MA 52: Quantum Magnets and Molecular Magnets (joint session TT/MA)

Time: Thursday 15:00–18:00 Location: HSZ 304

Invited Talk MA 52.1 Thu 15:00 HSZ 304

Linear magnets: a structure-property-relation for finding unquenched orbital moments — •Anton Jesche — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86135 Augsburg, Germany

The presence of orbital magnetic moments in rare-earth-elements is one of the major differences to transition metal compounds and is at the heart of magnetic anisotropy, stability, and functionality. A large crystal electric field effect acting on an unquenched orbital moment can lead to extremely large anisotropy and coercivity as experimentally verified for iron-doped lithium nitride [1]. In the dilute limit, those iron atoms can be considered as single-atom magnets and are ideal candidates to study the quantum dynamics of anisotropic spins [2]. This, together with the strong field dependence of the spin reversal, allows creating stable but switchable states that could act as a 'quantum bit' at elevated temperatures of 10 K. A recent Mössbauer study revealed dominant magnetic quantum tunneling at even higher temperatures [3]. The presence of orbital moments in iron-doped lithium nitride is not a coincidence and not a solitary case: based on the proposed structural motif of the 'linear chain', we have identified several other 'linear magnets' with similar physical properties: iron-doped Li_4SrN_2, $LiSr_2(CoN_2)$, $(Sr_6N)[FeN_2][CN_2]_2$, and K_2NiO_2.Implications and limitations of the linear coordination are discussed in relation to the electronic structure.

[1] M. Fix et al., PRB 97, 064419 (2018)
[2] M. Fix et al., PRL 120, 147202 (2018)
[3] S. A. Bräuninger et al., arXiv:1909.12774

MA 52.2 Thu 15:30 HSZ 304

The power of typicality applied to magnetic molecules and low-dimensional quantum spin systems — •Jürgen Schnack — Universität Bielefeld, Fakultät für Physik

Molecular or low-dimensional quantum spin systems often prevent an exact calculation of their magnetic properties due to a prohibitively large size of the related Hilbert spaces. Typicality-based approaches such as the finite-temperature Lanczos method allow to investigate rather large systems with unprecedented accuracy. This way quantum critical as well as magnetocaloric properties of large cyclic clusters could be elucidated [1]. For the kagome lattice antiferromagnet it became possible to model a lattice of size N=42 (!) quasi exactly. This enabled us to study in particular that the low-lying density of singlet states moves up in energy contrary to common believe [2]. In addition, we could demonstrate for lattices up to 72 sites that magnon crystallization occurs slightly below the saturation field, an effect driven by the existance of flat energy bands [3].

[1] A. Baniodeh et al., npj Quantum Materials 3,10 (2018)
[2] J. Schnack, J. Schulenburg, J. Richter, Phys. Rev. B 98, 094423 (2018)
[3] J. Schnack, J. Schulenburg, A. Honecker, J. Richter, arXiv:1910.10448

MA 52.3 Thu 15:45 HSZ 304

Resonant photon absorption in $GdPc_2$ molecular magnet — •Gheorghe Taran[1], Eufemio Moreno-Pineda[2], Edgar Bonet[3], and Wolfgang Wernsdorfer[1,2,3] — [1]Physikalisches Institute, KIT, Karlsruhe — [2]Institute of Nanotechnology (INT), Karlsruhe — [3]Néel Institute, CNRS, Grenoble, France

Single ion molecular magnets (SIMMs) champion a magnetic center (*e.g.* a 3d or 4f ion) whose properties are modulated by the coordinated organic ligands. Their relative simple structure makes the task of correlating structural characteristics to physical properties considerably easier and thus, opens the doors for chemical tailoring for technological applications that range from refrigeration to storage and processing of quantum information.

In this study, we investigate the resonant photon absorption in diluted single crystals of $GdPc_2$ SIMM using micro-SQUID technique at subkelvin temperatures. Combining the advantages of EPR (*e.g.* the ability to explore the anisotropy character of the magnetic interactions) and those of micro-SQUID techniques (*e.g.* time-resolved dynamics on a micro-second scale) we construct the map of resonant transitions in the [1:40] GHz frequency range. The transitions are analyzed in the framework of a single spin Hamiltonian describing the ground state, $S = 7/2$, of the $GdPc_2$ complex and the predictions are compared to the ones made by ab-initio calculations. The unprecedented resolution of the resonant frequency-field maps allows a critical evaluation of the state of the art ab-initio methods for ligand field estimations and sets the base for future investigations into the coherent dynamics.

MA 52.4 Thu 16:00 HSZ 304

Quantum magnetism in Boleite - an Archimedean Solid with strong magnetic frustration — Stefan Lebernegg[1,2], Jürgen Schnack[3], Oleg Janson[4], Johannes Richter[5], Jörg Sichelschmidt[2], Tobias Förster[6], Alexander Tsirlin[7], and •Helge Rosner[2] — [1]Technical University of Munich, 80335, Munich, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [3]Bielefeld University, Faculty of Physics, Universitätsstr. 25, D-33615 Bielefeld, Germany — [4]IFW Dresden Helmholtzstraße 20 01069 Dresden Germany — [5]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden Germany — [6]Dresden High Magnetic Field Laboratory — [7]Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Combined theoretical and experimental effort, applying electronic structure calculations and numerical simulations as well as chemical analysis, X-ray diffraction and magnetic measurements had to be joined by mineralogical expertise to unveil the quantum magnetism of the mineral Boleite. This mineral is a strongly frustrated quantum magnet with 24 spin 1/2 Cu sites arranged on the vortices of a truncated cube, one of the famous Archimedean solids. We find that the system with its typical 1/3 magnetization plateau can be well understood by two leading interactions and their "randomness" describing a certain distribution of these exchange interactions.

MA 52.5 Thu 16:15 HSZ 304

Multi band modelling of exchange couplings in edge-sharing Cu-O chains — •Dijana Milosavljevic[1], Oleg Janson[2], Jan Tomczak[3], and Helge Rosner[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Technical University of Vienna, Austria

One of the structural features that has a crucial role in the determination of the exchange coupling constant in chain containing compound is the Cu-O-Cu bond angle. However the angle is not the only factor. Equally important influence on the the exchange coupling has the presence of the side groups coupled to the O-ligands. To demonstrate this we show two representatives of edge sharing chain cuprates with similar Cu-O-Cu bond angles but drastically different exchanges. From detailed DFT studies and subsequently derived multi band tight binding models we find that the crucial parameter is the difference in onsite energies of ligand O $2p_x$ and O $2p_y$ orbitals parallel and perpendicular to the Cu-O chain. Using this parameter, a microscopic explanation for the drastically different magnetic exchanges can be established. To illustrate the crucial influence of side groups we provide examples of H-containing compounds where a rotation of H even leads to a sign change of the superexchange interaction from strongly ferromagnetic to strongly antiferromagnetic.

15 min. break.

MA 52.6 Thu 16:45 HSZ 304

Field tunability of BKT correlations in the square-lattice Heisenberg antiferromagnet CuPOF — •D. Opherden[1,2], C. P. Landee[3], F. Bärtl[1,2], M. Uhlarz[1], Y. Skourski[1], A. N. Ponomaryov[1], S. A. Zvyagin[1], J. Wosnitza[1,2], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Clark University, Worcester, Massachusetts, USA

The metal-organic compound $[Cu(pz)_2(2\text{-}OHpy)_2](PF_6)_2$ (CuPOF) is a molecular-based realization of the 2D square-lattice $S = \frac{1}{2}$ Heisenberg antiferromagnet with well-separated Cu(pz) layers and a moderate intraplane coupling $J/k_B = 6.8$ K. We present a focus study of the low-T phase transition to long-range order, performed via ^{1}H and ^{31}P nuclear magnetic resonance and bulk magnetometry. A weak in-

trinsic easy-plane anisotropy, revealed by magnetization data, yields a temperature-driven crossover of the spin-exchange anisotropy from isotropic Heisenberg to anisotropic XY-type behavior. The application of a magnetic field normal to the easy-plane yields a field-driven increase of the magnetic anisotropy with the occurrence of Berezinskii-Kosterlitz-Thouless correlations, revealed by results of the ^{31}P spin-lattice relaxation rate close to the transition temperature to long-range order. A detailed analysis of the temperature-dependent order parameter demonstrates the possibility for a continuous tuning of the spin-exchange anisotropy in CuPOF, from almost ideal isotropic Heisenberg to nearly XY-type exchange at elevated fields.

MA 52.7 Thu 17:00 HSZ 304

Y-, La- and Lu-Agardite, preparation, crystal structure, vibrational and low-dimensional magnetic properties — •Aleksandr M. Golubev[1], Eva Brücher[1], Armin Schulz[1], Reinhard K. Kremer[1], Robert Glaum[2], and Myung-Hwan Whangbo[3] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Institut für Anorganische Chemie, Universität Bonn, 53121 Bonn, Germany — [3]Department of Chemistry North Carolina State University Raleigh, North Carolina 27695-8204, USA

We have prepared polycrystalline samples of Y, La- and Lu-agardite with composition $RECu_6(OH)_6(AsO_4)_3 \cdot n\ H_2O$ (RE = Y, La, Lu; n ≈ 3) and characterized their structural and vibrational properties as well as the magnetic behavior of the Cu^{2+} entities. The arsenates $RECu_6(OH)_6(AsO_4)_3 \cdot n\ H_2O$ (RE = Y, La, Lu; n ≈ 3) are isostructural with the mineral mixite and crystallize with a hexagonal structure which contains ribbons of edge-sharing $[CuO_5]$ square-pyramids extending along the hexagonal axis. They interconnect via $(AsO_4)^{3-}$ groups to form hexagonal tubes of about 10 Å inner diameter. Such zeolite-like tubes host water molecules, which can be reversibly removed at moderate temperature (≈ 100 °C). Like in mixite the Cu^{2+} cations in $RECu_6(OH)_6(AsO_4)_3 \cdot n\ H_2O$ (RE = Y, La, Lu; n ≈ 3) exhibit low-dimensional antiferromagnetic properties the character of which is subject to changes in the Cu-O-Cu bonding distances and bonding angles due to the lanthanide contraction. DFT calculations indicate that the strongest spin exchange pathways couple the Cu^{2+} S=1/2 magnetic moments predominantly within the hexagonal tubes.

MA 52.8 Thu 17:15 HSZ 304

Quantum phase transitions of Ising ferromagnets in tilted transverse fields — •Heike Eisenlohr and Matthias Vojta — Institut für theoretische Physik, Technische Universität Dresden, Germany

Transverse-field Ising magnets constitute a paradigmatic example for quantum phase transitions, with experimental realisations in e.g. $LiHoF_4$ and $CoNb_2O_6$. Here we theoretically analyze the fate of the field-driven zero-temperature transition upon tilting the field away from the direction perpendicular to the easy axis. While the transition turns into a crossover if the ordered phase is single-domain, a sharp transition remains in the multi-domain case relevant for a ferromagnet. We characterize this transition in detail, also discussing effects of domain-wall motion. Upon including nuclear spin degrees of freedom, we are able to link our results to experiments on $LiHoF_4$.

MA 52.9 Thu 17:30 HSZ 304

Chemical design strategies and field-induced phases in antiferromagnetically coupled organic spin-dimer systems — •Bernd Wolf[1], Lars Postulka[1], Paul Eibisch[1], Ulrich Tutsch[1], Martin Baumgarten[2], and Michael Lang[1] — [1]Physics Institute, Goethe-University, SFB/TR49, D-60438 Frankfurt (M) — [2]Max-Planck-Institute for Polymer Research, SFB/TR49, D-55128 Mainz

Coupled antiferromagnetic spin-dimer systems based on the stable organic radical units nitronyl-nitroxide (NN) and imino-nitroxide (IN) are recognized as suitable candidates for exploring critical phenomena under well-controlled conditions. For these systems the *intra*- and *inter*-dimer magnetic exchange interactions can be modified in specific ways. Depending on the geometry of the *inter*-dimer couplings, various scenarios can be observed. We discuss the magneto-structural correlations of selected materials based on tolan molecules linked together with NN- and IN-units. Furthermore, using low-temperature ac susceptibility and specific heat measurements we characterize the field-induced magnetic phases of these materials and discuss their critical behavior. In addition, we present a new approach for designing intermolecular magnetic exchange interactions based on planar π-bridges of benzo[1,2 -*b*:4,5 -*b'*] dithiophene derivatives which connect the stable NN and IN radical units. Our results demonstrate that π-stacking of the planar bridges allows a good control of the *inter*-molecular magnetic exchange.

MA 52.10 Thu 17:45 HSZ 304

Field-induced magnetic phase in quasi-one-dimensional $YbAlO_3$ — •Stanislav Nikitin[1,2], Liusuo Wu[3], Aleksandr Sukhanov[1,2], Nikolay Pavlovskiy[4], Jianhui Xu[5], Manuel Brando[1], Leonid Vasylechko[6], and Andrey Podlesnyak[7] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Technical University Dresden, Germany — [3]Southern University of Science and Technology, Shenzhen, China — [4]Kirensky Institute of Physics, Krasnoyarsk, Russia — [5]Helmholtz-Zentrum Berlin, Berlin, Germany — [6]Lviv Polytechnic National University, Lviv, Ukraine — [7]Oak Ridge National Laboratory, TN , USA

The antiferromagnetic Heisenberg S = 1/2 chain in magnetic field is one of the simplest model, which exhibits quantum critical behavior. In finite magnetic field below the QPT, a weak interchain interaction can stabilize an incommensurate spin-density wave phase, which propagation vector can be continuously tuned by magnetic field.

$YbAlO_3$ is a quasi-1D spin chain compound, where Yb moments form spin chain along the *c*-axis. In this work we studied excitation spectrum and magnetic structure of this materials by means of neutron scattering in magnetic field. We found that the excitation spectra are well described by simple Heisenberg model in magnetic field. However, in contrast to the simple spin-density wave ordering with propagation vector $\mathbf{q} = 2k_F$ as predicted by the Heisenberg model, the magnetic structure shows more complex behavior and drastically changes at $M/3$ plateau. We discuss a possible theory explanation for this behavior.