TT 22: CE: Spin Systems and Itinerant Magnets

Time: Wednesday 9:30–13:15 Location: H21

TT 22.1 Wed 9:30 H21

Hydrodynamic Limit for the Spin Dynamics of the Heisenberg Chain — •Wolfram Brenig and Simon Grossjohann — Institute for Theoretical Physics, Technical University Braunschweig

We show that Quantum-Monte-Carlo calculations of the dynamic structure factor of the spin-1/2 antiferromagnetic Heisenberg chain at intermediate temperatures based on the stochastic series expansion method corroborate predictions for a diffusive behavior of the spin-dynamics at finite frequencies in the low-energy long wave-length limit. The temperature dependence of the scattering rate will be detailed and will be shown to be in good agreement with similar findings by bosonization and DMRG methods. Implications for NMR and spin-transport measurements will be discussed.

TT 22.2 Wed 9:45 H21

Non-abelian statistics in higher spin antiferromagnets — Burkhard Scharfenberger[1], Ronny Thomale[2], and •Martin Greiter[1] — [1]Institut für Theorie der Kondensierten Materie, KIT, 76128 Karlsruhe — [2]Department of Physics, Princeton University, Princeton, NJ 08544, USA

We conjecture, and provide some preliminary evidence, that spinons (and holons) in antiferromagnets with spin $S=2$ and higher generally obey non-abelian statistics (SU(2) level $k=2S$ anyons for S integer). The line of argument is as follows. In one dimension, a paradigm for a general $S=1$ spin chain (the AKLT chain) can be obtained by projecting two dimer (or Majumdar-Ghosh) chains with $S=1/2$ together. Similarly, we can obtain an $S=1$ spin liquid from projecting two $S=1/2$ chiral spin liquids together [M.Greiter, J.Low Temp. Phys. 126, 1029 (2002)]. In both cases, a discrete symmetry is violated for the $S=1/2$ models, which is restored for $S=1$. We assume that the $S=1$ spin liquid provides a paradigm of the disorderd $S=1$ antiferromagnet. If this is correct, we may further assume that an $S=2$ spin liquid generated by projecting two of these $S=1$ liquids together will in turn provide a paradigm of the disordered $S=2$ antiferromagnet. We provide evidence that the excitations of this $S=2$ spin liquid obey non-abelian statistics, and show that the degeneracy on a torus is $3\times 3=9$, as expected for two species of Ising (SU(2) level $k=1$) anyons with opposite chiralities.

TT 22.3 Wed 10:00 H21

An FRG approach for quantum antiferromagnets — •Johannes Reuther and Peter Wölfle — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Germany

We consider spin-1/2 Heisenberg antiferromagnets on two dimensional lattices. In particular we study the melting of magnetic order as an effect of frustration. Examples for such models are the J_1-J_2-model or the Heisenberg model on a triangular or Kagome lattice. The last two lattices are examples for geometrically frustrated systems. We rewrite the spin operators in the Hamiltonians in terms of auxiliary fermions which enable us to perform diagrammatic approximations. For the auxiliary particle constraint an exact projection scheme proposed by Popov and Fedotov is available. In order to sum up diagrams in a controlled way we apply the Functional Renormalization Group (FRG) in conjunction with a cutoff procedure called Katanin truncation. Calculating the magnetic susceptibility and the spin-spin correlations we are able to distinguish between magnetically ordered and paramagnetic phases. We find phase diagrams in good agreement with numerical studies.

TT 22.4 Wed 10:15 H21

Spin dynamics in nearly critical magnets with quenched disorder — •Matthias Vojta — Institut für Theoretische Physik, Universität zu Köln, Germany

Quanten phase transitions in quantum magnets, with coupled-dimer systems being prominent examples, have been extensively studied both experimentally and theoretically. In the absence of quenched disorder, the excitation spectrum near criticality is essentially understood. In contrast, relatively little is known about dynamical properties in the disordered case. Here we present numerical results for the fluctuation spectrum of coupled-dimer magnets with quenched disorder of random-mass type, obtained by a generalization of the bond-operator method. The results are directly applicable to doped dimer materials like (K,Tl)$CuCl_3$ and will also be discussed with an eye towards disordered stripe phases in cuprate superconductors.

TT 22.5 Wed 10:30 H21

Accurate spin susceptibilities for strongly correlated metals — •Lewin Boehnke[1], Olivier Parcollet[2], Michel Ferrero[3], and Frank Lechermann[1] — [1]1. ITP, Universität Hamburg, D-20355 Hamburg, Germany — [2]IPhT, CEA/DSM/IPhT-CNRS/URA 2306, CEA-Saclay, F-91191 Gif-sur-Yvette, France — [3]CPHT, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France

For many strongly correlated systems, the dynamical mean-field theory (DMFT) has proven its value as a numerically feasable and nevertheless physically sound approximation. In combination with the local density approximation (LDA), several material specific phenomena have been successfully studied. However, most of the former LDA+DMFT calculations in a manifest multi-orbital context were restricted to density-density interactions in the many-body hamiltonian and rather high temperatures. These restrictions rendered it difficult to accurately compute susceptibilities that are actually comparable with experimental data.

Due to the novel generation of continuous-time quantum-Monte-Carlo (CT-QMC) impurity solvers, these latter limitations have been lifted. Hence in this talk we want to present the computation of (frequency-dependent) spin susceptibilites for realistic correlated metals using the hybridization-expansion CT-QMC technique [1]. As a concrete example we will discuss the intriguing spin correlations in the strongly correlated Na_xCoO_2 system.

[1] P. Werner, A. Comanac, L. de' Medici, M. Troyer and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

TT 22.6 Wed 10:45 H21

Orbitally induced string formation in the spin-orbital polarons — •Krzysztof Wohlfeld[1], Andrzej M. Oles[2,3], and Peter Horsch[3] — [1]IFW Dresden, Germany — [2]Jagellonian University, Poland — [3]Max-Planck-Institut für Festkörperforschung, Germany

We study the spectral function of a single hole doped into an ab plane of a Mott insulator $LaVO_3$ with antiferromagnetic (AF) spin order of $S=1$ spins accompanied by alternating orbital (AO) order of active $\{yz,zx\}$ orbitals [1]. Starting from the respective t-J model, with spin-orbital superexchange and effective three-site hopping terms, we derive the polaron Hamiltonian and show that a hole couples simultaneously to the collective excitations of the AF/AO phase, magnons and orbitons. Next, we solve this polaron problem using the self-consistent Born approximation and find a stable quasiparticle solution — a spin-orbital polaron. We show that the spin-orbital polaron resembles the orbital polaron found in e_g systems, as e.g. in K_2CuF_4 or (to some extent) in $LaMnO_3$, and that the hole may be seen as confined in a string-like potential. However, the spins also play a crucial role in the formation of this polaron — we explain how the orbital degrees of freedom: (i) confine the spin dynamics acting on the hole as the classical Ising spins, and (ii) generate the string potential which is of the joined spin-orbital character. Finally, we discuss the impact of the results presented here on the understanding of the phase diagrams of the lightly doped cubic vanadates.

[1] K. Wohlfeld, A. M. Oleś, and P. Horsch, Phys. Rev. B **79**, 224433 (2009).

15 min. break

TT 22.7 Wed 11:15 H21

Dynamic topological spin clusters in the paramagnetic phase of MnSi. — •A. Hamann[1], D. Lamago[1,2], T. Wolf[1], H. v. Löhneysen[1], and D. Reznik[1] — [1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Laboratoire Léon Brillouin, CEA Saclay, France

At ambient pressure and below T_C spins in MnSi order in a helical ground state with the helix axis pinned by the crystal potential. At high pressure an exotic spin state forms referred to as partial order [1]. It is characterized by translational helical spin order but orientational disorder and the non-Fermi-liquid resistivity appears nearby in the phase diagram.

Our numerical calculations show that in the absence of the pinning potential isotropic near-neighbor chiral spin interactions of MnSi favor a glassy collection of topological spin clusters. These have the spectral signature of partial order. Their stability relative to the helical order increases with increasing temperature, and a competition with these clusters, not conventional fluctuations, melts the helical phase. Our detailed neutron scattering measurements fully confirm this prediction by identifying partial order at ambient pressure. We show that this partial order may explain most of the puzzling properties of MnSi including the two-component phase transition that was revealed by specific heat [2].

[1] C. Pfleiderer, D. Reznik et al., Nature **427**, 227 (2004)
[2] S. M. Stishov et al., Phys. Rev. B **76**, 052405 (2007)

TT 22.8 Wed 11:30 H21

Dynamics in the B-T phase diagram of MnSi measured with MIEZE — •Georg Brandl[1,2], Robert Georgii[1,2], Christian Pfleiderer[1], and Peter Böni[1] — [1]Physik Department E21, Technische Universität München, 85747 Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, Technische Universität München, 85747 Garching, Germany

MIEZE (Modulation of IntEnsity by Zero Effort) has been proposed some time ago as a variant of the NRSE technique [1], having the advantage of preparing the beam modulation before the sample. This allows measurements under experimental conditions causing depolarization, such as magnetic samples or samples in an applied magnetic field without losing signal intensity, while keeping the high resolution of the spin echo technique. Yet, despite being potentially very attractive the MIEZE technique has so far not been used to tackle real scientific problems. We report the development of a MIEZE set up on the very cold neutron beam line MIRA at the FRM II. We have used the MIEZE technique at MIRA to study the skyrmion lattice in the B20 compound MnSi [2], a novel magnetic state composed of particle-like spin textures with non-trivial topology that forms in an applied magnetic field. We have measured the linewidth of the magnetic scattering at the position of the magnetic satellites throughout the B-T-diagram of MnSi. The results give us a clue on the stability of the various magnetic structures of MnSi.

[1] R. Gähler, R. Golub, T. Keller, Physica B, 180, 899 (1992)
[2] S. Mühlbauer et al., Science 323, 915 (2009)

TT 22.9 Wed 11:45 H21

Quantum Phase Transitions in Single-Crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$: I. Crystal Growth, Magnetization and Specific Heat — •Andreas Bauer, Andreas Neubauer, Christian Franz, and Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85747 Garching, Germany

The helimagnetic transition in MnSi is suppressed under substitutional doping with Fe and Co on the Mn site. We report a comprehensive study of the magnetization and specific heat of single-crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$. With increasing concentration x the magnetic phase diagram remains essentially unchanged, exhibiting three phases (helical order, conical order and the Skyrmion lattice phase). In addition an extended cross-over regime exists between the paramagnetic and the helimagnetic state. When suppressing the magnetic modulations in an applied magnetic field, it is possible to infer the evolution of the underlying weakly ferromagnetic state as a function of x. In contrast to the pressure depencence of pure MnSi, which shows a first order quantum phase transition, we observe strong evidence for ferromagnetic quantum criticality.

TT 22.10 Wed 12:00 H21

Quantum Phase Transitions in Single-Crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$: II. Small Angle Neutron Scattering — •Tim Adams[1], Sebastian Mühlbauer[1], Andreas Bauer[1], Andreas Neubauer[1], Christian Franz[1], Robert Georgii[2], Peter Böni[1], and Christian Pfleiderer[1] — [1]Technische Universität München, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, Garching, Germany

We report a comprehensive small angle neutron scattering study of the evolution of the magnetic phase diagram in $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$. With increasing concentration x the magnetic phase diagram remains essentially unchanged, exhibiting a well defined helimagnetic, conical and Skyrmion lattice phase up to $X \approx 0.5x_c$, where x_c is the critical concentration for which the helimagnetic transition temperature vanishes. Surprisingly, for concentrations $x \to x_c$ the magnetisation, susceptibility and specific heat are still akin the magnetic phase diagram of pure MnSi, but small angle neutron scattering suggests the emergence of complex spin textures. Similarities and differences with the pressure-temperature phase diagram of pure MnSi and the doped semiconductor $Fe_{1-x}Co_xSi$ will be discussed.

TT 22.11 Wed 12:15 H21

Quantum Phase Transitions in Single-Crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$: III. Magnetoresistance and Hall effect — •Christian Franz — Physik Department E21, Technische Universität München, München, Germany

Complex spin textures with non-trivial topology may generate anomalous contributions in the Hall conductivity, the so-called topological Hall effect, that provide direct evidence of non-vanishing winding numbers. We report a comprehensive study of the evolution of the spin structures and spin textures in $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$ by means of the magnetoresistance and the Hall effect. Our study identifies the A-phase, located just below the helimagnetic transition, as a sykrmion lattice for a wide range of x. Combining the bulk properties and small angle neutron scattering with our Hall effect data additionally suggests the formation of non-trivial spin textures in parameter regimes outside the A phase when approaching quantum criticality under Fe- and Co-doping. Similarities and differences with pure MnSi and the doped semiconductor $Fe_{1-x}Co_xSi$ will be discussed.

TT 22.12 Wed 12:30 H21

Low-dimensional magnetic properties of anhydrous (black) dioptase. — •J. M. Law[1], C. Hoch[1], M.-H. Whangbo[2], and R. K. Kremer[1] — [1]Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204, U.S.A.

Hydrous dioptase, $CuSiO_3{\cdot}H_2O$ is a low-dimensional quantum antiferromagnet. From a theoretical and experimental investigation it was proposed that hydrous dioptase is close to a quantum critical point.[1] Anhydrous dioptase, $CuSiO_3$ has a very similar magnetic lattice. We carried out a single-crystal structure determination and investigated the magnetic properties of anhydrous dioptase by carrying out specific heat and magnetic susceptibility measurements and performed a spin dimer analysis based on extended Hückel tight-binding calculations. We found that anhydrous dioptase conforms very well to a $S{=}1/2$ antiferromagnetic quantum chain model with uniform nearest-neighbor exchange interaction. Intra-chain interaction is by two orders of magnitude smaller than inter-chain superexchange and leads to long-range antiferromagnetic ordering at about 5 K.

[1] C. Gros *et al.*,*Europhys. Lett.* **2002**, *60*, 276.

TT 22.13 Wed 12:45 H21

Probing spin correlations in the highly frustrated magnets $CdCr_2O_4$ and $ZnCr_2O_4$ — •Christian Kant[1], Joachim Deisenhofer[1], Torsten Rudolf[1], Franz Mayr[1], Florian Schrettle[1], Vladimir Tsurkan[1,2], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chisinau, Republic of Moldova

The spinel systems $CdCr_2O_4$ and $ZnCr_2O_4$ can be regarded as paradigms for highly frustrated systems where antiferromagnetic nearest-neighbor Heisenberg exchange leads to inherent frustration and considerable degeneracy of the magnetic ground state.

We performed optical, magnetic susceptibility, and specific heat measurements on single crystals of both compounds. From the magnetic susceptibility we estimate the nearest-neighbor and next-nearest neighbor exchange constants. The spin-spin correlation functions is derived from the magnetic susceptibility and the magnetic contribution to the specific heat. Comparing the frequency shift of the infrared optical phonons above T_N, we obtain the spin-phonon coupling constant in both systems.

TT 22.14 Wed 13:00 H21

High pressure studies in $Ca_3Ru_2O_7$ — •Oliver Welzel[1], Naoki Kikugawa[2], Andrew Mackenzie[3], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]National Institute for Materials Science, 1-2-1 Sengen, Tsukuba 305-0047, Japan — [3]Scottish Universities Physics Alliance, School of Physics & Astronomy, University of St Andrews, UK

The bilayer ruthenate $Ca_3Ru_2O_7$ undergoes first a magnetic transition (T_N = 56 K) and then a structural transition (T_S = 48 K) on cooling. Most of the Fermi surface is gapped out at low temperature, leading to a very low carrier density and small Fermi surface pockets. Pressure suppresses both T_N and T_S and, for $p > 3.5$ GPa, induces a third low temperature state, which has been known to be robust up to at least 7.5 GPa.

A detailed investigation of the unusual low temperature states of $Ca_3Ru_2O_7$ across the pressure-temperature-field phase diagram requires reliable access to hydrostatic pressures up to and beyond 10 GPa. We apply lithographic patterning and sputtering processes to anvil pressure cells in order to produce complex but robust lead patterns, which are integrated into the anvil surface. Patterns include multi-turn coils as well as eight-lead configurations for resistivity measurements.

Resistivity data in $Ca_3Ru_2O_7$ is presented, which indicates that the high pressure ordered state is fully suppressed at $p_c \simeq 9.5$ GPa. Beyond p_c, the in-plane resistivity follows a $T^{5/3}$ power-law down to below 1 K, suggesting ferromagnetic quantum criticality