TT 42: Correlated Electrons: Frustrated Magnets - Strong Spin-Orbit Coupling 2

Time: Wednesday 9:30–13:00 Location: HSZ 304

TT 42.1 Wed 9:30 HSZ 304

Thermal transport in Kitaev spin systems — •Wolfram Brenig and Alexandros Metavitsiadis — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We study the dynamical thermal conductivity of Kitaev spin models on two-leg ladders and honeycomb lattices. In contrast to the majority of conventional one-dimensional spin systems, we show the ladder to represent the rare case of a perfect heat insulator. This is a direct consequence of fractionalization of spins into mobile Majorana matter and static Z_2 gauge fields. Our findings rest on complementary calculations of the current correlation function, comprising a mean-field treatment of thermal gauge fluctuations, a complete summation over all gauge sectors, as well as exact diagonalization of the original spin model. On the honeycomb lattice results will be presented from high temperature numerical diagonalization and from low temperature perturbation theory.

TT 42.2 Wed 9:45 HSZ 304

Three-band Hubbard model for Na_2IrO_3: Topological insulator, zigzag antiferromagnet, and Kitaev-Heisenberg material — •Stephan Rachel[1], Manuel Laubach[1], Ronny Thomale[2], and Johannes Reuther[3] — [1]TU Dresden, Institut für Theoretische Physik — [2]Universität Würzburg, Institut für Theoretische Physik — [3]FU Berlin & Helmholtz-Zentrum Berlin

Na_2IrO_3 was one of the first materials proposed to feature the Kane-Mele type topological insulator phase. About the same time it was claimed that the very same material is in a Mott insulating phase which is described by the Kitaev-Heisenberg (KH) model. First experiments indeed revealed Mott insulating behavior in conjunction with antiferromagnetic long-range order. Further refined experiments established antiferromagnetic order of zigzag type which is not captured by the KH model. Since then several extensions and modifications of the KH model were proposed in order to describe the experimental findings. Here we suggest that adding charge fluctuations to the KH model represents an alternative explanation of zigzag antiferromagnetism. Moreover, a phenomenological three-band Hubbard model unifies all the pieces of the puzzle: topological insulator physics for weak and KH model for strong electron-electron interactions. And at moderate interaction strength we find a zigzag antiferromagnet.

TT 42.3 Wed 10:00 HSZ 304

Honeycomb-lattice Heisenberg-Kitaev model in a magnetic field: Spin canting, metamagnetism, and vortex crystals — •Lukas Janssen[1], Eric C. Andrade[2], and Matthias Vojta[1] — [1]Technische Universität Dresden, Germany — [2]Universidade de São Paulo, Brazil

The Heisenberg-Kitaev model is a paradigmatic model to describe the magnetism in honeycomb-lattice Mott insulators with strong spin-orbit coupling, such as A_2IrO_3 (A = Na, Li) and α-$RuCl_3$. In this talk, I present in detail the physics of the Heisenberg-Kitaev model in an external magnetic field. Using the combined results of Monte-Carlo simulations and spin-wave theory the classical phase diagram for different directions of the magnetic field is mapped out. Broken SU(2) spin symmetry renders the magnetization process rather complex, with sequences of phases and metamagnetic transitions. In particular, various large-unit-cell and multi-Q phases including a vortex-crystal phase occur for a field in the [111] direction. I also discuss quantum corrections in the high-field phase.

[1] L. Janssen, E. C. Andrade, and M. Vojta, arXiv:1607.04640 [cond-mat.str-el] (PRL accepted).

TT 42.4 Wed 10:15 HSZ 304

Spectroscopic investigations of a novel Iridate - a possible reference material for Kitaev physics — Philipp Benrath[1], Angela Möller[1], Vladimir Gnezdilov[2,3], and •Peter Lemmens[2] — [1]IAC-AC, JGU Mainz — [2]TU-BS, Braunschweig — [3]ILTP, Kharvov

In $Na_2Ir(OH)_6$ there exist a D3d point group symmetry with an uniaxial threefold symmetry of the iridium complex. In our search for nonabelian anyons (fractionalized excitations)[1] we performed a systematic Raman scattering investigation of its excitation spectrum. Evidence for a symmetry reduction and its relation to other distorted Kitaev materials are discussed.

Work supported by RTG-DFG 1952/1, the Laboratory for Emerging Nanometrology, TU Braunschweig, and NTH Contacs in Nanosystems.

[1] A. Glamazda, P. Lemmens, S.-H. Do, K.-Y. Choi, Nature Commun. 7, 12286 (2016).

TT 42.5 Wed 10:30 HSZ 304

Electronic structure of α-$RuCl_3$ from electron spectroscopy — •Andreas Koitzsch[1], Carsten Habenicht[1], Eric Müller[1], Martin Knupfer[1], Bernd Büchner[1,2], Hem Kandpal[1,3], Jeroen van den Brink[1,4], Domenic Nowak[5], Anna Isaeva[5], and Thomas Doert[5] — [1]IFW Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, Germany — [3]Indian Institute of Technology, Roorkee, India — [4]Institute for Theoretical Physics, TU Dresden, Germany — [5]Department of Chemistry and Food Chemistry, TU Dresden, Germany

Novel ground states might be realized in honeycomb lattices with strong spin–orbit coupling. Here we study the electronic structure of α-$RuCl_3$, in which the Ru ions are in a d^5 configuration and form a honeycomb lattice, by angle-resolved photoemission, x-ray photoemission and electron energy loss spectroscopy supported by density functional theory and multiplet calculations. We find that α-$RuCl_3$ is a Mott insulator with significant spin-orbit coupling, whose low energy electronic structure is naturally mapped onto J_{eff} states. This makes α-$RuCl_3$ a promising candidate for the realization of Kitaev physics. Relevant electronic parameters such as the Hubbard energy U, the crystal field splitting $10Dq$ and the charge transfer energy Δ are evaluated.

TT 42.6 Wed 10:45 HSZ 304

Field-induced changes of the thermodynamic properties of the honeycomb system α-$RuCl_3$ — •A.U.B. Wolter[1], L.T. Corredor[1], M. Geyer[1], K. Nenkov[1], R. Hühne[1], S.-H. Do[3], K.-Y. Choi[3], Y.S. Kwon[4], A. Isaeva[5], D. Nowak[5], T. Doert[5], L. Janssen[6], M. Vojta[6], and B. Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany — [3]Department of Physics, Chung-Ang University, Seoul 156-756, Republic of Korea — [4]Department of Emerging Materials Science, DGIST, Daegu 711-873, Republic of Korea — [5]Department of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany — [6]Institute for Theoretical Physics, TU Dresden, 01062 Dresden, Germany

α-$RuCl_3$ with its honeycomb lattice and strong spin-orbit coupling has been at the center of attention in the last two years, since it has been proposed as a prime candidate to study fractionalized Kitaev physics despite its zigzag antiferromagnetic ground state. The thermal fractionalization of quantum spins in a Kitaev model has been predicted to be experimentally observable in e.g. the specific heat, and transport properties. We studied the thermodynamic behavior of this system by means of a detailed specific heat investigation in applied magnetic fields up to 14 T. Our studies reveal an angular dependent suppression of the long-range magnetic order in applied magnetic fields, as well as a pronounced suppression of the specific heat at low temperatures and high fields, suggesting the appearance of a gapped state. This scenario is discussed in light of a detailed entropy analysis in both regimes.

TT 42.7 Wed 11:00 HSZ 304

Anisotropic Ru^{3+} magnetism in the honeycomb system α-$RuCl_3$ — •Maximilian Geyer[1,2], Laura Theresa Corredor Bohorquez[1], Sebastian Gass[1], Synho Do[3], Kwangyong Choi[3], Yong Seung Kwon[3], Anna Isaeva[4], Domenic Nowak[4], Thomas Doert[4], Anja U.B. Anja U.B. Wolter[1], and Bernd Büchner[1,2] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany — [3]Department of Physics, Chung-Ang University, Seoul 156-756, Republic of Korea — [4]Department of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany

The interplay between electronic correlations and spin-orbit coupling in heavy transition metal compounds has been intensively studied in the last years due to their interesting properties and unusual ground states like quantum spin liquids. Particularly, α-$RuCl_3$ shows interesting properties, which can be attributed to its proximity to a Kitaev spin liquid state. We report on magnetization measurements for α-$RuCl_3$ single crystals grown by means of chemical vapor transport reactions. The main focus lies on angular dependent measurements and the behavior of α-$RuCl_3$ in high magnetic fields in order to understand the highly anisotropic magnetism in this layered compound.

15 min. break.

TT 42.8 Wed 11:30 HSZ 304

Transport studies of the Kitaev-Heisenberg compound α-$RuCl_3$ — •Richard Hentrich[1,2], Bernd Büchner[1,2], Domenic Nowak[3], Anna Isaeva[3], Thomas Doert[3], Jennifer Sears[4], Young-June Kim[4], Paula J. Kelley[5], Stephen E. Nagler[5], and Christian Hess[1,2] — [1]IFW Dresden, Germany — [2]Center for Transport and Devices of Emergent Materials, TU Dresden, Germany — [3]Inorganic Chemistry Department II, TU Dresden, Germany — [4]Department of Physics, University of Toronto, Canada — [5]Oak Ridge National Laboratory, USA

α-$RuCl_3$ is a material composed of weakly van der Waals bound honeycomb layers of edge sharing $RuCl_6$ octahedra with the central atom being in a $J_{\text{eff}} = 1/2$ state. This kind of strongly frustrated spin structure is a candidate for Kitaev-Heisenberg physics which features non-trivial, fractionalised excitations.
Thermal transport measurements are known as a valuable tool to probe elementary excitations of systems with low dimensional spin structure and are possibly suited to detect Majorana fermionic contributions to the net heat conductivity.
We observe strong suppression of the phononic in-plane thermal conductivity of α-$RuCl_3$ single crystals at low temperatures in zero magnetic field. However, upon applying an external magnetic field the heat conductivity is strongly enhanced. We interpret our findings in terms of a field-induced quantum phase transition.

TT 42.9 Wed 11:45 HSZ 304

Single, double, and triple spin-orbit excitons in α-$RuCl_3$ — •Nick Borgwardt[1], Alessandro Revelli[1], Maria Hermann[2], Petra Becker[3], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für theoretische Physik, Universität zu Köln — [3]Abteilung Kristallographie, Institut für Geologie und Mineralogie, Universität zu Köln

Spin-orbit-assisted d^5 Mott insulators with local j=1/2 moments are discussed as realizations of the Kitaev model which hosts Majorana fermion excitations. In promising candidate materials such as $RuCl_3$, lattice distortions give rise to a mixing of j=1/2 and 3/2 character which may spoil the picture. The so-called spin-orbit exciton corresponds to an excitation to the j=3/2 state and is very sensitive to the character of the relevant states. In the literature, features in Raman scattering, neutron scattering, and infrared absorption data were reported in the relevant frequency range of one to a few hundred meV. We challenge the reported interpretations and demonstrate that our infrared data show single, double, and triple spin-orbit excitons. These novel and unusual excitations are directly connected to the microscopic processes relevant for the Kitaev coupling.

TT 42.10 Wed 12:00 HSZ 304

Raman Spectroscopy on the putative Kitaev Material $RuCl_3$ — •Thomas Koethe[1], Sebastian Kaul[1], Raphael German[1], Petra Becker[2], Markus Grüninger[1], and Paul van Loosdrecht[1] — [1]Institute of Physics 2, University of Cologne — [2]Institute for Geology and Mineralogy, University of Cologne

The famous Kitaev model with bond-directional Ising-type interactions on tricoordinated lattices allows for an exotic spin liquid ground state and Majorana fermion excitations. Real materials like the spin-orbit driven Mott insulator $RuCl_3$ usually show an additional isotropic Heisenberg interaction competing with the Kitaev interactions. Raman spectroscopy is an excellent tool to investigate unconventional states of matter and provides information not only about the electronic ground state of the material, whose $j = 1/2$ nature is a requirement for the Kitaev physics, but also about the nature of the excitations. Though we observe a low energy scattering continuum, our results do not seem to be compatible with current theoretical predictions for the Majorana continuum. We do see, however, a Fano-type phonon continuum coupling which may be compatible with theoretical expectations. Electronic excitations at higher energies challenge the previously proposed electronic structure of the material.

TT 42.11 Wed 12:15 HSZ 304

Effect of symmetry and local distortions on fractionalized excitations in Kitaev Systems — •Peter Lemmens[1], Vladimir Gnezdilov[1,2], Alexander Glamazda[1,2,3], S.-H. Do[3], K.-Y. Choi[3], Angela Möller[4], Friedrich Freund[5], and Philipp Gegenwart[5] — [1]TU-BS Braunschweig — [2]ILTP Kharkov — [3]CAU Seoul — [4]IAC-AC, JGU Mainz — [5]EP-VI, ZEKM, Augsburg

In Kitaev physics the role of symmetry is crucial. A prerequisite of the Kitaev model demands uniaxial threefold symmetry of the iridium complex. [1,2] Therefore, the comparison of different systems representing the Kitatev model on different honeycomb-like lattices [3] is an important topic. We performed Raman scattering investigations on the continuum of fractionalized excitations to understand the role of symmetry, local distortions and dimensionality. In detail, we will report on data of α-$RuCl_3$ as well as 2D/3D $(Na,Li)_2IrO_3$ and related compounds.

Work supported by RTG-DFG 1952/1, the Laboratory for Emerging Nanometrology, TU Braunschweig, and NTH Contacs in Nanosystems.
[1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009)
[2] M. Becker, M. Hermanns, B. Bauer, M. Garst and S. Trebst, Phys. Rev. B 91, 155135 (2015)
[3] A. Glamazda, P. Lemmens, S.-H. Do, K.-Y. Choi, Nature Commun. 7, 12286 (2016).

TT 42.12 Wed 12:30 HSZ 304

Disorder and topology in a periodically driven Kitaev model — •Mykola Maksymenko[1,2], Maria-Theresa Rieder[2], Ion Cosma Fulga[2], Netanel Lindner[3], and Erez Berg[2] — [1]Institute for Condensed Matter Physics of NAS of Ukraine, Lviv-79011, Ukraine — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, 76100, Israel — [3]Physics Department, Technion, 320003 Haifa, Israel

We investigate a periodically driven 2D Kitaev model in which anisotropic exchange integrals are boosted at consecutive time intervals. This model shows a rich phase diagram consisting of novel anomalous topological phases. Unlike the static Kitaev model some of the phases, can host pairs of Majorana modes at a single vortex defect or lattice dislocation. We characterize the different phases using weak and strong scattering-matrix invariants defined for the corresponding fermionic model and investigate their stability to different types of disorder.

TT 42.13 Wed 12:45 HSZ 304

Topological Superconductivity in the Extended Kitaev-Heisenberg Model — •Johann Schmidt, Tomas Löthman, and Annica M. Black-Schaffer — Uppsala Universitet, Uppsala, Schweden

We extend the discussion of superconductivity in the Kitaev-Heisenberg model by taking into account the recently proposed symmetric off-diagonal exchange term Γ. The new interaction term contributes further to the triplet superconductivity triggered by the Kitaev exchange. While a positive Γ bolsters the already reported time-reversal symmetric p-wave state with its transition to a topologically non-trivial state at high doping levels, new superconducting orders emerge for negative values of Γ. Of particular interest is a region at intermediate doping which breaks time-reversal symmetry and can be classified by a Chern number of ± 2.