TUT 4: Tutorial: Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics (joint session O/TUT)

This tutorial is designed for students, early-career researchers, and anyone interested in the foundational principles and practical methods for simulating magnetic materials. The journey begins with an introduction to the fundamentals of spin lattice Hamiltonians and their various forms, including a detailed discussion of their derivation (Lecture 1). Next, we explore state-of-the-art techniques for extracting magnetic exchange interactions from first-principles calculations through an engaging overview (Lecture 2). The final session (Lecture 3) delves into atomistic spin-dynamics simulations using the SPIRIT code, a versatile tool compatible with both smartphones and laptops. Throughout, we will emphasize the theoretical framework underpinning these approaches. The participants will have the freedom to explore a large range of phenomena, such as domain walls, skyrmions, and their dynamics under applied currents or torques.

Time: Sunday 16:00–18:15 Location: H10

Tutorial TUT 4.1 Sun 16:00 H10

Derivation of the spin-lattice Hamiltonian: Heisenberg, beyond Heisenberg, DMI, nematic exchange — •Hiroshi Katsumoto — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52428 Jülich, Germany

Magnetization textures, such as domain walls, skyrmions, or hopfions, are very active areas of condensed matter physics. These magnetic textures are usually explained based on the Heisenberg and the relativistic Dzyaloshinskii-Moriya interaction (DMI). Comparisons with experiments have shown that, in many cases, these interactions are insufficient, and a whole range (sometimes called a zoo) of higher-order symmetric and antisymmetric interactions have been proposed. In this tutorial, based on four elemental ingredients: Coulomb interaction, indistinguishability of electrons, spin, and spin-orbit interaction (SOI), I present a framework for systematically constructing exact spin-lattice models containing all spin Hamiltonians, including higher-order terms dependent on spin quantum numbers and lattice size. Examples of spin Hamiltonians for spin-1/2 and spin-1 systems up to four lattice sites are discussed. The tutorial also explores higher-order relativistic exchange interactions derived from SOI. I consider perturbations up to the 2^{nd} order of SOI and organize (anti)symmetric interactions. Finally, the classicalization of quantum spin relevant to magnetism in solids is discussed, culminating in a spin-lattice model that provides a theoretical framework for extracting material-dependent exchange interactions via numerical calculations and enables the modeling of magnetic textures. – DFG supports the work through SPP-2137 Skyrmionics.

Tutorial TUT 4.2 Sun 16:45 H10

Computing magnetic exchange interactions using DFT — •Manuel dos Santos Dias — Scientific Computing Department, STFC Daresbury Laboratory, United Kingdom

Magnetic materials are an unending source of fascinating physical behaviour which have fundamental appeal but also important technological applications. In order to understand, quantify and predict the properties of magnetic materials, we need information about the magnetic exchange interactions (introduced in the preceding tutorial), which control how the different magnetic atoms interact with each other and respond to external stimuli. This tutorial will give an overview on first-principles approaches to the calculation of magnetic exchange interactions using density functional theory (DFT). First I will outline how the properties of magnetic materials can be computed with and what capabilities are offered by different DFT codes. Next I will discuss how to map DFT calculations to spin models and when such a mapping is expected to work, followed by a discussion of the two main approaches to compute magnetic exchange interactions: the infinitesimal rotation method and the spin cluster expansion. Lastly, I will explain how to obtain simple information from the computed magnetic exchange interactions, such as the magnetic ground state and the spin wave spectrum, and how to connect to atomistic spin dynamics (for instance using the Spirit code covered in the next tutorial), Monte Carlo and micromagnetic simulations.

Tutorial TUT 4.3 Sun 17:30 H10

Hands-on atomistic spin-dynamics simulations with Spirit — •Thorben Pürling[1,2] and Moritz Sallermann[1,2,3] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, D-52425 Jülich — [2]Physics Department, RWTH-Aachen University, D-52062 Aachen — [3]University of Iceland

Atomistic spin-dynamics is a powerful, fascinating and educational simulation approach to studying the stability and dynamics of mesoscopic spin-textures such as skyrmions on the basis of atomistic spin-models. It can be used as digital twin to experiments.In this tutorial, participants will be introduced to the atomistic spin model and learn interactively how to perform atomistic spin simulations using the Spirit code [1]. We will cover common computational methods employed in atomistic spin simulations, emphasizing their practical application through the Spirit software framework [2]. The majority of the session will be dedicated to engaging exercises, where participants will work through example problems using Jupyter notebooks that interface directly with Spirit. Participants are encouraged to come with basic knowledge of Python and bring their charged laptops to fully engage in the tutorial. We provide a website [3] to keep you updated such that you arrive at the tutorial prepared for a hands-on experience.
We acknowledge funding from the ERC grant 856538 (project "3D MAGIC").

[1] Gideon P. Müller *et al.*, 10.5281/zenodo.7746551 (2024)
[2] https://spirit-code.github.io
[3] https://spirit-code.github.io/dpg-regensburg2025