MA 17: Computational Magnetism II

Time: Tuesday 9:30–12:45 Location: EB 202

MA 17.1 Tue 9:30 EB 202

Rational design of RE-free magnets from first principles via Bayesian optimisation — •Fabian Eilers, Stephan Erdmann, Halil Ibrahim Sözen, and Thorsten Klüner — Institute of Chemistry, Carl-von-Ossietzky University of Oldenburg, D-26129 Oldenburg, Germany

The design of new rare-earth-free permanent magnetic materials to replace the powerful, but critically limited, rare earth-based magnets remains a a major challenge for the scientific community. Here we report on the rational design of new RE-free magnets using Bayesian optimisation. We attempt to improve the magnetic properties and phase stability of Fe2P-based magnetic materials by optimising the chemical composition and the lattice configuration of the unit cell. This problem involves global optimisation in a high configuration space. Bayesian optimisation can be used as a sequential design strategy to effectively explore this high configuration space. In an active learning approach, new trials are generated by sampling based on the expected improvement of the Gaussian process surrogate model. Trial evaluation is then performed via first-principles calculations using the Korringa-Kohn-Rostoker and Coherent Potential Approximation (KKR-CPA) method.

MA 17.2 Tue 9:45 EB 202

Efficient Implementation of the Minimum Mode Following Method for magnetic systems — •Hendrik Schrautzer[1,2], Moritz Sallermann[1,3,4], Stefan Heinze[2], Hannes Jónsson[1], and Pavel F. Bessarab[1] — [1]University of Iceland, Reykjavik, Iceland — [2]Christian-Albrechts-University, Kiel, Germany — [3]Forschungszentrum Jülich and JARA, Jülich, Germany — [4]RWTH Aachen University, Aachen, Germany

Magnetic systems hosting topological textures have been of great technological and fundamental interest in recent years. Identifying the lifetime of metastable states, predicting hitherto unknown states, and computing their kinetics are essential tasks [1]. Identifying first-order saddle points on the energy surface is paramount in this context, and the potential for identifying magnetic systems through the implementation of the Minimum Mode Following approach is significant [2]. However, the main computational challenge lies in determining the eigenmodes of the Hessian, which means that embedding these methods in adaptive kinetic Monte Carlo simulations has not yet been achievable. We introduce an efficient implementation of a Riemannian optimization of the Rayleigh Quotient on the Grassmann manifold, which achieves high accuracy determination of extremal eigenmodes without requiring explicit second-order Hessian information. The efficiency of the method is demonstrated by computing various transitions in a complex multistable skyrmionic system.

1: F. Muckel et al., Nat. Phys. 17.3 (2021):395-402
2: G. P. Müller et al., Phys. Rev. Lett. 121.19 (2018):197202

MA 17.3 Tue 10:00 EB 202

Mixed valence nature of the Ce 4f state in $CeCo_5$ — •Ruiwen Xie and Hongbin Zhang — Group of Theory of Magnetic Materials, Technical University of Darmstadt, Darmstadt, Germany

Cerium-based intermetallics are currently attracting much attention as highly promising alternatives to conventional permanent magnets that contain a scarce rare earth element like neodymium. Furthermore, the mixed valency nature of Ce, as unveiled by experimental XPS and BIS spectra, broadens the scope for another intriguing field of investigation. Here we apply a charge fully self-consistent approach combining density functional theory and dynamical mean-field theory (DFT+DMFT) to investigate the magnetization and electronic structure of the $CeCo_5$ system. In addition, the Ce-4f valence state fluctuations are evaluated and compared within pristine $CeCo_5$ and Cu-doped $CeCo_5$. Contrasting behaviours of Cu doping effects on the two Wyckoff positions of Co are found, which is expected to contribute to the experimentally reported nonmonotonic change of the magnetic anisotropy with increasing Cu alloying content in $Ce(Co_{1-x}Cu_x)_5$ alloys.

MA 17.4 Tue 10:15 EB 202

Is the ground state of Anderson's impurity model a recurrent neural network? — •Jonas B. Rigo[1] and Markus Schmitt[1,2] — [1]Forschungszentrum Jülich, Institute of Quantum Control (PGI-8), D-52425 Jülich, Germany — [2]University of Regensburg, 93053 Regensburg, Germany

When the Anderson impurity model (AIM) is expressed in terms of a Wilson chain it assumes a hierarchical Renormalization group structure that translates to a ground state with features like Friedel oscillations and the Kondo screening cloud [1]. Recurrent neural networks (RNNs) have recently gained traction in the form of Neural Quantum States (NQS) ansätze for quantum many body ground states and they are known to be able to learn such complex patterns [2]. We explore RNNs as an ansatz to capture the AIM's ground state for a given Wilson chain length and investigate its capability to predict the ground state on longer chains for a converged ground state energy.

[1] Affleck, Ian, László Borda, and Hubert Saleur. "Friedel oscillations and the Kondo screening cloud." Physical Review B 77.18 (2008): 180404.

[2] Hibat-Allah, Mohamed, et al. "Recurrent neural network wave functions." Physical Review Research 2.2 (2020): 023358.

MA 17.5 Tue 10:30 EB 202

High-throughput calculation of magnetic exchange interactions using DFT — •Jan Priessnitz and Dominik Legut — IT4Innovations, VSB-TU Ostrava, Ostrava, Czechia

Ab-initio calculation of magnetic properties is an invaluable tool in development of novel magnetic materials. Magnetism in these materials can often be modeled using the classical Heisenberg model, with exchange interaction being the most significant term, determining the ground state magnetic ordering as well as critical temperature, magnon spectrum, etc. Knowing the exchange interactions is a prerequisite for larger-scale spin-dynamic or micromagnetic calculations.

Exchange interactions are usually calculated via density functional theory (DFT), either through energy variation of the ground state (Green's functions), or by calculating the total energies of multiple magnetic configurations and fitting them into the Heisenberg model Hamiltonian. Neither method is completely foolproof, limiting the high-throughput use case.

In this talk, I'm going to focus on the total energy method, presenting a new approach for selecting a suitable set of excited magnetic configurations, including an algorithm that can efficiently traverse the exponentially-growing magnetic configuration space. This improvement allows us to use the total energy method even in otherwise difficult cases, e. g., calculating long-range interactions in metallic systems.

Furthermore, I'll introduce OstravaJ, a Python package that fully automates the exchange interaction calculation, employing in principle any non-collinear electronic structure DFT code, e.g. VASP.

MA 17.6 Tue 10:45 EB 202

Machine learning-based prediction of transfer integrals in undoped cuprates — •Denys Kononenko[1], Ulrich K. Rössler[1], Jeroen van den Brink[1,2], and Oleg Janson[1] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, 01069, Germany — [2]Institute for Theoretical Physics, TU Dresden, Dresden, 01069, Germany

Undoped cuprates represent an abundant class of magnetic insulators characterized by a complex interplay of chemistry and quantum fluctuations, resulting in diverse magnetic behaviors. Comprehending the magnetism in these materials requires understanding the underlying spin model.

Antiferromagnetic superexchange is the dominant magnetic coupling in cuprates which is estimated through electronic transfer integrals, computed using density functional theory (DFT) within the Wannier basis. However, these calculations are computationally cumbersome. We present an alternative approach based on Artificial Neural Networks (ANN) trained on high-throughput DFT calculations. The ANN predicts transfer integrals solely based on the crystal structure, offering a more efficient and less computationally demanding method. Descriptors within the ANN model capture spatial configuration and the chemical composition of the local crystalline environment.

The ANN model is a powerful tool for predicting transfer integrals and rapidly screening the relevant spin model in undoped cuprates. This development opens new avenues for designing and exploring novel materials with tailored magnetic properties.

15 min. break

MA 17.7 Tue 11:15 EB 202

Deep learning of phase transitions for quantum spin chains from correlation aspects — •Ming-Chiang Chung — National Chung-Hsing University, Taichung, Taiwan

Using machine learning (ML) to recognize different phases of matter and to infer the entire phase diagram has proven to be an effective tool given a large dataset. In our previous proposals, we have successfully explored phase transitions for topological phases of matter at low dimensions either in a supervised or an unsupervised learning protocol with the assistance of quantum information related quantities. In this work, we adopt our previous ML procedures to study quantum phase transitions of magnetism systems such as the XY and XXZ spin chains by using spin-spin correlation functions as the input data. We find that our proposed approach not only maps out the phase diagrams with accurate phase boundaries, but also indicates some new features that have not been observed in the field of machine learning before. In particular, we define so-called relevant correlation functions to some corresponding phases that can always distinguish between those and their neighbors.

[1]Y. H. Tsai, M.Z. Yu, Y.H. Hsu, and M.C. Chung, Phys. Rev. B 102, 054512 (2020). [2]Y.H. Tsai, K.F. Chiu, Y.C. Lai, K.J. Su, T.P. Yang, T.P. Cheng, G.Y. Huang, and M.C. Chung, Phys. Rev. B 104, 165108 (2021). [3]Ming-Chiang Chung, Guang-Yu Huang, Ian P. McCulloch, and Yuan-Hong Tsai, Phys. Rev. B 107, 214451 (2023)

MA 17.8 Tue 11:30 EB 202

Translationally Invariant Formalism for the Computation of Orbital Magnetization — •Seung-Ju Hong and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea

The computation of orbital magnetization [1,2] is implemented in various codes, such as Wannier90 and Wannierberri. However, for an accurate computation, there are some remaining practical issues. One of the issues is the violation of translational invariance in the finite difference formula, that is, the results change under lattice vector translation of selected atoms or arbitrary translation of the whole system.

Recently, a translationally invariant formalism for the position matrix elements was developed [3]. In this talk, we will discuss the extension of translational invariance of the other Wannier matrix elements needed for the computation of orbital magnetization. The results show that the convergence is much better with the translationally invariant formulae and, thus, demonstrate that the use of translationally invariant formalism is necessary for the accurate computation of orbital magnetization.

[1] T. Thonhauser, Davide Ceresoli, David Vanderbilt, and R. Resta, Phys. Rev. Lett. 95, 137205 [2] M. G. Lopez, David Vanderbilt, T. Thonhauser, and Ivo Souza, Phys. Rev. B 85, 014435 [3] J.-M. Lihm, M. Ghim, and C.-H. Park, *Accurate calculation of position matrix elements for Wannier interpolation, Part 1: translational invariance,* Wanner 2022 Developers Meeting, Trieste, Italy (2022). https://indico.ictp.it/event/9851/

MA 17.9 Tue 11:45 EB 202

Kondo cloud of a partially screened impurity coupled to s-wave superconductor — •Anand Manaparambil[1], Catalin Pascu Moca[2,3], Gergely Zarand[2], and Ireneusz Weymann[1] — [1]Adam Mickiewicz University, Poznan, Poland — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]University of Oradea, Oradea, Romania

Magnetic impurities coupled to a band of conduction electrons generate a many-body correlated state known as the Kondo state. The correlations in the Kondo state extend to large length scales compared to the size of the impurity. In general, the Kondo cloud has been predicted to extend up to micrometers in size and recent experiments have confirmed the presence of such large screening clouds. In the presence of superconducting correlations, such screening clouds have been shown to exist even outside the Kondo phase. In this work, we study a large spin Kondo model coupled to an s-wave superconductor. We show that there exists an underscreened Kondo doublet to an unscreened triplet phase transition according to the dominant energy scale. We observe different behaviors of the screening in both of the phases predicted analytically by the renormalized perturbation theory(RPT) and confirmed numerically using the Numerical Renormalization Group(NRG) methods. The spatial extension of the correlations estimated from the equal-time spin-spin correlation function calculated using the Density Matrix Renormalization Group (DMRG) corroborates the presence of screening clouds in both phases.

MA 17.10 Tue 12:00 EB 202

Ab-initio study of x-ray circular dichroism in chiral solids: disentangling magnetic and natural cross-sections — •Alberto Marmodoro[1,2], Ondrej Sipr[1,2], Sergiy Mankovsky[3], and Hubert Ebert[3] — [1]Institute of Physics (FZU), AS CR Prague, Czech Republic — [2]New Technologies Center (NTC), University of West Bohemia, Plzen, Czech Republic — [3]Ludwig Maximilians University (LMU), Munich, Germany

Circular dichroism in x-ray absorption (XCD), i.e. the different cross-section for a left or right circularly polarized beam, can arise from a variety of mechanisms.

Ferromagnetic order leads to a magnetic signal (XMCD) which mainly arises from dipole-allowed transitions and which follows a well-known cosine dependence with respect to azimuthal angle between beam and magnetic moments.

Even in the absence of atomic magnetic moment, a chiral arrangement of the atoms lead among other chirality induced spin-selectivity effects (CISS) to a "natural" signal (XNCD) [1-2], which involves instead higher order terms in electron-photon interaction and which also follows a different angular dependence.

We use fully-relativistic multiple scattering / Green's function methods (KKR-GF) and density functional theory (DFT) plus enhancements for core-hole effects, in order to numerically study this phenomenology in e.g. Strukturbericht B20 compounds, and to offer some predictions for the different impact of finite temperature effects [3] onto the two above components of XCD.

MA 17.11 Tue 12:15 EB 202

Automating ab initio modeling applied to muon spin rotation and relaxation spectroscopy — •Miki bonacci[1], Ifeanyi John Onuorah[2], Roberto De Renzi[2], Giovanni Pizzi[1], and Pietro Bonfa'[2] — [1]Paul Scherrer Institut, Switzerland — [2]Universita' degli studi di Parma, Italy

Muon spin spectroscopy is a precise experimental tool used to characterize several physical phenomena, from magnetic to superconducting phases [1]. For an accurate characterization, first-principles simulations are crucial to supply experimental measurements with an accurate prediction of muon resting sites in samples and the associated magnetic fields [2]. Furthermore, in silico characterizations readily discern cases where the muon probe itself plays a significant role [3]. These simulations, requiring deep expertise, are thus not easily accessible by non-expert users. Here, we propose the full automation of ab-initio muon characterization in crystalline solids. The predictive power of DFT is exploited by means of ad-hoc workflows implemented in AiiDA [4], encoding all the expertise needed to perform accurate computational muon spectroscopy. A user-friendly graphical interface, embedded in the AiiDAlab platform [5], is demonstrated, offering an intuitive means to conduct muon simulations routinely alongside experiments. We conclude by validating some well-known cases to demonstrate the predictive power of our simulations.

MA 17.12 Tue 12:30 EB 202

Energy-efficient control of magnetic states — Mohammad Badarneh[1], Grzegorz Kwiatkowski[1], and •Pavel Bessarab[1,2] — [1]Science Institute, University of Iceland, Reykjavik, Iceland — [2]Linnaeus University, Kalmar, Sweden

Control of magnetization switching is critical for the development of novel technologies based on magnetic materials. Transitions between magnetic states can follow various pathways which are not equivalent in terms of energy consumption and duration. In this study, we propose a general theoretical approach based on the optimal control theory to design external stimuli for efficient switching between target magnetic states. The approach involves calculation of optimal control paths (OCPs) for the desired change in the magnetic structure. Following an OCP involves rotation of magnetic moments in such a way that the strength of the external stimulus is minimized, but the system's internal dynamics is effectively used to aid the switching. All properties of the control pulses including temporal and spatial shape can be derived from OCPs in a systematic way. Various applications of OCP calculations are presented, including energy-efficient switching of a nanomagnet by means of external magnetic field [1] or electric current [2], spin-wave assisted magnetization reversal in nanowires [3], and optimal skyrmion motion in synthetic antiferromagnets.

[1] G.J. Kwiatkowski et al., Phys. Rev. Lett. 126, 177206 (2021).

[2] S.M. Vlasov et al., Phys. Rev. B 105, 134404 (2022).
[3] M.H.A. Badarneh et al., Nanosyst. Phys. Chem. Math. 11, 294 (2020).