MA 10: Electron Theory of Magnetism and Correlations/Other Theory

Time: Monday 15:00–18:00 Location: EB 107

MA 10.1 Mon 15:00 EB 107

Broken-symmetry magnetic phases in two-dimensional triangulene crystals — João C. G. Henriques[1,2], Gonçalo Catarina[3], David Jacob[4], Alejandro Molina-Sánchez[5], •António T. Costa[1], and Joaquín Fernández-Rossier[1] — [1]International Iberian Nanotechnology Laboratory, Braga, Portugal — [2]Universidade de Santiago de Compostela, Santiago de Compostela, Spain — [3]Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [4]Universidad del País Vasco, San Sebastián, Spain — [5]University of Valencia, Valencia, Spain

We provide a theory of magnetic phases in 2D triangulene crystals, using both Hubbard model and density functional theory (DFT) calculations. We consider centrosymmetric, non-centrosymmetric and nitrogen-doped triangulene crystals. In the undoped cases, DFT and mean-field Hubbard model predict the emergence of broken-symmetry antiferromagnetic and ferrimagnetic phases. We also compute the spin wave spectrum of these crystals.The results are in excellent agreement with the predictions of a Heisenberg spin model derived from multi-configuration calculations for the unit cell.

For the N-doped case we show that the low energy excitations include strongly coupled spin and orbital degrees of freedom. The key ingredient is the existence of orbital degeneracy, which forces us to leave the benzenoid/half-filling scenario. We find a rich interplay between orbital and spin degrees of freedom that confirm the need to go beyond the spin-only paradigm.

MA 10.2 Mon 15:15 EB 107

Exploring Temperature-Dependent Magnetic Properties in NiO: A First Principles Study — •Ravi Kaushik[1,2], Ryota Ono[3], and Sergey Artyukhin[1] — [1]Italian Institute of Technology, Genova 16163, Italy — [2]University of Genova. Genova, Italy — [3]National Institute for Materials Science, Ibaraki, Japan

Knowing the magnetic Hamiltonian parameters, such as Heisenberg exchange constants, is crucial for describing magnetic properties of materials. Such parameters can be efficiently calculated using Density Functional Theory, which operates at T=0. Magnetic materials exhibit a complex interplay between spin, orbital, and lattice degrees of freedom, and magnetic exchange interactions are influenced by thermally excited phonons. Here we develop a method to compute the change in exchange constants with temperature, and test it on a paradigm antiferromagnet, NiO. Our approach is based on a special displacement method, which should be modified to use two specific configurations with opposite displacements, to average out the exchange contribution, linear in phonon amplitude. The results enable the calculation of magnetic exchange constants and modelling of magnetic systems, at finite temperatures and set the stage for more intricate studies in systems with complex interdependencies.

MA 10.3 Mon 15:30 EB 107

Analysis of the topology of NiS2 based on magnetic topological quantum chemistry — •Mikel Iraola[1,2], Iñigo Robredo[1,3], Martina Sondini[4], Titus Neupert[4], and Maia Vergniory[1,3] — [1]Donostia International Physics Center, Donostia-San Sebastián, Spain — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]University of Zürich, Zürich, Switzerland

NiS2 exhibits a non-collinear antiferromagnetic ordering that preserves the translational symmetry of the paramagnetic structure. Furthermore, previous theoretical works have reported that spin-orbit coupling and strong electronic interactions might play an important role in the electronic properties of the compound. Recently, experimental analyses have reported evidences of surface transport, hinting at the potential existence of surface conducting states of topological origin. This rich phenomenology makes NiS2 an interesting testbed to explore the interplay between magnetism, electron interactions and topology. In this work, we combine ab initio simulations and symmetry-based arguments to investigate the bulk and surface electronic structures of NiS2 within the framework of magnetic topological quantum chemistry.

MA 10.4 Mon 15:45 EB 107

Electronic and magnetic structures of $AgCrX_2$ (X=S, Se, Te) through first-principles density functional theory — •Seo-Jin Kim[1], Gesa Siemann[2], Chiara Bigi[2], Phil King[2], Giovanni Vinai[3], Vincent Polewczyk[3], Haijing Zhang[1], Michael Baenitz[1], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]SUPA, University of St. Andrews, St. Andrews, UK — [3]IOMCNR, Laboratorio TASC, Trieste, Italy

We present a comprehensive study of the electronic and magnetic structures of $AgCrX_2$ (X=S, Se, Te) using first-principles density functional theory. The dichalcogenide $AgCrX_2$ forms a layered triangular lattice akin to delafossite systems, but it lacks inversion symmetry. This absence contributes to unique properties, such as the spin-polarized surface state [1] and the unconventional anomalous Hall effect [2] in $AgCrSe_2$. Our previous experiments on $AgCrSe_2$ revealed a complex magnetic spin texture with a long cycloidal coupling in the plane and an anti-parallel coupling between layers below T_N=32K [3]. This investigation aims to analyze electronic structure variations resulting from different covalency introduced by substituting chalcogen atoms. Additionally, using hopping parameters extracted by the Wannier function approach, we explore the intricate interplay between crystal and magnetic structures across all compounds of the series.

[1] G.-R. Siemann et al., npj Quantum Mater. 8, 61 (2023). [2] S.-J. Kim et al., arXiv:2307.03541, Advanced Science (accepted; 2023). [3] M. Baenitz et al., Physical Review B, 104, 134410 (2021).

MA 10.5 Mon 16:00 EB 107

Instabilities towards weak ferromagnetism and spin spirals in the non-collinear anti-ferromagnet Mn_3Sn. — Lars Nordström[1], Anders Bergman[1], and •Ramon Cardias[2] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Instituto de Física, Universidade Federal Fluminense, 24210-346, Niterói RJ, Brazil

From accurate electronic structure calculations of the non-collinear antiferromagnet Mn_3Sn, the magnetic exchange interactions are obtained and used to study instabilities of the magnetic structure as well as to calculate the spectra of collective excitations. The initial antiferromagnetic structure with coplanar local magnetic moments rotated by 240° due to the frustration within the Kagome-like structure, is shown to be first unstable towards a magnetic structure with incomplete compensation of the antiferromagnetic moments, leading to a small ferromagnetic moment. In addition this structure in turn is further unstable towards a formation of an in-commensurate spiral. Both these instabilities are analysed and their origin is discussed in a more general context.

MA 10.6 Mon 16:15 EB 107

Two-particle self-consistent approach for broken symmetry phases — •Lorenzo Del Re — Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany

Spontaneous symmetry breaking of interacting fermion systems constitutes a major challenge for many-body theory due to the proliferation of scattering channels once degenerate in the symmetric phase. One example is given by the ferro/antiferromagnetic broken symmetry phase (BSP) of the Hubbard model, where vertices in the spin-transverse and spin-longitudinal channels become independent with a consequent increase in the computational power for their calculation.

Here we generalize the formalism of the non-perturbative Two-Particle-Self-Consistent method (TPSC) to treat broken SU(2) magnetic phases of the Hubbard model. We show how in the BSP, the sum-rule enforcement of susceptibilities must be accompanied by a modified gap equation resulting in a renormalisation of the order parameter, vertex corrections and the preservation of the gap-less feature of the Goldstone modes.

We then apply the theory to the antiferromagnetic phase of the 3D-Hubbard model in the cubic lattice at half-filling. We compare our results of double occupancies and staggered magnetisation to the ones obtained using Diagrammatic Monte Carlo showing good quantitative agreement between the two methods.

We argue how vertex corrections play a central role in lowering the Higgs resonance with respect to the quasi-particle excitation gap in the spin-longitudinal susceptibility, yielding a well visible Higgs-mode.

15 min. break

MA 10.7 Mon 16:45 EB 107

Magneto structural correlations in the binary compound Cr_3Se_4 — •Helge Rosner, Seojin Kim, Yurii Prots, Marcus Schmidt, and Michael Baenitz — Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

Cr_3Se_4 crystallises in a monoclinic lattice, structurally closely related to the rhombohedral chalcogenite delafossite-like systems $ACrX_2$ with A = Na, Cu, Ag and X = S, Se. In contrast to these intrinsically semiconducting materials with a nonmagnetic monovalent A site, in Cr_3Se_4 the distorted triangular $CrSe_2$ layers are separated by a formally trivalent and magnetic ion. Motivated by the reported exotic physical properties of the ternary $ACrX_2$ compounds, like multiferroic behaviour, unconventional magnetic ordering or anomalous Hall conductivity, we present here an ongoing joint experimental and theoretical study of the related binary material Cr_3Se_4. The metallic system undergoes an antiferromagnetic ordering at about 160 K which is strongly coupled to the crystal lattice. Density functional band structure calculations show that the conduction bands originate from strongly hybridised Cr-Se states with sizeable spin-orbit interaction. In a detailed comparison, we will highlight the similarities and differences between Cr_3Se_4 and the chalcogenite delafossites.

MA 10.8 Mon 17:00 EB 107

Paramagnons in $Na_xCa_{2-x}CuO_2Cl_2$ from a Quantum Cluster Approach using Matrix-Product States — •Abhiroop Lahiri[1], Sebastian Paeckel[2], Thomas Köhler[3], and Benjamin Lenz[1] — [1]IMPMC UMR-7590,CNRS, Sorbonne Université, Paris, France — [2]Ludwig-Maximilians-Universität München, Germany — [3]Uppsala Universitet, Uppsala, Sweden

In recent years, advances in the field of resonant inelastic x-ray scattering (RIXS) have rendered the measurement of paramagnons in doped cuprates feasible. In certain cases, the collective low-energy excitations seen in the RIXS map can be described to a good approximation by the dynamical spin structure factor. In this talk, we will show a comprehensive study of this quantity for a doped Hubbard-type model, tailored via ab initio simulations to the cuprate $Na_xCa_{2-x}CuO_2Cl_2$. In our calculations, we choose different quantum clusters and employ matrix-product states (MPS) to describe the cluster wave-function. This efficient way of representing the essential part of the Hilbert space allows us to treat cluster sizes within density matrix renormalization group that go beyond the scope of standard exact diagonalization solvers. In particular, our approach is based on a recently developed band-Lanczos method optimized for the use of MPS. We finally compare our results to the literature, in particular to cluster dynamical mean-field theory calculations and RIXS measurements of the material.

MA 10.9 Mon 17:15 EB 107

Modeling non-local Coulomb interaction in 2D Van der Waals materials using the DFT+$U+V$ method — •Wejdan Beida[1,2], Gustav Bihlmayer[1], Gregor Michalicek[1], Daniel Wortmann[1], Ersoy Sasioglu[3], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Physics Department, RWTH-Aachen University, 52062 Aachen, Germany — [3]Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle (Saale), Germany

For bilayer graphene it was found the non-local Coulomb interaction, denoted as V, is crucial for the description of the electronic structure [1]. In this presentation, we extend the investigation to 2D van der Waals materials characterized by covalent bonds between magnetic 3d-transition metal atoms and atoms possessing polarizable and delocalized p-electrons. To address this, we have theoretically formalized the incorporation of this interaction into a Hamiltonian model system and found renormalization of the magnetic interactions. Subsequently, we have implemented this theoretical framework into our FLEUR code [2], which is based on the Full-potential Linearized Augmented Plane Wave method. We comprehensively examined the impact of V on the electronic properties using the DFT+$U+V$ approach. V-values have been determined from microscopic theory on the level of constrained random phase approximation.

[1] Wehling, T. O., et al. Physical Review Letters 106.236805 (2011).
[2]FLEUR: https//doi.org/10.5281/zenodo.7778444

MA 10.10 Mon 17:30 EB 107

Quantum kinetic equation and thermal conductivity tensor for bosons — •Léo Mangeolle[1,2,3], Lucile Savary[1,2], and Leon Balents[2] — [1]ENS de Lyon, CNRS, Laboratoire de Physique, 46 allée d'Italie, 69007 Lyon, France — [2]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106 — [3]Technical University of Munich, School of Natural Sciences, Physics Department, 85748 Garching, Germany

We obtain a systematic derivation of the semi-classical kinetic equation for neutral bosons from their full quantum kinetic equation. It incorporates the semi-classical topological dynamics of wavepackets in the form of geometric properties of the energy eigenstates, such as the Berry phases and curvatures, generalized to phase space. This makes it possible to treat inhomogeneous systems, including boundaries, textures, etc., in a compact and natural manner. We compute the associated observable quantities, such as energy and current densities, away from equilibrium. In particular, the thermal conductivity tensor, which describes the energy current induced by a temperature gradient, is exactly obtained. This provides a self-contained and exact derivation of the intrinsic thermal Hall effect of neutral bosons such as phonons and magnons, in agreement with Kubo formula results while being considerably more intuitive, and naturally avoiding subtleties associated with magnetization currents. I will eventually present a few calculations using the derived quantum kinetic equation: - the local thermal Hall current of topological magnons in a collinear antiferromagnet, - the energy density and local currents in a skyrmion lattice.

MA 10.11 Mon 17:45 EB 107

Exploration of magnetism and flat bands in novel Kagome magnets — •Ryo Misawa[1], Rinsuke Yamada[1], Ryota Nakano[1], Milena Jovanovic[2], Maxim Avdeev[3], Taka-hisa Arima[4,5], Yusuke Nambu[6,7,8], Leslie Schoop[9], and Max Hirschberger[1,4] — [1]Dep. of Applied Physics, Univ. of Tokyo, Japan — [2]Dep. of Chemistry, North Carolina State Univ., USA — [3]ANSTO, Australia — [4]RIKEN CEMS, Japan — [5]Dep. of Advanced Materials Science, Univ. of Tokyo, Japan — [6]Inst. Materials Res., Tohoku Univ., Japan — [7]FOREST, Japan Science and Technology Agency, Japan — [8]Organization for Advanced Studies, Tohoku Univ., Japan — [9]Dep. of Chemistry, Princeton Univ., USA

Kagome metals, a class of materials intrinsically possessing both Dirac cones and flat bands, have shown their versatility as a platform for exotic quantum phases of matter, such as superconductivity and charge order. However, the interplay between flat bands and magnetism remains unexplored. We will talk about our exploration of novel Kagome magnets, where the magnetic contributions come from rare-earth elements, and flat bands arise near the Fermi energy from the transition metal.