TT 17: Poster Session Correlated Electrons 1

Time: Monday 15:00–19:00 Location: P2/EG

TT 17.1 Mon 15:00 P2/EG

RMn_2Ge_2 (R = Nd, Sm, Dy): Single crystal growth and characterization — •Michelle Ocker, Robert Möller, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

The compounds RMn_2Ge_2, where R is a rare earth element, crystallize in the body centered tetragonal $ThCr_2Si_2$ structure type and exhibit a complex magnetic behaviour. At high temperature, the magnetism is determined by the ordering of the Mn-Mn layer, while at low temperatures it is dominated by the ordering of the rare earths local moments [1, 2]. There are many studies of polycrystalline samples or small single crystals, but large and pure single crystals suitable for spectroscopic studies are missing. In this contribution, we present the details of the growth by Czochralski method from a levitating melt of RMn_2Ge_2 (R=Nd, Sm, Dy) single crystals and their structural, chemical and physical characterization.

[1] G. Guanghua, M.V. Eremin, A. Kirste, N.P. Kolmakava, A.S. Lagutin, R.Z. Lebitin, M von Ortenberg and A.A. Sidorenko, Journal of Experimental and Theoretical Physics, **93**, 796 (2001)
[2] N. P. Kolmakova, A. A. Sidorenko, and R. Z. Levitin, Low Temperature Physics 28, 653 (2002).

TT 17.2 Mon 15:00 P2/EG

Crystal growth and characterization of materials with the $ThCr_2Si_2$ structure type — •Susanna Rongstock, Ali Scherzad, Alexej Kraiker, Doan-My Tran, Sebastian Witt, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, Germany

We present the single crystal growth of different intermetallic compounds within the LnT_2Si_2 family (with Ln = lanthanides and T = Rh, Ir), by employing a high-temperature metal-flux technique. The habitus of the obtained crystals is platelet like with the crystallographic c direction perpendicular to the surface [1]. The magnetic properties of these crystals were characterized by magnetization, heat-capacity, thermopower and resistivity measurements. These crystals form the materials basis for a thorough study of exciting surface properties by angle-resolved photoemission spectroscopy [2,3].

[1] K. Kliemt *et al.*, Cryst. Res. Technol., 1900116 (2019).
[2] A. Chikina *et al.*, Phys. Rev. B. 95, 155127 (2017).
[3] A. Generalov *et al.*, Phys. Rev. B. 98, 115157 (2018).

TT 17.3 Mon 15:00 P2/EG

Crystal growth and characterization of $CeCo_2P_2$ and $EuFe_2P_2$ — •Thanh Duc Nguyen, Johannes Hellwig, Marius Peters, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

The ternary phosphides $CeCo_2P_2$ and $EuFe_2P_2$ are compounds that belong to the '122'-systems crystallizing in the $ThCr_2Si_2$ structure type. $CeCo_2P_2$ is an antiferromagnet due to the ordering of cobalt atoms at $T_N = 440$ K [1]. $EuFe_2P_2$ is a ferromagnet due to the ordering of divalent europium atoms with a Curie temperature of $T_C = 27.5$ K [3]. We synthesized both compounds in tin-flux using either quartz or niobium ampoules [2]. In this way, large platelet-like $CeCo_2P_2$ single crystals of several mm lateral size were created. For the europium system the crystals are smaller. Electrical transport measurements and a magnetic characterization were done for both compounds. In addition, $CeCo_2P_2$ is a candidate for the investigation of its surface states by ARPES.

[1] Yong Tian et al., Physica B: Condensed Matter, 512, 75, (2017)
[2] Kliemt et al., Cryst. Res. Technol., 1900116, (2019)
[3] E. Mörsen et al., Journal of Physics and Chemistry of Solids, 49, 7, (1987)

TT 17.4 Mon 15:00 P2/EG

Scanning Tunneling Microscopy on $Eu_5In_2Sb_6$: a nonsymmorphic antiferromagnetic insulator — •Maria Victoria Ale Crivillero[1], Sahana Roessler[1], Priscila F. S. Rosa[2], and Steffen Wirth[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany. — [2]Condensed Matter and Magnet Science Group, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.

Motivated by theoretical predictions of non-trivial Fermi surface topology stabilized by the non-symmorphic symmetry in the Zintl phase $Ba_5In_2Sb_6$, we investigated the magnetic analogue $Eu_5In_2Sb_6$. The inclusion of Eu gives rise to a complex magnetic behavior. At low temperatures, two magnetic transitions ($T_{N_1} \approx 14$ K and $T_{M_2} \approx 7$ K), revealed in our magnetization, heat-capacity and transport measurements, point to such an intricate magnetic structure. Interestingly, the emergence of colossal magnetoresistance (CMR) suggests the formation of magnetic polarons.

We performed complementary STM/STS measurements. To this end, we attempted to cleave the samples *in situ* in UHV and at low temperatures along the a, b and c-axis. $Eu_5In_2Sb_6$ crystallizes in an orthorhombic structure (*Pbam*), characterized by infinite $[In_2Sb_6]^{10-}$ double chains along the c-axis. In the (010) plane, we obtained striped patterns that can be correlated to the double-chains stacking. The attempted cleavage along the a-axis revealed a more complex pattern, which could be indicative of cleavage along the $(1\bar{1}0)$ plane. So far, no clear experimental evidence of surface states was observed.

TT 17.5 Mon 15:00 P2/EG

Evidence of fully-gapped superconductivity in the locally noncentrosymmetric heavy-fermion system $CeRh_2As_2$ — •Seunghyun Khim[1], Manuel Brando[1], Jacintha Banda[1], Oliver Stockert[1], Zurab Guguchia[2], Robert Scheuermann[2], and Christoph Geibel[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Villigen PSI, Switzerland

Recently, we have discovered unconventional superconducting behavior in $CeRh_2As_2$. The upper critical field (H_{c2}) which exceeds by far the Pauli limit indicates the Rashba-type spin-polarized electronic structure originating from the lack of local inversion symmetry. Coexistence of superconductivity with a possible quadrupolar order is suggestive of multipolar quantum criticality. Here, we present a study of the superconducting state of $CeRh_2As_2$ using muon spin rotation/relaxation (μSR) experiments. Results of transverse-field μSR experiments confirm bulk superconductivity and suggest a fully-gapped superconductivity order parameter. We discuss this finding together with the low-temperature specific-heat data.

TT 17.6 Mon 15:00 P2/EG

Optical Spectroscopy of $CeRh_2As_2$ and $LaRh_2As_2$ — Shinichi Kimura[1,2], Seunghyun Khim[3], and •Jörg Sichelschmidt[3] — [1]Graduate School of Frontier Biosciences, Osaka University, Suita 565-0871, Japan — [2]Department of Physics, Graduate School of Science, Osaka University, Toyonaka 560-0043, Japan — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$CeRh_2As_2$ is a new heavy-fermion superconductor ($T_C \simeq 0.25$ K) which crystallizes in the $CaBe_2Ge_2$-type structure where inversion symmetry is locally broken at the Ce site. It is discussed to be a model system to investigate the influence of Rashba-type interactions on heavy-fermion superconductivity. We present results of optical reflectivity on $CeRh_2As_2$ and $LaRh_2As_2$ for temperatures down to 10 K. In the far-infrared energy region $CeRh_2As_2$ shows a strong spectral weight redistribution with decreasing temperature which is a typical feature found in heavy-fermion materials. The spectra of $LaRh_2As_2$ show an unexpected strong temperature dependence which has not been observed in other counterparts of heavy-fermion materials. The phonon peaks of both compounds show unusually strong softening. Furthermore, the phonon frequency is higher in the Ce-system than in the La-system, in contrast to expectation. We discuss these observations in terms of the lack of local inversion symmetry in the crystal structure.

TT 17.7 Mon 15:00 P2/EG

Monte Carlo Study of Field-Induced Multipolar Phases in the Kondo Material $PrTi_2Al_{20}$ — •Frederic Freyer[1], Simon Trebst[1], SungBin Lee[2], Yong Baek Kim[3], and Arun Paramekanti[3] — [1]University of Cologne, 50937, Germany — [2]Korea Advanced Institute of Science and Technology, Daejeon, 34141, Korea — [3]University of Toronto, Toronto, Ontario, Canada M5S 1A7

Multispin interactions have long been appreciated as a possible microscopic driver for the formation of spin liquids or other forms of

unconventional magnetic ordering, e.g. in the proximity of the Mott transition. Here we discuss the role of such multispin interactions in the Kondo material $PrTi_2Al_{20}$, which exhibits a rich phase phase diagram including intertwined quadrupolar orders, superconductivity and non-Fermi-liquid behavior. Our focus is on magnetic-field induced phase transitions in the quadrupolar ordered state, which have recently been experimentally probed by the Nakatsuji group. Via extensive Monte Carlo simulations we demonstrate that three-spin interactions between the local moments play an important role to explain the observed field dependence of the quadrupolar regime, in the context of a relatively simple O(2) spin model.

TT 17.8 Mon 15:00 P2/EG

Carrier relaxation dynamics in Kondo insulator YbB_{12} — •Amrit R Pokharel[1], Steinn Y Agustsson[1], Fumitoshi Iga[2], Toshiro Takabatake[2], Hidekazu Okamura[3], and Jure Demsar[1] — [1]Johannes Gutenberg University Mainz, Germany — [2]Graduate School of Advanced Sciences of Matter, Hiroshima University, Japan — [3]Graduate School of Advanced Technology and Science, Tokushima University, Japan

We investigate the photoexcited quasiparticle relaxation dynamics in Kondo insulator YbB_{12} by means of time resolved all-optical pump-probe spectroscopy. In particular, we focus on temperature and excitation density dependent studies to address the temperature dependent changes in the low energy electron structure associated with the interplay/hybridization between the Yb 4f-levels and the conduction band electrons. At low temperatures, both the rise-time and recovery of the photoinduced reflectivity changes show dramatic temperature and excitation density dependence. The results are well accounted by the presence of the 15 meV indirect hybridization gap. While the static optical conductivity studies suggest the fully opening of gap around 20 K, our data implies its presence to much higher temperatures of the order of 150 K. Both, the dependence of build-up and its recovery on excitation density can be in detail accounted for by the phenomenological Rothwarf-Taylor model, describing the carrier relaxation across the narrow electronic gap, bottlenecked by the re-absorption of emitted phonons with energy larger than the gap.

TT 17.9 Mon 15:00 P2/EG

Interplay of spin-orbit coupling and spin-orbital superexchange — •Pascal Strobel and Maria Daghofer — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart, 70550 Stuttgart, Germany

In strongly correlated materials with a t_{2g}^4 electron configuration the interplay of superexchange, tetragonal crystal field splitting, and spin-orbit coupling is supposed to support a superposition of singlet and triplet states from the spin-orbit coupling Hamiltonian. This property is often referred to as excitonic magnetism. Ca_2RuO_4 is argued to be a promising candidate for hosting this excitonic magnetism by Raman scattering data [1] as well as numerical results from the variational cluster approach [2]. In order to get a comparison to neutron scattering data [3], we derive an effective hopping Hamiltonian via second order perturbation theory which gives rise to a Kugel-Khomskii type model. Using exact diagonalization we obtain spectra of the magnetic structure factor which show a high agreement with the experiment. With this model it is possible for us to investigate the influence of the parameters appearing in the Kugel-Khomskii type Hamiltonian in the regime of non zero spin-orbit coupling.
[1] Phys. Rev. Lett.119, 067201 (2017)
[2] arXiv:1910.13977v2 (2019)
[3] Phys. Rev. Lett.115, 247201 (2015)

TT 17.10 Mon 15:00 P2/EG

Crystal growth and characterization of the frustrated spinsystems $(Cs_{2-x}Rb_x)CuCl_4$ — •Sarah Krebber, Christian Klein, and Cornelius Krellner — Goethe-Universität Frankfurt am Main, Max-von-Laue-Straße 1, D-60438 Frankfurt am Main

Crystals of the antiferromagnetic insulator Cs2CuCl4 and the substitution series $(Cs_{2-x}Rb_x)CuCl_4$ (x = 0, 0.1, 0.2) were grown by vertical Bridgman method. The controlled substitution of cesium atoms with the smaller rubidium, causes chemical pressure on the crystal lattice [1]. The magnetic properties are caused by Jahn-Teller distorted ($CuCl_4$) tetrahedra, which are arranged in layers separated by the alkali atoms. In these layers the localized Cu^{2+} spins form a triangular lattice, where the spins interact through exchange couplings. The resulting geometric frustration leads to quantum spin liquid properties at low temperatures. In addition to the growth and characterization of $(Cs_{2-x}Rb_x)CuCl_4$, we discuss the structural changes in the lattice parameters and the magnetic behavior of the substituted system in comparison to the well-known parent compound Cs_2CuCl_4. Furthermore we report an experimental study of the low-temperature specific heat and magnetic susceptibility of the substitution series $Cs_2CuCl_{4-x}Br_x$ (x = 0, 1, 2, 4) [2].
[1] H.T. Witteveen et al., Mater. Res. Bull. 9, 345 (1974)
[2] U.Tutsch et al., PRL 123, 147202 (2019)

TT 17.11 Mon 15:00 P2/EG

Multiple Spin-Orbit Excitons and the Electronic Structure of α-$RuCl_3$ — •Philipp Warzanowski[1], Nick Borgwardt[1], Karolin Hopfer[1], Thomas Koethe[1], Petra Becker[2], Vladimir Tsurkan[3,4], Alois Loidl[3], Maria Hermanns[5], Paul H. M. van Loosdrecht[1], and Markus Grüninger[1] — [1]Inst. of Physics II, University of Cologne — [2]Sect. Crystallography, Inst. of Geology and Mineralogy, University of Cologne — [3]Exp. Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [4]Inst. of Applied Physics, Chisinau, Moldova — [5]Dept. of Physics, Stockholm University, AlbaNova University Center, Sweden

α-$RuCl_3$ is widely discussed as a proximate Kitaev spin-liquid material. This scenario builds upon spin-orbit entangled $j = 1/2$ moments which arise in a t_{2g}^5 electron configuration with strong spin-orbit coupling λ and a large cubic crystal field. Despite the keen interest in α-$RuCl_3$, the low-energy electronic structure is still puzzling. In particular the origin of infrared absorption features at 0.30, 0.53, and 0.75 eV is still a matter of debate. Also the energy of the spin-orbit exciton, the excitation from $j = 1/2$ to $j = 3/2$, and thus λ are controversial. Combining infrared absorption and Raman data, we attribute the infrared features to single, double, and triple spin-orbit excitons, yielding $\lambda = 0.16\,\text{eV}$ and a non-cubic crystal field splitting $\Delta = 42\,\text{meV}$. These results support the $j = 1/2$ picture despite of the crystal field distortion. The strength of the double excitation can be understood by the same hopping interactions that also establish dominant Kitaev exchange [1].
[1] P. Warzanowski *et al.*, arXiv:1911.09337

TT 17.12 Mon 15:00 P2/EG

Magnetic field effects on Kitaev spin liquids — •Christoph Berke, Ciaran Hickey, and Simon Trebst — University of Cologne

Frustrated quantum magnets can give rise to unconventional spin-liquid ground states. Paradigmatic examples are two- and three-dimensional Kitaev systems. The characteristic bond-directional interactions are realized in a number of spin-orbit entangled Mott insulators that, in the presence of magnetic fields, show no indications of long-range order. Here, we study quantum phase transitions in the Kitaev model on different lattices under a magnetic field with an emphasis on the topological nature of Majorana excitations. Our interest is particularly in the emergence of intermediate phases, expected to appear for *AFM* couplings between the Kitaev spin liquid and the field polarized phase.

TT 17.13 Mon 15:00 P2/EG

Heat transport in the Kitaev spin-liquid candidate α-$RuCl_3$ — •Matthias Gillig[1], Richard Hentrich[1], Xiaochen Hong[1], Maria Roslova[2], Anna Isaeva[1,2], Thomas Doert[2], Bernd Büchner[1,3], and Christian Hess[1,3] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, Germany

α-$RuCl_3$ is a prime candidate to be close to the realization of the Kitaev model in a real material. The model is of interest due to its exact solution with a spin-liquid ground state and emerging Majorana excitations. Additional Heisenberg and off-diagonal terms in the Hamiltonian of α-$RuCl_3$ distinguish it from a pure Kitaev system which leads to an antiferromagnetically ordered ground state below T = 7 K. By applying a magnetic field above 8 T parallel to the honeycomb plane the ordered phase can be suppressed and a new phase emerges which is predicted to have spin-liquid character. We have performed detailed studies on the longitudinal and transverse heat transport in α-$RuCl_3$ for magnetic fields applied parallel and perpendicular to the honeycomb plane to explore the field-induced phase.

TT 17.14 Mon 15:00 P2/EG

Anisotropic field-induced ordering in the triangular-lattice quantum spin liquid $NaYbSe_2$ — •K. M. Ranjith[1], S. Luther[2,3], T. Reimann[2], B. Schmidt[1], Ph. Schlender[4], J. Sichelschmidt[1], H. Yasuoka[1], A. M. Strydom[5], Y. Skourski[2],

J. Wosnitza[2,3], H. Kühne[2], Th. Doert[4], and M. Baenitz[1] — [1]MPI for Chemical Physics of Solids, Dresden, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [3]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [4]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany — [5]Highly Correlated Matter Research Group, University of Johannesburg, South Africa

High-quality single crystals of $NaYbSe_2$, which resembles a perfect triangular-lattice antiferromagnet without intrinsic disorder, are investigated by magnetization and specific-heat, as well as the local probe techniques nuclear magnetic resonance and electron spin resonance. The low-field measurements confirm the absence of any spin freezing or long-range magnetic order down to 50 mK, which suggests a quantum spin liquid ground (QSL) state with gapless excitations. An instability of the QSL state is observed upon applying magnetic fields. The absence of magnetic long-range order at zero fields is assigned to the effect of strong bond-frustration, arising from the complex spin-orbit entangled $4f$ ground state. Finally, we derive the highly anisotropic magnetic phase diagram, which is discussed in comparison with the existing theoretical models for spin-$\frac{1}{2}$ triangular-lattice antiferromagnets.

TT 17.15 Mon 15:00 P2/EG

Spin dynamics in the quasi-2D Honeycomb material $Na_2Co_2TeO_6$ probed by Electron Spin Resonance — •Christoph Wellm[1,2], Vladislav Kataev[1], Bernd Büchner[1,2], Weiliang Yao[3], and Yuan Li[3,4] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01069 — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01062 — [3]International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — [4]Collaborative Innovation Center of Quantum Matter, Beijing 100871, China

We report an electron spin resonance (ESR) study on single crystals of $Na_2Co_2TeO_6$, a layered honeycomb material providing a possible realization of Kitaev physics [1]. Similar to previously conducted magnetization measurements [1], ESR data reveals magnetic anisotropy and interesting, complex angular and temperature dependent behavior. In addition, low-energy magnetic excitations can be examined. Our results contribute to a thorough understanding of the magnetic properties and spin correlations in the title compound.
[1] W. Yao and Y. Li, Proc. Natl. Acad. Sci., arXiv:1908.09427

TT 17.16 Mon 15:00 P2/EG

DFT calculations and spin dynamics of the quantum spin liquid candidate $Na_2BaCo(PO_4)_2$ — •Christoph Wellm[1,2], Willi Roscher[1], Vladislav Kataev[1], Oleg Janson[1], Bernd Büchner[1,2], Robert J. Cava[3], and Ruidan Zhong[3] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01069 — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01062 — [3]Department of Chemistry, Princeton University, Princeton, US-08544

The recently synthesized triangular lattice magnet $Na_2BaCo(PO_4)_2$ shows effective S = 1/2 behavior with strong quantum fluctuations persistent down to 50 mK in absence of long-range order, rendering it a promising candidate for the quantum spin liquid (QSL) ground state [1,2]. In this joined work, DFT calculations and ESR measurements provide a microscopic insight into the leading magnetic interactions and spin dynamics of the system. Using the full-potential code FPLO, the leading magnetic exchanges, the spin orbit coupling constant and the trigonal crystal field splitting are evaluated. ESR hints at a temperature-dependent magnetic moment in line with magnetization data, and shows enhanced spin-spin correlations at low-temperatures. The theoretical findings are compared to the new experimental results.

TT 17.17 Mon 15:00 P2/EG

The present understanding of anisotropic exchange interactions in linarite and other frustrated edge-sharing chain cuprates — •Stefan-Ludwig Drechsler[1], Satoshi Nishimoto[1,2], Helge Rosner[3], Alexander Tsirlin[4], Rolf Schumann[2], and Ullrich Roessler[1] — [1]IFW-Dresden, Dresden, Germany — [2]TU Dresden, Germany — [3]MPI-cPfS, Dresden, Germany — [4]Experimental Phys. IV, University of Augsburg, Germany

Based on various recent experimental data /1-3/ and novel DFT calculations we discuss the interplay of symmetric and antisymmetric exchange anisotropies in the context of the rich $B-T$ phase diagram, in particular, with the focus on the high-field region, the asymptotic saturation, and the possibility of sizable multipolar (nematic and higher order) fluctuations. Consequences of the XYZ-anisotropy and the presence of Dzyaloshinskii-Moriya (DM) interactions including DFT estimates are taken into account. In the vicinity of the magnetic ordering a phenonmenological Ginzburg-Landau analysis is applied, too.
[1] L. Heintze *et al.* Phys. Rev. B **99** , 094436 (2019)
[2] E. Cemal *et al.* Phys. Rev. Lett. **120**, 067203 (2018)
[3] S.K. Gotovko *et al.* Phys. Rev. B **100**, 174412 (2019)

TT 17.18 Mon 15:00 P2/EG

Dynamical Monte Carlo Simulations with Applications in Dipolar Spin Ice and Open Floquet Systems — •Martin Gembe, Jan Attig, and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Many-body systems subject to a periodic drive have triggered an enormous research interest, as fluctuations induced by this drive can lead to a variety of exotic phenomena such as time crystals or novel topological states. These phenomena are by definition not accessible within ordinary stationary quantum mechanics but require large-scale full dynamic quantum simulations. In this work, we present dynamical Monte Carlo simulations based on the classical single spin flip Metropolis algorithm in order to study such systems out of equilibrium in the classical limit. With this algorithm, we explore the dynamics of emerging magnetic monopoles in dipolar spin ice in an external magnetic AC field, which exhibits a critical speeding up near the monopole liquid-gas transition. Secondly, we study an open Floquet system, in which analytically it is found that rapid periodic oscillations of the couplings drive the system away from criticality.

TT 17.19 Mon 15:00 P2/EG

Thermodynamic classification of 3D Kitaev spin liquids — •Tim Eschmann[1], Petr A. Mishchenko[2], Kevin O'Brien[1], Troels A. Bojesen[2], Yasuyuki Kato[2], Maria Hermanns[3,4], Yukitoshi Motome[2], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne — [2]Department of Applied Physics, University of Tokyo — [3]Department of Physics, Stockholm University — [4]Nordita, KTH Royal Institute of Technology and Stockholm University

Kitaev models are prototypical spin models in which the spins fractionalize, and the emergent spin liquid ground state is composed of Majorana fermions coupled to a $\mathbb{Z}_2$ gauge field. At low temperatures, the $\mathbb{Z}_2$ gauge field is generally assumed to exhibit an ordered ground state, characterized by the presence or absence of $\mathbb{Z}_2$ fluxes through the elementary lattice plaquettes. In 3D, this ground state is separated from the paramagnetic phase through a thermal phase transition, at which the (gapped) vison excitations proliferate. Here, we further the understanding of this "gauge physics" by a comprehensive classification of the thermodynamics of a family of elementary 3D Kitaev models. Based on large-scale, sign-free quantum Monte Carlo simulations, we verified that the ground state flux sectors of these systems are entirely determined by their elementary plaquette length - extending the applicability of Lieb's theorem to a number of lattice geometries beyond its original scope. As manifestation of the close interplay of vison-physics and gauge-ordering transition, we report a (linear) correlation between the critical temperature and the size of the vison gap.