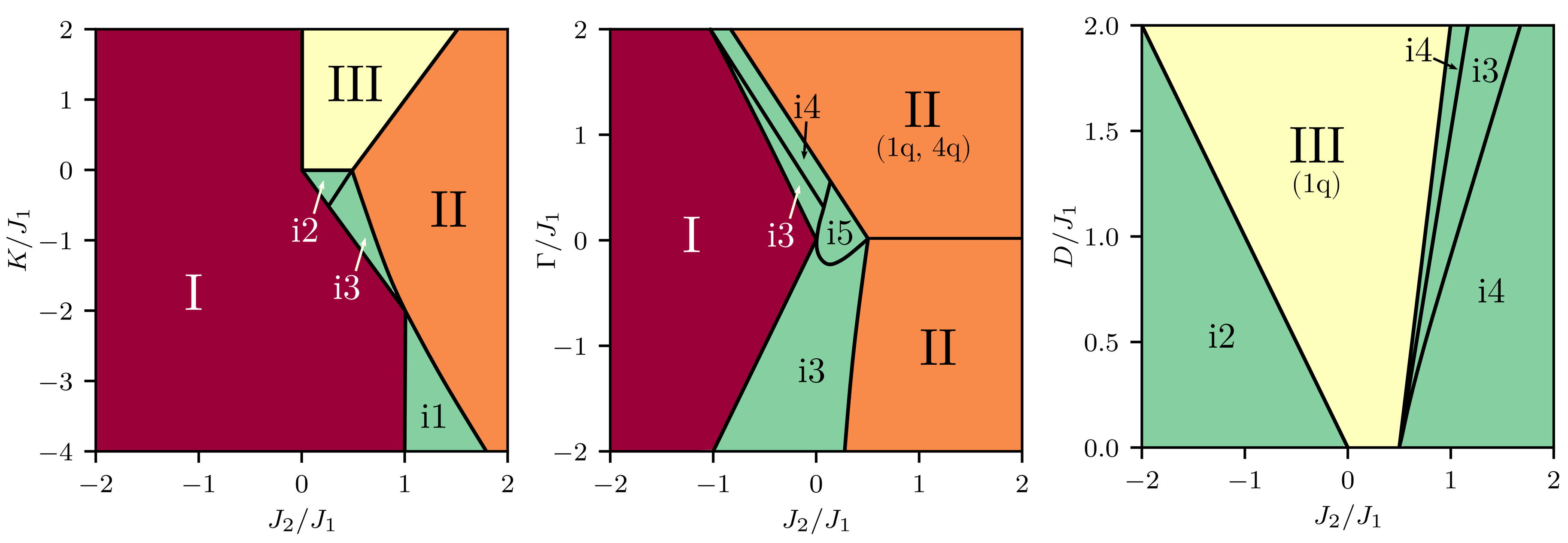




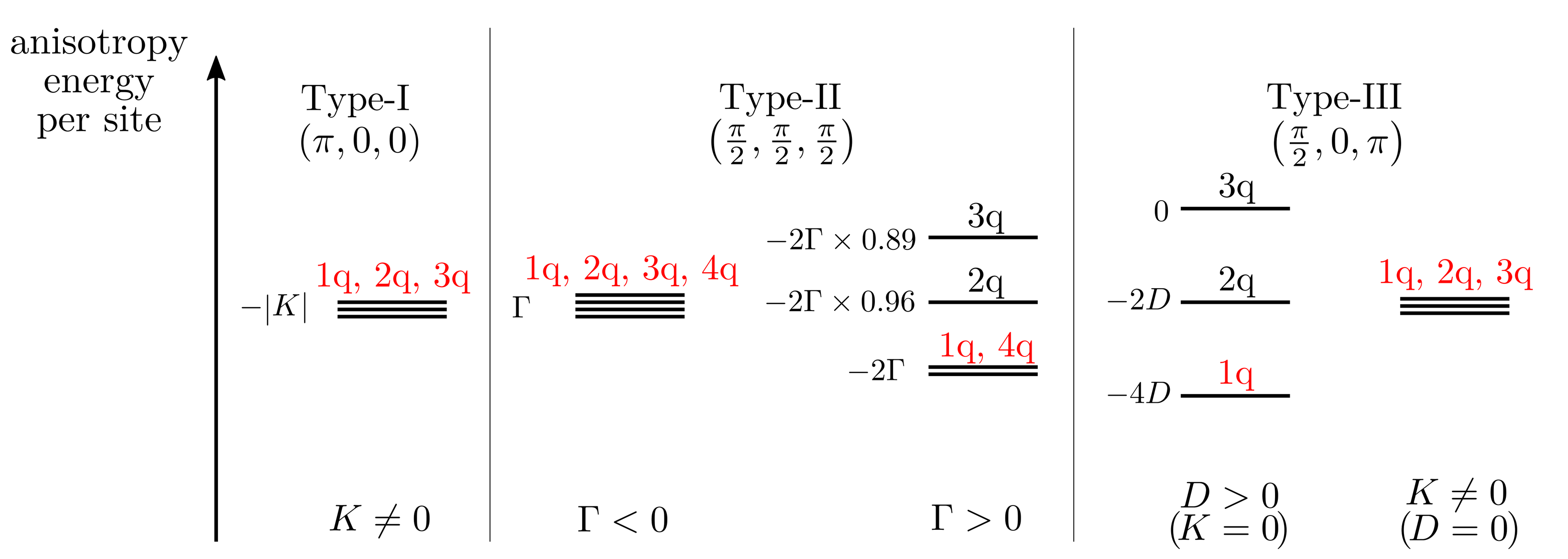
$\gamma = x \quad \alpha, \beta = y, z$
$\gamma = y \quad \alpha, \beta = z, x$
$\gamma = z \quad \alpha, \beta = x, y$

3. Anisotropy-induced classical ground states

In the (J_1, J_2, K, Γ, D) space, the optimal ordering wavevector (**q**) is computed using the Luttinger-Tisza method, resulting in a rich phase diagram with various commensurate (I, II, III) and incommensurate (i1 to i5) orders:



Do the anisotropic interactions lift the single-q/multi-q degeneracy? Not completely:

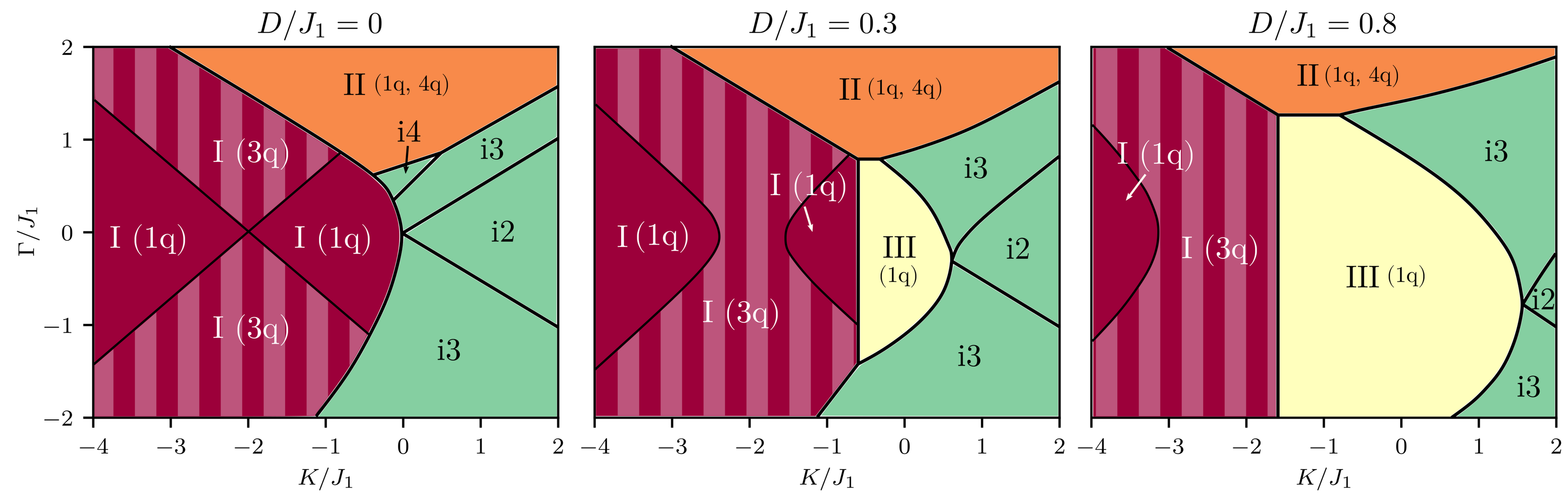


4. Quantum fluctuations and order-by-disorder

Among states with the same classical energy, **quantum fluctuations** favor the state which minimizes the zero-point energy: this is quantum **order-by-disorder**. The zero-point energy is computed using a real-space perturbative approach → effective biquadratic interaction:

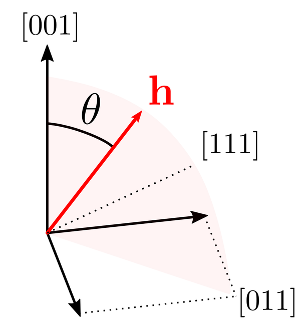
$$\delta H_{\text{biq}} = -\frac{1}{4h_0 S^2}\sum_{ij}(S_i^\mu A_{ij}^{\mu\nu} S_j^\nu)^2$$

In the isotropic case, quantum fluctuations select the single-q (collinear) states. For significant anisotropy, a triple-q type-I state can be favored:

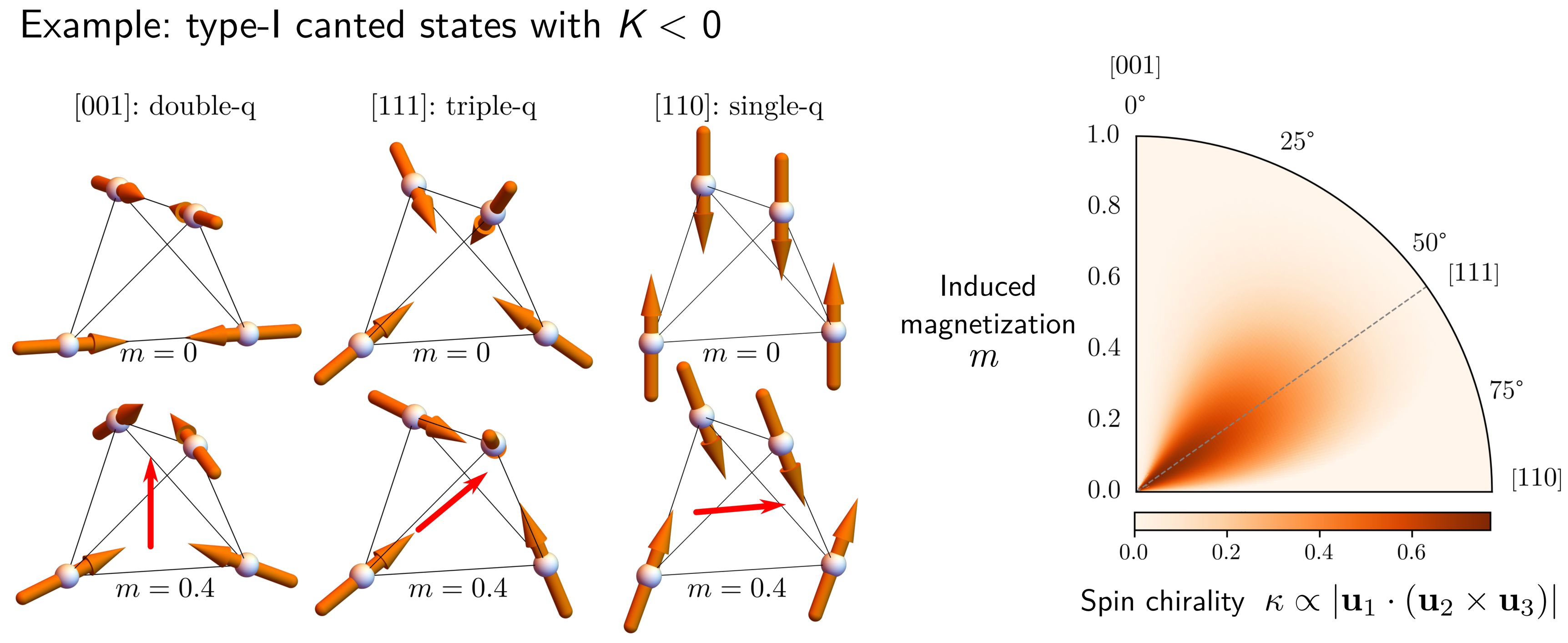


5. Field-induced ground states

The ground state degeneracy is also lifted by a **small external magnetic field h**: canting the spins in direction of the field costs some anisotropy energy. Different states are selected depending on field direction (θ) with respects to the crystal axes.



Example: type-I canted states with $K < 0$

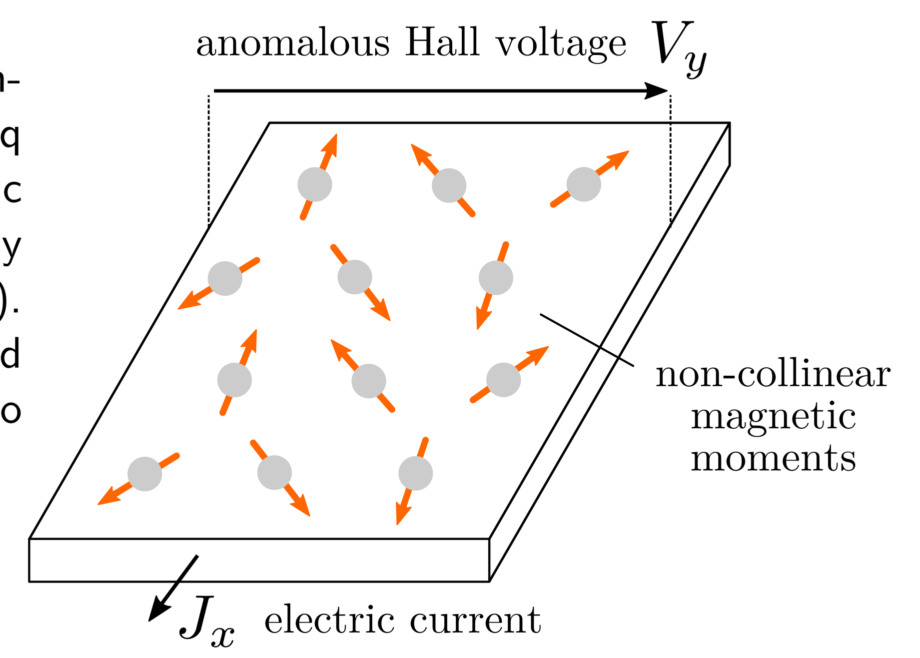


6. Conclusions and outlook

In half-Heusler antiferromagnets, several anisotropic exchange couplings are expected and lead to various orders.

- The accidental degeneracy between collinear/non-collinear states persists in presence of anisotropy.
- Inversion symmetry-breaking DM interaction selects a non-collinear (type-III, 1q) state.
- Quantum fluctuations + strong anisotropy → non-coplanar type-I states.
- Possibility to control the ground state *via* a tunable magnetic field.

When coupled to itinerant electrons, non-collinear configurations such as multi-q states may play a role in the electric transport of half-Heuslers, most notably in the **anomalous Hall effect** (AHE). Electrons hopping between misaligned spins can acquire Berry phases leading to an intrinsic AHE.



References

[1] S-S. Diop, G. Jackeli, L. Savary, “*Anisotropic exchange and non-collinear antiferromagnets on a noncentrosymmetric fcc structure as in the half-Heuslers*”, arXiv:2107.04906 (2021)

Acknowledgements

This work was funded by the ERC under the European Union's Horizon 2020 research and innovation programme (Grant No. 853116, acronym TRANSPORT) and by the NSF (Grant No. NSF PHY-1748958). We acknowledge support by the Max-Planck-UBC-UTokyo Centre for Quantum Materials.