MA 34: Computational Magnetism I

Time: Wednesday 15:00–18:30 Location: HSZ/0004

MA 34.1 Wed 15:00 HSZ/0004

GPU acceleration of atomistic spin dynamics simulations — Mariia Mohylna[1], Anders Bergman[2], Arkadijs Slobodkins[2], Olle Eriksson[2], Anna Delin[1], and •Johan Hellsvik[1] — [1]KTH Royal Institute of Technology, Stockholm, Sweden — [2]Uppsala University, Uppsala, Sweden

The Uppsala Atomistic Spin Dynamics (UppASD) [1,2] code implements algorithms for modelling magnetic materials on microscopic and mesoscopic length scales. In our recent implementation, kernels for magnetic field calculation for bilinear spin-spin pair interaction and one numerical integrator have been implemented with the CUDA programming model for use on NVIDIA GPUs, and the HIP programming model for AMD GPUs. Benchmarks for the simulation of bulk bcc Fe and the spin glass CuMn establish firmly the proposition of high speed-up for magnetization dynamics simulation on GPU hardware. The superior performance of the GPU implementations highlights the compatibility of spin-related problems with GPU architecture.

[1] The UppASD code https://github.com/UppASD/UppASD [2] Atomistic spin-dynamics; foundations and applications, O. Eriksson, et al. (Oxford University Press, 2017).

MA 34.2 Wed 15:15 HSZ/0004

Spin waves in double-layered antiferromagnets: insights from chain models and application to CrN — Seo-Jin Kim[1], Zdeněk Jirák[2], Jiří Hejtmánek[2], Karel Knížek[2], Helge Rosner[1], and •Kyo-Hoon Ahn[2] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czechia

The stability and magnonic properties of double-layered antiferromagnets are examined using two model systems, the linear chain (LC) and the railroad trestle (RT) geometry, and compared with the behavior of the real solid CrN. In the LC, the spin-paired order ($\cdots ++-- \cdots$) requires alternating ferromagnetic and antiferromagnetic (AFM) exchanges, whereas in the RT geometry an analogous order remains stable even with purely AFM interactions under specific analytical conditions. In CrN, the rock-salt structure causes strong magnetic frustration because each Cr atom has twelve symmetry-equivalent AFM nearest neighbors. Below $T_N = 287$ K, however, a magnetostructural transition to an orthorhombically distorted phase generates four distinct Cr-Cr distances and, consequently, a broad distribution of exchange strengths. This diversification suppresses frustration and stabilizes the double-layered AFM order. We trace this behavior to the competition between Cr–Cr direct exchange and 90° Cr–N–Cr superexchange, both exhibiting characteristic power-law dependencies on the interatomic distances. Finally, using *ab initio* exchange parameters, we derive the magnon spectrum and the temperature evolution of the ordered moments.

MA 34.3 Wed 15:30 HSZ/0004

Magnetoelastic behavior calculations in tetragonal systems — •Jakub Sebesta and Dominik Legut — IT4Innovations, VSB-TU Ostrava, 17.listopadu 2172/15, 708 00 Ostrava-Poruba, Czech Republic

In modern devices, various energy conversion effects are used for efficient operation. One of these effects represents magnetoelasticity – the conversion between the magnetic and mechanical energy. It is widely used in sensors or actuators *e.g.* force or torque sensors, fuel injectors, micro-pump, etc. So far, high symmetry systems, such as ferromagnetic 3d elements or rare-earth-based Laves phases, have been studied especially. In contrast ,here we provide a theoretical investigation of magnetoelastic behavior in tetragonal systems, focusing on the determination of the magnetoelastic properties influenced by the magnetic structure, and investigating the source of the observed modification. Eventually, we discussed a simple theoretical model for the magnetoelasticity in the considered systems.

[1] J. Sebesta et al. Magnetoelasticity - magnetic structure interrelation - tetragonal MnPt system study, Arxiv 2503.14693

MA 34.4 Wed 15:45 HSZ/0004

Ontology-driven Metadata for Multiscale Magnetism: The mammos-entity tool — •Andrea Petrocchi[1], Swapneel Amit Pathak[1], Martin Lang[1], Samuel J. R. Holt[1], Wilfried Hortschitz[2], Santa Pile[2], Martin Dobiasch[2], Thomas Schrefl[2], and Hans Fangohr[1] — [1]MPSD, Hamburg, Germany — [2]UWK, Krems, Austria

In science numerical values are interpretable only when their units and semantic meanings are known. Ontologies are able to identify physical quantities (i.e. using unique labels) and the provenance of data (i.e. the source and process creating it). The magnetic materials ontology is developed within the MaMMoS project and defines magnetic material properties and their interrelationships across various length scales.

In this talk, we present the core capabilities and limitations of mammos-entity, a Python package focused on one essential subset of information (called entity) needed for reliable data exchange: value, unit, and ontology label. This package facilitates working with entities programmatically, streamlines reading and writing data enriched with units and ontology identifiers as metadata and improves FAIRness of data. The aim is to make semantic annotation of data simple enough for everyday use. The mammos-entity package emerges from the magnetism community but supports all quantities defined in the EMMO (https://emmc.eu/emmo/).

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MA 34.5 Wed 16:00 HSZ/0004

Prediction of Iron Atom Magnetic Moments in Fe-Al Alloys via SOAP-based Neural Network Models — •Vojtěch Rálišš[1,2], Martin Friák[1], Jan Fikar[1], and Aleš Horák[2] — [1]Institute of Physics of Materials, v.v.i., Czech Academy of Sciences, Brno, Czech Republic — [2]Faculty of Informatics, Masaryk University, Brno, Czech Republic

We investigate neural network approaches for predicting local magnetic moments of iron atoms in Fe-Al disordered alloys using a dataset of 227 unit cells (27–216 atoms) with Al concentrations of 0–60%, totaling 6880 Fe atoms (mean: $2.013\,\mu_B$, std: $0.424\,\mu_B$) from DFT calculations.

Local environments are encoded using SOAP descriptors with a cutoff capturing the first three coordination shells, yielding rotation- and translation-invariant features. Our feedforward neural network achieves MAE = $0.0436\,\mu_B$ on the test set, significantly outperforming a first-neighbor baseline (MAE = $0.121\,\mu_B$) and CHGNet (MAE = $0.215\,\mu_B$), while requiring far less memory and compute time.

These results demonstrate the effectiveness of SOAP-based neural networks for fast, accurate prediction of electronic properties in metallic alloys, with implications for large-scale computational screening and local magnetic phenomena studies.

MA 34.6 Wed 16:15 HSZ/0004

Material Parameter Determination with Deep Learning — •Jack Smith[1,2], Dieter Suess[1], and Florian Slanovc[2] — [1]University of Vienna, Vienna, Austria — [2]Silicon Austria Labs, Villach, Austria

Measuring a set of material parameters from stray field measurements presents a challenging inverse problem. In this work, we introduce a data-driven approach for this task using a probabilistic neural network.

A standard regression approach can fail to capture the non-uniqueness of this task, leading to unphysical predictions. To mitigate this, we model the conditional probability distribution of the material parameters and measured stray field. We use a mixture density network (MDN)[1], which combines a neural network with a mixture density model, to model this conditional probability distributions. To capture spatial correlations, we employ a convolutional neural network feature extractor that projects the stray field map into a high-dimensional latent space before probabilistic decoding with the MDN.

We demonstrate that this method can extract ground-truth parameters with high accuracy, even for visually indistinguishable stray fields. It also provides a quantifiable uncertainty, identifying regimes where the stray field solution is non-unique and traditional inversion methods would fail.

[1] C. M. Bishop, Mixture density networks (1994).

MA 34.7 Wed 16:30 HSZ/0004

Automated Magnetism Analysis via Tensorial Interacting Spins — •Haichang Lu[1,2] and Stefan Blügel[3,4] — [1]Fert Bei-

jing Institute, MIIT Key Laboratory of Spintronics, School of Integrated Circuit Science and Engineering, Beihang University, Beijing, 100191, China — [2]Engineering Department, Cambridge University, Cambridge CB2 1PZ, UK — [3]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [4]Institute for Theoretical Physics, RWTH Aachen University, 52062 Aachen, Germany

Analyzing and describing magnetism in materials with localized moments requires accurate and generalizable spin models that go beyond conventional scalar or vector exchange interactions. Here we present *AMATIS*: an automated computational workflow that systematically incorporates tensorial spin interactions (non-relativistic and relativistic) into the effective Hamiltonian. Grounded in quantum spin properties and group theoretical analysis, tensorial components are extracted from the constrained least-squares fitting, ensuring fidelity to *ab initio* data. An integrated Monte Carlo module allows for the simulation of finite-temperature magnetic thermal equilibrium properties. We demonstrate the utility of this workflow on a series of two-dimensional magnetic materials and a van der Waals heterostructure, revealing the full spectrum of relevant tensorial interactions and their impact on magnetic properties. This approach offers a robust, high-throughput pathway from atomic structure to magnetic behavior, advancing the predictive design of novel magnetic materials.

15 min break

MA 34.8 Wed 17:00 HSZ/0004

Forestalled phase separation as the precursor to stripe order and superconductivity — •Aritra Sinha and Alexander Wietek — Max Planck Institute for the Physics of Complex Systems

Stripe order is a key feature of the cuprate phase diagram and appears as the ground state of the two-dimensional Fermi-Hubbard and t-J models in relevant regimes. With increasing temperature, stripe and superconducting orders give way to the strange metal and pseudogap phases, whose microscopic origins remain unclear. Using advanced tensor-network simulations, we try to identify the real-space mechanisms behind this evolution. iPEPS reveals a strong peak in the uniform charge susceptibility above the stripe phase near hole doping p=0.1, sharpening on cooling. METTS simulations on finite cylinders trace this peak to fluctuating charge clusters, resembling incipient phase separation into hole-rich and hole-poor regions-ultimately prevented by stripe order at low temperature. In the doped Mott regime of the t-t'-J model, we find that fluctuating domain walls of doped holes act as precursors to superconductivity. At low T, transient mergers of hole-rich regions create larger clusters containing superconducting condensates, which gradually phase-lock upon cooling into a coherent, stripe-aligned d-wave superconductor. Together, these results suggest a unified picture where charge and pairing fluctuations evolve into stripe order and superconductivity, clarifying their intertwined roles in strongly correlated systems.

MA 34.9 Wed 17:15 HSZ/0004

Anisotropic Ligand-Mediated Magnetic Interactions in Strongly Correlated Layered Antiferromagnet $GdTe_3$ — •Sergii Grytsiuk[1], Patrik Thunström[2], Mikhail I. Katsnelson[1], and Malte Rösner[1] — [1]Radboud University, Institute for Molecules and Materials, Nijmegen, The Netherlands — [2]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

In this study, we investigate the magnetic properties of $GdTe_3$ through first-principles calculations and spin-dynamics simulations. We reveal that its complex phase diagram arises from the interplay between the antiferromagnetic isotropic exchange of Gd localized f- and delocalized d-states and the substantial anisotropic exchange with Te ligand-conducting p-states. Despite the half-filled nature of Gd-f states suggesting a lack of magnetocrystalline anisotropy (MCA), we identify that the anisotropic coupling of it with ligand states serves as the primary source of MCA. This coupling is significantly influenced by the magnetic ordering of neighboring localized spins and is sensitive to charge density waves (CDW). It can also be tuned via magnetic field, temperature, and pressure. By linking the ligand spin-orbit coupling and induced magnetic moments to the effective interactions among localized spins, we successfully reproduce the experimental magnetic susceptibility across varying temperatures, magnetic fields, and pressures.

MA 34.10 Wed 17:30 HSZ/0004

operator Lanczos approach enabling neural quantum states as real frequency impurity solvers — •Jonas Rigo[1] and Markus Schmitt[1,2] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control, 52425 Jülich, Germany — [2]University of Regensburg

To understand the intricate exchange between electrons of different bands in strongly correlated materials, it is essential to treat multi-orbital models accurately. For this purpose, dynamical mean-field theory (DMFT) provides an established framework, whose scope crucially hinges on the availability of efficient quantum impurity solvers. Here we present a real-frequency impurity solver based on neural quantum states (NQS) combined with an operator-space Lanczos construction. NQS are an asymptotically unbiased variational ground-state ansatz that employs neural networks to capture long-range correlations on complicated graph structures. We leverage this ability to solve complex multi-orbital impurity problems using a systematically improvable segmented commutator operator Lanczos (SCOL) construction. Our benchmarks on both the single-orbital Anderson model and the multi-orbital Hubbard–Kanamori impurity Hamiltonian reveal excellent ground state precision and the capacity to resolve key features of zero temperature spectral functions and self-energies. These promising results open avenues for extending DMFT to more challenging problems.

MA 34.11 Wed 17:45 HSZ/0004

Theoretical study of doping and pressure effects in organic magnets — Rohit Pathak[1,2], Isabella Rudengren[1,2], Torbjörn Wigren[1], Anna Delin[2,3], Olle Eriksson[1,2], Niklas Wahlström[1,2], and •Vladislav Borisov[1,2] — [1]Uppsala University, Sweden — [2]Wallenberg Initiative Materials Science for Sustainability, Sweden — [3]KTH Royal Institute of Technology, Stockholm, Sweden

Technologically important permanent magnets used nowadays rely on rare-earth elements and are associated with negative environmental impact and high energy costs, when produced. On the other hand, organic magnets are known, which can solve these problems, but their applications are limited due to low ordering temperature and coercivity. In this work, we aim to explore further the class of organic magnets to find ways of improving their magnetic properties, which would allow their applications and potentially even partial replacement of inorganic magnets. Also, fundamental aspects of organic magnets are studied in terms of delocalized nature of magnetism. Using first-principles electronic structure theory and atomistic spin dynamics (UppASD code [1]), we model magnetic properties of different compounds including the effects of chemical doping and mechanical pressure to understand the structural and chemistry-related trends. Machine-learning models for property prediction and structure reverse engineering will be applied to make the search for new magnets feasible.

1. B. Skubic, J. Hellsvik, L. Nordström, and O. Eriksson, A method for atomistic spin dynamics simulations: implementation and examples, J. Phys.: Condens. Matter. 20, 315203 (2008).

MA 34.12 Wed 18:00 HSZ/0004

Ground-state phases and excitation spectra of dipole conserving spin-half chain — •Prabhakar Prabhakar[1], Soumya Bera[1], and Giuseppe De Tomasi[2] — [1]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India — [2]CeFEMA-LaPMET, Departamento de Fisica, Instituto Superior Tecnico, Universidade de Lisboa, Portugal

We explore the ground state phase diagram of a translationally invariant, non-integrable one-dimensional spin chain with dipole conservation. The model is typically realized in quantum simulators, such as cold-atom setups, in the presence of a large, tilted electric field. Despite the strong kinetic constraints imposed by dipole conservation, which prevent the propagation of isolated spin excitations and suppress single-spin order, the system stabilizes an antiferromagnetic dipole-ordered ground state. However, at a large Ising interaction strength, the model shows a phase transition to a spin-ordered phase. Using exact diagonalization along with density matrix renormalization group simulations, we examine the associated phases with different antiferromagnetic order parameters, the entanglement spectrum, and the dynamical spectral function.

MA 34.13 Wed 18:15 HSZ/0004

Implementation of spin-current density functionals in VASP — •Fabien Tran, Marie-Therese Huebsch, and Martijn Marsman — VASP Software GmbH, A-1090, Vienna, Austria

The implementation of spin-current density functionals (SCDF) in VASP is reported. SCDFs, which depend on the spin kinetic-energy density and spin current density, are intended for non-collinear calculations and can capture a non-zero local exchange-correlation spin torque. Results obtained with various SCDFs, namely TDRU [Tancogne-Dejean *et al.*, Phys. Rev. B **107**, 165111 (2023)], nc-mSCAN [Desmarais *et al.*, Phys. Rev. Lett. **134**, 106402 (2025)] and HTM [Huebsch *et al.*, arXiv:2501.04124 (2025)] will be presented.