# TT 42: Poster: Correlated Electrons I

Time: Wednesday 15:00–18:00

TT 42.1 Wed 15:00  $\mathrm{P2}/\mathrm{OG2}$ 

Single crystal growth and characterization of CeCoIn<sub>5</sub> and Ce<sub>2</sub>IrIn<sub>8</sub> — •ANJA PHILIPP, KRISTIN KLIEMT, and CORNELIUS KRELLNER — Max-von-Laue-Straße 1

The heavy-fermion series  $\operatorname{Ce}_n \operatorname{T}_m \operatorname{In}_{3n+2}$  (n=1,2; T = Co, Rh, Ir) with the unique tetragonal crystal structure, leading to a quasi-two dimensional Fermi surface, received growing attention over the past decades [1],[2],[3]. In these compounds, there are strong electronic interactions between conduction electrons and localized 4f-electrons of the Ce ions, which lead to a variety of interesting phenomena like spin and valence fluctuations, Kondo effect, magnetic order, non Fermi-liquid behaviour and unconventional superconductivity [3].

In this contribution, the results of the self-flux growth of  $CeCoIn_5$ and  $Ce_2InIr_8$  single crystals are shown. The crystallographic orientation of the single crystals was determined using microscopy and Laue X-ray diffraction. The physical properties like resistivity, heat capacity and magnetic susceptibility down to 2K were measured for both compounds and were analyzed in this work.

[1] R.T. Maculso et al., Chem Mater. 15, 1394 (2003)

[2] G.D. Morris et al., Phys. Rev. B 69, 214415 (2004)

[3] A. Ikeda et al., Phys. Soc. Jap. 70, 2248 (2001)

TT 42.2 Wed 15:00 P2/OG2 Search for superconductivity in CeSb<sub>2</sub> under chemical pressure — •JAN WEBER, KRISTIN KLIEMT, and CORNELIUS KRELLNER — Max-von-Laue Straße 1, 60438 Frankfurt am Main, Physikalisches Institut

Recently, an unconventional superconducting state was discovered at a pressure-induced magnetic quantum critical point in the Kondo-lattice system  $CeSb_2[1]$ . Under normal pressure  $CeSb_2$  crystallizes in the orthorombic SmSb<sub>2</sub> structure (Space group 64) [2]. At high pressures, the crystal structure changes and  $CeSb_2$  adopts the ZrSi<sub>2</sub> - structure (Space group 63)[1]. This change in structure precedes the superconductivity around the magnetic quantum critical point. In this contribution, we present first attempts to replace the physical pressure using adequate substituents to reproduce the high-pressure structure at ambient pressure.

[1] O.P. Squire et. al., arXiv:2211.00975 [cond-mat.str-el] (2022)

[2] R. Wang et. al., Inorg. Chem. 6, 1685 (1967)

TT 42.3 Wed 15:00 P2/OG2 Searching for the critical endpoint in cobalt-doped EuRh<sub>2</sub>Si<sub>2</sub> — •FRANZISKA WALTHER, ALEXEJ KRAIKER, KRISTIN KLIEMT, and CORNELIUS KRELLNER — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

The ternary europium-based intermetallic compounds with the ThCr<sub>2</sub>Si<sub>2</sub>-type structure show a variety of intriguing physical properties due to the coupling between lattice and electronic degrees of freedom. Eu ions can be present in a magnetic divalent or non-magnetic trivalent state. Under variation of temperature and pressure, it's possible to enforce a valence transition associated with a change of the unit cell volume [1]. At ambient pressure, EuRh<sub>2</sub>Si<sub>2</sub> orders antiferromagnetically below  $T_N = 24$  K in a stable divalent state [2], whereas the isoelectronic related compound EuCo<sub>2</sub>Si<sub>2</sub> is nearly trivalent und indicates no magnetic ordering [1]. EuRh<sub>2</sub>Si<sub>2</sub> undergoes a pressureinduced first order valence transition [3]. We expect the second order critical endpoint in the pressure range from 1.7 to 2.1 GPa, where the first-order phase transition terminates and critical elasticity may occur. We want to approach the critical endpoint by applying chemical pressure through substituting Rh in EuRh<sub>2</sub>Si<sub>2</sub> with Co. We report on the growth of samples of the  $Eu(Rh_{1-x}Co_x)_2Si_2$  -system and the characterization of their physical and chemical properties.

[1] Y. Onuki et al., J. Phys. Soc. Japan 89, 102001 (2020)

[2] S. Seiro, C. Geibel, J. Phys.: Condens. Matter 26, 046002, (2014)
[3] F. Honda *et al.*, J. Phys. Soc. Japan 85, 063701 (2016)

#### TT 42.4 Wed 15:00 P2/OG2

Symmetry-broken low-temperature state in the Kondo system  $Ce_2Rh_2Ga - \bullet SAJAL$  NADUVILE THADATHIL<sup>1,2</sup>, J STIRNAT<sup>1,2</sup>, P DEVI<sup>1</sup>, M BAENITZ<sup>3</sup>, A STRYDOM<sup>4</sup>, D SOHOLOV<sup>4</sup>, J WOSNITZA<sup>1,2</sup>, and T HELM<sup>1</sup> - <sup>1</sup>Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Germany - <sup>2</sup>Institute of Solid State and Materials Physics, TU Dresden, Germany —  $^3{\rm Max}$  Planck Institute for Chemical Physics of Solid, Dresden, Germany —  $^4{\rm University}$  of Johannesburg, South Africa

Cerium-based heavy-fermion conductors often exhibit unconventional transport and thermodynamic properties related to 4f-electron physics. Ce<sub>2</sub>Rh<sub>2</sub>Ga exhibits a structural phase transition around  $T_{\rm p} \approx 130$  K from an orthorhombic to monoclinic crystal structure accompanied by an extreme anisotropy in its electrical conduction. Recent nuclear quadrupole resonance studies on polycrystals found evidence for the emergence of two inequivalent Ce ions below 2 K with different electronic environments that may provide grounds for multion Kondo physics [1]. Here, we present results from magnetotransport studies on micron-sized devices cut from single crystals. We investigated the anisotropy between 0.3 and 300 K in fields up to 16 T. Below 5 K, the angular dependence of the magnetoresistance exhibits a significant change in its rotational anisotropy, indicating a broken symmetry. These findings may provide further evidence for multi-ion Kondo physics in Ce<sub>2</sub>Rh<sub>2</sub>Ga.

[1] Sh. Yamamoto et al., Phys. Rev. B 106, 115125 (2022)

TT 42.5 Wed 15:00 P2/OG2 Spin excitations in the field-induced phase of Ce<sub>2</sub>Bi — •Nikolai Pavlovskii<sup>1</sup>, Anton Kulbakov<sup>1</sup>, Aleksandr Sukhanov<sup>1</sup>, Michael Smidman<sup>2</sup>, Federico Mazza<sup>3</sup>, and Dmytro Inosov<sup>1</sup> — <sup>1</sup>TU Dresden, Dresden, Germany — <sup>2</sup>Zhejiang University, Hangzhou, China — <sup>3</sup>Vienna University of Technology, Austria

The compound Ce<sub>2</sub>Bi represents a rare example of the heavy fermion materials that exhibit the coexistence of an antiferromagnetic magnetic (AFM) order and a tricritical point (TCP) in their temperature-magnetic field phase diagram. This combination is unusual because the TCP typically occurs in the ferromagnetic (FM) heavy fermion materials. In AFMs, the magnetic order can in many cases be continuously suppressed to zero temperature at a quantum critical point (QCP) by tuning pressure, magnetic fields, or chemical substitution. In the case of FMs, the situation is usually different. There, a QCP is generally avoided by changing the character of the magnetic magnetic magnetic number to the first order, which induces a TCP. Using neutron time-of-flight spectroscopy, we observed two weakly-dispersed magnetic excitations modes in Ce<sub>2</sub>Bi below Neel temperature that seem to show a nontrivial response to the applied magnetic field.

TT 42.6 Wed 15:00 P2/OG2 Transverse-field susceptibility of spin freezing at the mesoscale quantum phase transitions in LiHoF<sub>4</sub> — •MICHAEL LAMPL, ANDREAS WENDL, FELIX RUCKER, and CHRISTIAN PFLEI-DERER — Physik-Department, Technical University of Munich, 85748 Garching, Germany

The perhaps best understood example of a quantum critical point is the response of the dipolar Ising ferromagnet LiHoF<sub>4</sub> under a transverse field [1-3]. When tilting the magnetic field away from the hard axis such that the Ising symmetry is always broken, a line of well-defined phase transitions emerges from the transverse-field quantum critical point, characteristic of further symmetry breaking, and in stark contrast to a crossover expected microscopically [4]. Detailed theoretical modelling in excellent agreement with experiment identifies this line of phase transitions as mesoscale quantum criticality. We report an experimental study of the transverse-field susceptibility of this mesoscale quantum criticality into a regime of spin freezing under large field tilting angles. Our observations will be compared with the characteristics of spin freezing, kinetic arrest, and quantum annealing observed in heavily diluted LiHo<sub>x</sub>Y<sub>1-x</sub>F<sub>4</sub>.

[1] D. Bitko et al., Phys. Rev. Lett. 77, 940 (1996)

[2] H. M. Ronnow et al., Science **308**, 389 (2005)

[3] P. B. Chakraborty et al., Phys. Rev. B 70, 144411 (2004)

[4] A. Wendl et al., Nature **609**, 65 (2022)

TT 42.7 Wed 15:00 P2/OG2 Phase diagram study of the Falicov-Kimball model on the two-dimensional Kagome lattice — Younes Javanmard<sup>1</sup> and •Ammar Nejatri<sup>2</sup> — <sup>1</sup>Leibniz Universität Hannover, Hannover, Germany — <sup>2</sup>Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich

Location: P2/OG2

Wednesday

The Falicov-Kimball Model (FKM) is a relatively simple model of coupled quantum and classic degrees of freedom, in the middle of the spectrum between the Hubbard and the Anderson models. A number of studies have revealed its rich phase diagram in two-dimensional lattices, e.g. square and triangular lattices [1,2]. In a square lattice with half-filling, depending on the interaction strength and temperature, FKM exhibits a rich variety of phases: At sufficiently low temperatures, there is a charge density wave (CDW) phase; at high temperatures and weak interactions, a weakly localized phase appears which becomes an Anderson-localized phase in the thermodynamic limit; at high temperatures and strong interactions, a Mott insulating phase emerges [1]. In addition, there are two other phases called "quantum liquid" and "classical liquid" in triangular lattices and away from half-filling at sufficiently low temperatures and weak interactions [2].

We set up a Monte Carlo algorithm for the two-dimensional FKM away from the half-filling regime on a Kagome lattice to study this model's rich phase diagram, and to extend the previous studies regarding the consequences of geometry on the emegent quantum phases and the corresponding phase transitions.

[1] Phys. Rev. Lett. 117, 146601

[2] Phys. Rev. Lett. 122, 197601

### TT 42.8 Wed 15:00 P2/OG2

Quantum-critical properties of random transverse-field Ising models extracted by quantum Monte Carlo methods — •CALVIN KRÄMER, ANJA LANGHELD, JAN KOZIOL, MAX HÖRMANN, and KAI PHILLIP SCHMIDT — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

The transverse-field Ising model with quenched disorder is studied in one and two dimensions at zero temperature by stochastic series expansion quantum Monte Carlo simulations. Using a sample-replication method we are able to determine distributions of pseudo-critical points, from which critical shift and width exponents  $\nu_{s/w}$  are extracted by finite-size scaling. The scaling of the averaged magnetisation at the critical points is used further to determine the order-parameter critical exponent  $\beta$ . The dynamical scaling in the Griffiths phase is investigated by measuring the local susceptibility in the disordered phase and the critical exponent z' is extracted.

### TT 42.9 Wed 15:00 P2/OG2

Numerical investigation of the Ising model in a light-induced quantized transverse field — •ANJA LANGHELD and KAI PHILLIP SCHMIDT — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Friedrich-Alexander Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We investigate the Ising model in a light-induced quantized transverse field [1] with a particular focus on antiferromagnetic, potentially frustrated Ising interactions. Using exact diagonalization, we provide data for the antiferromagnetic chain in a longitudinal field that is inconsistent with earlier results coming from mean-field considerations [2]. In order to study the model on frustrated, two-dimensional lattice geometries, we extend the mean-field calculation and develop a quantum Monte Carlo update based on the recently introduced wormhole update [3], for which the photons are integrated out. By this means, the photons induce a retarded spin-spin interaction in imaginary time that is also non-local in space in contrast to the Ising interaction inherent to the model.

- [1] J. Rohn et al., Phys. Rev. Research 2, 023131 (2020)
- [2] Y. Zhang et al., Sci. Rep. 4, 4083 (2014)
- [3] M. Weber et al., Phys. Rev. Lett. 119, 097401 (2017)

### TT 42.10 Wed 15:00 P2/OG2

High-order series expansions and crystalline structures for Rydberg atom arrays — •ANTONIA DUFT, JAN KOZIOL, MATTHIAS MÜHLHAUSER, PATICK ADELHARDT, and KAI PHILLIP SCHMIDT — Friedrich-Alexander-Universität Erlangen-Nürnberg

We investigate a model of hardcore bosons on the links of a Kagome lattice subject to a long-range decaying van-der-Waals interaction. This model is known to be the relevant microscopic description of Rydberg atom arrays excited by a detuned laser field which has been realized in experiments recently. Particular interest lies on this system as it is an engineerable quantum platform which has been predicted to to host a topological phase. We investigate the quantum phase diagram for different limiting cases with a main focus on the low interaction-strength limit where we apply high-order linked cluster expansions. TT 42.11 Wed 15:00 P2/OG2

Superexchange and spin-orbit coupling in the half-filled  $t_{2g}$  shell — •MARCO SCHÖNLEBER, DANIEL PRANJIC, and MARIA DAGHOFER — Insitut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

Strongly correlated and spin-orbit coupled  $t_{2g}$  systems have been extensively investigated. By coupling orbital and spin angular momentum into one quantity, spin-orbit coupling (SOC) tends to reduce orbital degeneracy, e.g. for the widely studied case of one hole in the  $t_{2g}$  shell. However, the opposite has to be expected at half filling. Without spin-orbit coupling, all orbitals are half filled, no orbital degree of freedom is left and coupling to the lattice can be expected to be small. At dominant spin-orbit coupling, in contrast, one of the j = 3/2 states is empty and the system couples to the lattice. We investigate this issue. One finding is that the low-energy manifold evolves smoothly from the four S = 3/2 states in the absence of SOC to the four j = 3/2 states with dominant SOC. These fur states are always separated from other states by a robust gap. We then discuss relevant superexchange models.

TT 42.12 Wed 15:00 P2/OG2 From linear to circular polarized light - Floquet engineering in Kitaev-Heisenberg materials with Lissajous figures — •PASCAL STROBEL<sup>1</sup> and MARIA DAGHOFER<sup>1,2</sup> — <sup>1</sup>Institute for Functional Matter and Quantum Technologies, University of Stuttgart, 70550 Stuttgart, Germany — <sup>2</sup>Center for Integrated Quantum Science and Technology, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Floquet engineering is a promising tool for tuning magnetic interactions in the candidate Kitaev material  $\alpha$ -RuCL<sub>3</sub>. Amplitude and frequency of the time periodic light field are able to modulate both sign and strength of Kitaev-, Heisenberg-, and  $\Gamma$ -interactions present in  $\alpha$ -RuCl<sub>3</sub>. This paves the way of possibly driving  $\alpha$ -RuCL<sub>3</sub> into the sought after Kitaev spin-liquid phase.

We want to discuss possibilities of Floquet engineering with arbitrary polarized light in  $\alpha$ -RuCl<sub>3</sub>. In order to do so, we describe the influence of arbitrary polarization via an effective model including Lissajous figures. This model is derived via perturbation theory up to fourth order. Starting from linear and circular polarized light we bridge the gap between those two limiting cases. Moreover we study more complex Lissajous figures and general trends arising for them.

TT 42.13 Wed 15:00 P2/OG2 Complete field-induced spectral response of the spin-1/2triangular-lattice antiferromagnet  $CsYbSe_2 - \bullet Stanislav$ NIKITIN<sup>1</sup>, T. XIE<sup>2</sup>, A. A. EBERHARTER<sup>7</sup>, J. XING<sup>2</sup>, S. NISHIMOTO<sup>3,4</sup>, M. Brando<sup>5</sup>, P. Khanenko<sup>5</sup>, J. Sichelschmidt<sup>5</sup>, A. A. Turrini<sup>1</sup> D. G.  $\mathrm{Mazzone^1},$  P. G.  $\mathrm{Naumov^1},$  L. D.  $\mathrm{Sanjeewa^2},$  A. S.  $\mathrm{Sefat^2}$ B. NORMAND<sup>1,6</sup>, A. M. LAUCHLI<sup>1,6</sup>, and A. PODLESNYAK<sup>2</sup> — <sup>1</sup>Paul Scherrer Institut, Switzerland — <sup>2</sup>Oak Ridge National Laboratory, USA — <sup>3</sup>TU Dresden, Germany — <sup>4</sup>IFW, Germany — <sup>5</sup>MPI CPfS, Germany — <sup>6</sup>EPFL, Switzerland — <sup>7</sup>Universitat Innsbruck, Austria The spin 1/2 triangular lattice Heisenberg antiferromagnet remains on of the most attractive models to explore highly entangled quantum spin states in proximity to magnetic order. In my presentation I will discuss our recent results on CsYbSe<sub>2</sub>. This materials exhibits strong two-dimensional magnetic behavior in absence of exchange and structural disorder and its spin Hamiltonian is well described by  $J_1-J_2$ AFM Heisenberg model. We performed comprehensive INS measurements over the whole field scale starting from zero field up to the saturation and observed that corresponding excitation spectra evolve from continuum-like to relatively sharp spin-wave modes in the upup-down phase, then back to continua and back to spin waves. We further support our observation by cylinder MPS calculation, which reproduce all observed features with semi-quantitative accuracy. Thus our comprehensive experimental and theoretical analysis of the fieldinduced spin excitations in the CsYbSe<sub>2</sub> provides valuable insight into the dynamics of a broad class of quantum many-body systems.

TT 42.14 Wed 15:00 P2/OG2 Low energy, mobile excitations in herbertsmithite revealed by magnetothermal conductivity — •RALF CLAUS, JAN BRUIN, YOSUKE MATSUMOTO, JÜRGEN NUSS, MASAHIKO ISOBE, and HI-DENORI TAKAGI — Max Planck Institute for Solid State Research, Stuttgart, Germany

We report the magnetothermal conductivity k(B) of the Kagome quan-

tum spin liquid candidate herbertsmithite  $(\text{ZnCu}_3(\text{OH})_6\text{Cl}_2)$  in the temperature range from 100 mK to 70 K with applied magnetic fields up to 12 T for heat flow parallel and perpendicular to the Kagome planes. We identify both phonon and magnetic contributions to k and find that the latter is only present for heat flow within the Kagome planes. These 2D magnetic contributions persist down to at least 200 mK, consistent with the presence of low-lying quantum spin liquid excitations with a gapless excitation spectrum.

#### TT 42.15 Wed 15:00 P2/OG2

Field-tuned critical fluctuations in the triangular-lattice delafossite NaYbO<sub>2</sub> probed by <sup>23</sup>Na NMR — •S. LUTHER<sup>1,2</sup>, K. M. RANJITH<sup>3,4</sup>, D. OPHERDEN<sup>1</sup>, S. KHIM<sup>3</sup>, H. YASUOKA<sup>3</sup>, J. WOSNITZA<sup>1,2</sup>, M. BAENITZ<sup>3</sup>, and H. KÜHNE<sup>1</sup> — <sup>1</sup>Hochfeld-Magnetlabor Dresden, HZDR — <sup>2</sup>Institut für Festkörper- und Materialphysik, TU Dresden —  ${}^{3}$ MPI-CPfS, Dresden —  ${}^{4}$ IFW Dresden The frustrated triangular-lattice delafossite NaYbO<sub>2</sub> is a promising candidate for realizing a quantum spin liquid (QSL) ground state. The combination of a strong spin-orbit coupling and crystalline-electricfield effects leads to a magnetic anisotropy and a pseudospin-1/2 state of the Yb<sup>3+</sup> ions at low temperatures. The absence of magnetic order and emergence of pronounced low-energy spin fluctuations have been shown by several experimental techniques, such as specific heat, inelastic neutron scattering, and muon spin relaxation. We present <sup>23</sup>Na NMR investigations of the low-temperature spin correlations by means of spectroscopy and  $1/T_1$  measurements of polycrystalline NaYbO<sub>2</sub>. At small magnetic fields and low temperatures, a strongly increased  $1/T_1$  rate, as well as the absence of significant spectral line broadening suggest the presence of a QSL ground state with critical fluctuations at the verge of a magnetic instability. Above about 1 T, a crossover regime with persistent strong spin fluctuations and an onset of static magnetic ordering is observed. For fields above about 2 T, the formation of fieldinduced long-range magnetic order yields a strongly suppressed  $1/T_1$ rate and an inhomogeneously broadened spectral lineshape.

#### TT 42.16 Wed 15:00 P2/OG2

Disorder effects in spiral spin liquids —  $\bullet$  PEDRO MONTEIRO CÔNSOLI and MATTHIAS VOJTA — Institut für Theoretische Physik, TU Dresden

Spiral spin liquids are a special kind of paramagnetic state that features a subextensive classical ground-state degeneracy related to a family of spin spirals whose ordering wave vectors form a submanifold of momentum space. As the number of their theoretical and experimental realizations grows, there is cumulative evidence that, under additional perturbations, spiral spin liquids constitute a promising platform for the emergence of exotic phases of matter and excitations, including quantum spin liquids, multiple-q states, and skyrmions. However, little is known about their response to quenched disorder. In this poster, we investigate how various types of defects affect the classical ground-state manifold of a spiral spin liquid on the honeycomb lattice. Among our results, we describe how different order-by-disorder mechanisms can arise, compete among themselves, and lead to spin-glass physics in these systems.

# $TT \ 42.17 \quad Wed \ 15:00 \quad P2/OG2$

Second-harmonic generation in the Kitaev model — •OLESIA KRUPNITSKA<sup>1,2</sup> and WOLFRAM BRENIG<sup>1</sup> — <sup>1</sup>Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — <sup>2</sup>Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 1 Svientsitskii Street, Lviv, 79011, Ukraine

Optical spectroscopies are important probes for elementary excitations of quantum magnets. In the present study, we investigate secondharmonic generation in the hexagonal Kitaev model induced by external electric fields. The prime interest is to identify fingerprints of fractionalization as has been shown to exist in this model in terms of Majorana particles and gauge excitations. For that purpose second order response functions are calculated within the equation of motion approach. Analytical results for the spectrum will be presented in the homogeneous gauge sector and exchange anisotropy and temperatures of Majorana fermions will be analyzed. The impact of gauge flux excitation will be speculated upon.

# $TT \ 42.18 \quad Wed \ 15:00 \quad P2/OG2$

Magnetostriction in frustrated planar quantum magnets — •ALEXANDER SCHWENKE and WOLFRAM BRENIG — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

Using the numerical linked cluster expansion (NLCE) focussing on the single-site representation, we study the field-induced thermodynamic and magnetoelastic properties of paradigmatic frustrated planar spin models. Results are presented for the energy, the specific heat and the magnetization. Employing simple magnetoelastic modelling we calculate the linear magnetostriction coefficient versus temperature and external magnetic field. In particular we consider magnetostriction at field-induced quantum phase transitions. Results obtained for the generalized Kitaev honeycomb model are extended to include findings on the anisotropic triangular Heisenberg antiferromagnet.

TT 42.19 Wed 15:00 P2/OG2 Continuous similarity transformation for critical phenomena: bilayer antiferromagnetic Heisenberg-model and  $J_1 - J_2$ model — •MATTHIAS R. WALTHER<sup>1</sup>, DAG-BJÖRN HERING<sup>2</sup>, GÖTZ S. UHRIG<sup>2</sup>, and KAI P. SCHMIDT<sup>1</sup> — <sup>1</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Theoretische Physik I, Staudtstraße 7, 91058 Erlangen — <sup>2</sup>Technische Universität Dortmund, Department of Physics, Condensed Matter Theory, Otto-Hahn-Str. 4, 44227 Dortmund

We apply continuous similarity transformations (CSTs) to the bilayer antiferromagnetic Heisenberg model and the antiferromagnetic  $J_1 - J_2$ model on the square lattice. The bilayer Heisenberg model features a well studied, continuous phase transition in the O(3) universality class between a gapless Néel phase and a gapped paramagnetic dimer phase (valence bond solid). The  $J_1 - J_2$  features a gapless Néel phase for  $J_1 \gg J_2$ , a gapless columnar phase for  $J_2 \gg J_1$  and an intermediate phase whose nature is still under debate. We start in both models from the magnetically ordered, collinear phases and approach the quantum phase transitions indicating the breakdown of these long-range ordered phases. The CST flow equations are truncated in momentum space by the scaling dimension d so that all contributions with  $d \leq 2$  are taken into account. We determine critical points by studying the breakdown of the ordered phases and try to determine critical exponents from the flow of the couplings, the ground-state magnetization and the groundstate energy.

TT 42.20 Wed 15:00 P2/OG2 Continuous similarity transformation for critical phenomena: easy-axis antiferromagnetic XXZ model — •DAG-BJÖRN HERING<sup>1</sup>, MATTHIAS R. WALTHER<sup>2</sup>, KAI P. SCHMIDT<sup>2</sup>, and GÖTZ S. UHRIG<sup>1</sup> — <sup>1</sup>Technische Universität Dortmund, Department of Physics, Condensed Matter Theory, Otto-Hahn-Str. 4, 44227 Dortmund — <sup>2</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Theoretische Physik I, Staudtstraße 7, 91058 Erlangen

We apply continuous similarity transformations (CSTs) to the easyaxis antiferromagnetic XXZ-model on the square lattice. The CST flow equations are truncated in momentum space by the scaling dimension d so that all contributions with  $d \leq 2$  are taken into account. The resulting quartic magnon-conserving effective Hamiltonian is analyzed in the zero-, one-, and two-magnon sector. In this way, a quantitative description of the ground-state energy, the one-magnon dispersion and its gap as well as of two-magnon bound states is gained for anisotropies ranging from the gapped Ising model to the gapless Heisenberg model. We discuss the critical properties of the gap closing as well as the evolution of the one-magnon roton mininum. The excitation energies of two-magnon bound states are calculated and their decay into the twomagnon continuum is determined via the inverse participation ratio.

TT 42.21 Wed 15:00 P2/OG2 Quantum criticality of the frustrated transverse-field Ising model on a triangular lattic using enhanced perturbative continous unitary transformations — •LUKAS SCHAMRISS<sup>1</sup>, MATTHIAS R. WALTHER<sup>1</sup>, DAG-BJÖRN HERING<sup>2</sup>, and KAI P. SCHMIDT<sup>1</sup> — <sup>1</sup>Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — <sup>2</sup>Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany

Ising models in a transverse field are paradigmatic models for quantum phase transitions of various universality classes which occur depending on the lattice geometry and the choice of antiferromagnetic of ferromagnetic coupling. We investigate the quantum phase diagram of the bilayer antiferromagnetic transverse field Ising model on a triangular lattice with an Ising-type interlayer coupling. Without a field, the model is known to host a classically disordered ground state, and in the limit of decoupled layers it exhibits the 3dXY transition of the corresponding single layer model. Our starting point for the unknown parts of the phase diagram is a high-order perturbative calculation from the limit of isolated dimers. Enhanced perturbative continuous unitary transformations (epCUTs) are used to derive series expansions for the ground state and the energy gap. These are refined by directly evaluated epCUTs (deepCUTs) which provide estimates which coincide with the perturbative series up to its respective order and add a non-perturbative correction. These allow to draw conclusions about the nature of occurring phase transitions.

TT 42.22 Wed 15:00 P2/OG2

Quantum simulation of transverse field Ising model using numerical linked cluster expansions with variational quantum eigensolver — •SUMEET SUMEET, MAX HÖRMANN, and KAI P. SCHMIDT — Institut für Theoretische Physik I Friedrich-Alexander-Universität Erlangen-Nürnberg

With the advancements in quantum technologies it has become in-

evitable to investigate the potential existence of quantum advantage for the paradigmatic models of quantum-many body physics. One of the very basic models is the transverse field Ising model that can be simulated on a quantum computer to compute properties such as the ground-state energy of a spin system. This problem, when tackled on a classical computer, leads to an exponential surge in the cost of computation with increasing system size. The advent of classical-quantum hybrid algorithms has shifted the focus to investigate the solution to this problem with algorithms such as the variational quantum eigensolver (VQE) which is considered reasonably good for obtaining the ground-state energies of quantum many-body systems in the NISQ era. In this work, we exploit the Hamiltonian variational ansatz for calculating the ground-state energy and fidelity of the transverse-field Ising model on one- and two-dimensional geometries. We devise strategies to compute the ground-state energy in the thermodynamic limit on quantum computers. In that regard, we apply numerical linked cluster expansions (NLCE) to VQE in order to simulate infinite spin systems using calculations on finite graphs. Further, we extend this approach to geometrically frustrated systems.