TT 50: Correlated Electrons: Frustrated Magnets - Theory

Time: Wednesday 15:00–19:15 Location: H18

TT 50.1 Wed 15:00 H18

Thermal conductivity of the Kitaev spin ladder — •Wolfram Brenig and Alexandros Metavitsiadis — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We analyze the thermal conductivity of the Kitaev spin model on a two leg ladder, which constitutes an exactly solvable example for a Z_2 spin liquid. Using a mapping to Majorana particles, the thermal transport is described in terms of matter fermions interacting with a Z_2 gauge field. Findings for the transport coefficient within linear response theory will be discussed in the long wave length limit, at finite frequency, and arbitrary temperature. For the zero flux sector analytic results will be presented, while finite flux densities will be treated numerically. The results will be contrasted against known thermal conductivities of other integrable spin models. Speculations on the impact of including an additional isotropic Heisenberg exchange will be made.

TT 50.2 Wed 15:15 H18

Classification of gapless Z_2 spin liquids in three-dimensional Kitaev models — •Kevin O'Brien, Maria Hermanns, and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

The formation of spin liquids in frustrated quantum magnets makes for an exciting prospect due to their hosting fractionalized excitations and emergent gauge fields. Unfortunately, they are notoriously difficult to study as there are often no good analytical methods available and Quantum Monte Carlo simulations are hindered by the infamous sign problem. The Kitaev honeycomb model is a notable exception of a frustrated spin model which is exactly solvable and which hosts a number of distinct quantum spin liquid ground states. As such, it allows for a rare opportunity to study the physics of spin liquids with full analytical tractability.

Here we study the fractionalization of magnetic moments into Majorana fermions and a Z_2 gauge field in a generalization of the Kitaev honeycomb model to a number of three-dimensional, tricoordinated lattices. While the excitations of the gauge field are always gapped, the Majorana fermions may form a gapless dispersion with either topologically protected Weyl nodes, symmetry protected nodal lines, or full 2D Fermi surfaces. We show that the nature of these Majorana (semi)metals can be deduced from an elementary analysis of the projective time-reversal and inversion symmetries for a given lattice, allowing us to classify the gapless spin liquids of three-dimensional Kitaev models.

TT 50.3 Wed 15:30 H18

Detailed phase diagram of Kitaev-Heisenberg model — •Dorota Gotfryd[1,2], Juraj Rusnacko[3], Jiri Chaloupka[3], and Andrzej M. Oles[2,4] — [1]Institute of Theoretical Physics, University of Warsaw, Poland — [2]Marian Smoluchowski Institute of Physics, Jagellonian University, Poland — [3]Central European Institute of Technology, Masaryk University, Czech Republic — [4]Max-Planck-Institut FKF, Germany

We present detailed phase diagram for the Kitaev-Heisenberg (KH) model [1] obtained by two approaches: ED and ED with cluster mean field introduced in [2]. While the evolution of ordered moments resulting from second method allows for more direct order/disorder phase transition analysis – we deliberately break SU(2) symmetry, spin correlation functions, spin-structure factor and dynamical spin susceptibility obtained from ED provide more details about the nature of two distinct spin liquid regions.

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[1] J. Chaloupka and G. Khaliullin, PRB **92**, 043032 (2015)
[2] A. F. Albuquerque et al., PRB **84**, 024406 (2011).

TT 50.4 Wed 15:45 H18

Quantum disordered insulating phase in the frustrated cubic-lattice Hubbard model — •Stephan Rachel[1], Manuel Laubach[1,2], Darshan Joshi[1], Johannes Reuther[3], Ronny Thomale[2], and Matthias Vojta[1] — [1]TU Dresden, Institut für Theoretische Physik — [2]Universität Würzburg, Institut für Theoretische Physik — [3]FU Berlin & Helmholtz-Zentrum Berlin

In the quest for quantum spin liquids in three spatial dimensions (3D), we study the half-filled Hubbard model on the simple cubic lattice with hopping processes up to third neighbors. Employing the variational cluster approach (VCA), we determine the zero-temperature phase diagram: In addition to a paramagnetic metal at small interaction strength U and various antiferromagnetic insulators at large U, we find an intermediate-U antiferromagnetic metal. Most interestingly, we also identify a non-magnetic insulating region, extending from intermediate to strong U. Using VCA results in the large-U limit, we establish the phase diagram of the corresponding J_1–J_2–J_3 Heisenberg model. This is qualitatively confirmed – including the non-magnetic region – using spin-wave theory. Further analysis reveals a striking similarity to the behavior of the J_1–J_2 square-lattice Heisenberg model, suggesting that the non-magnetic region hosts a 3D spin-liquid phase.

TT 50.5 Wed 16:00 H18

Quantum paramagnet in the Heisenberg model on the cubic lattice: a case study of a novel method for three-dimensional quantum magnetism — •Yasir Iqbal[1], Stephan Rachel[2], Ronny Thomale[1], and Johannes Reuther[3,4] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilian's University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute for Theoretical Physics, Technische Universität Dresden, D-01062 Dresden, Germany — [3]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, D-14195 Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany

A holy grail in quantum magnetism is the search for quantum spin liquids in strongly correlated systems. In particular, $2D$ quantum spin systems have been convincingly shown, both experimentally and theoretically, to host spin liquids. In contrast to $2D$, where there are by now powerful numerical methods available, the case of $3D$ remains out of reach of most numerical methods, or restricted to very small systems. We discuss recent developments of the pseudo-fermion functional renormalization group (PF-FRG) method enabling an efficient study of $3D$ systems. We use this framework to investigate the spin-1/2 quantum Heisenberg $J_1 - J_2 - J_3$ antiferromagnetic model on the simple cubic lattice, and obtain the phase diagram, which reveals the existence of a quantum paramagnetic phase over an extended region in parameter space, with a featureless spin susceptibility profile. A state-of-the-art implementation enables simulation of very large systems

15 min. break

TT 50.6 Wed 16:30 H18

Finite temperature dynamics of spin-1/2 chains with symmetry breaking interactions — Alexander C. Tiegel[1], •Salvatore R. Manmana[1], Thomas Pruschke[1], and Andreas Honecker[2] — [1]Institut f. Theor. Physik, Univ. Göttingen, 37077 Göttingen — [2]LPTM, Université de Cergy-Pontoise, France

I will discuss recent developments for flexible matrix product state (MPS) approaches to calculate finite-temperature spectral functions of low-dimensional strongly correlated quantum systems. The main focus will be on a Liouvillian formulation [1]. The resulting algorithm does not specifically depend on the MPS formulation, but is applicable for any wave function based approach which can provide a purification of the density matrix, opening the way for further developments of numerical methods. Based on MPS results for various spin chains, in particular systems with Dzyaloshinskii-Moriya interactions caused by spin-orbit coupling and dimerized chains, I will discuss how symmetry breaking interactions change the nature of the finite-temperature dynamic spin structure factor obtained in ESR [2] and neutron scattering experiments.

[1] A.C. Tiegel et al., PRB **90**, 060406(R) (2014)
[2] A.C. Tiegel et al., arXiv:1511.07880 (submitted to PRB)

TT 50.7 Wed 16:45 H18

Quantum Monte Carlo in the spin dimer-basis — •Jonas Stapmanns[1], Andreas Honecker[2], and Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics RWTH Aachen University, Aachen, Germany — [2]Laboratoire de Physique Théorique et Modélisation Université de Cergy-Pontoise, Pontoise, France

Quantum Monte Carlo simulations of frustrated spin systems are usually plagued by a severe sign-problem. However, due to its dependence on the employed computational basis, it can be feasible to reduce or even avoid the sign-problem by an appropriate local basis choice. Here, we consider in particular the possibility of simulating dimerized quantum spin systems based on a spin dimer-basis formulation of the stochastic series expansion algorithm. We discuss this simulation scheme and present results for thermodynamic properties of the fully-frustrated spin-1/2 Heisenberg ladder as well as for the fully-frustrated square lattice bilayer Heisenberg model.

TT 50.8 Wed 17:00 H18

Phase diagram of frustrated spin ladders with ring exchange interaction — •Alexandros Metavitsiadis[1] and Sebastian Eggert[2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]Physics Department and Research Center OPTIMAS, Technical University of Kaiserslautern, Germany

The ground state properties of spin ladders are studied, emphasizing the role of frustration. We present a unified field theory calculation for ladders with different geometries and using the renormalization group we deduce their phase diagrams in the presence of in-chain next nearest neighbor interactions as well as plaquette ring exchange interactions. We find the magnetically ordered states, Haldane and rung singlet, in addition to dimerized patterns, columnar dimer and staggered dimer. Lastly, we show that the interplay of the larger unit cell and the ring exchange interaction induces a ferro-antiferromagnetic state, otherwise expected at much higher energy scales.

TT 50.9 Wed 17:15 H18

The infinite-PEPS algorithm: improvements, and its application to spin-S Kagome quantum antiferromagnets in a field — •Roman Orus[1], Phien Ho[2], Johann Bengua[2], Hoang Tuan[2], Philippe Corboz[3], Thibaut Picot[4], Marc Ziegler[1], and Didier Poilblanc[4] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]University of Technology Sydney, Sydney 2007, Australia — [3]Institute for Theoretical Physics, University of Amsterdam, Science Park 904 Postbus 94485, 1090 GL Amsterdam, The Netherlands — [4]Laboratoire de Physique Theorique, IRSAMC, CNRS and Université de Toulouse, UPS, F-31062 Toulouse, France

The infinite Projected Entangled Pair States (iPEPS) algorithm has become a useful tool in the calculation of ground state properties of 2d quantum lattice systems in the thermodynamic limit. Here I will present results concerning iPEPS in two directions. In the first part of my talk I will explain how to overcome some of the current limitations of the method by using a gauge fixing and a "fast full update" of the tensors, implying dramatic computational savings, and improved overall stability. In the second part, I will explain how the method can be applied to obtain the phase diagrams of Spin-S Heisenberg quantum antiferromagnets on the Kagome lattice, up to S = 2.

TT 50.10 Wed 17:30 H18

Application of the DMRG in two dimensions: a parallel tempering algorithm — •Shijie Hu[1], Jize Zhao[2], Axel Pelster[1], Xuefeng Zhang[1], and Sebastian Eggert[1] — [1]Department of Physics and Research Center Optimas, Technical University Kaiserslautern, 67663 Kaiser- slautern, Germany — [2]Institute of Applied Physics and Computational Mathematics, Beijing 100088, China

The Density Matrix Renormalization Group (DMRG) is known to be a powerful algorithm for treating one-dimensional systems. When the DMRG is applied in two dimensions, however, the convergence becomes much less reliable and typically ”metastable states” may appear, which are unfortunately quite robust even when keeping a very high number of DMRG states. To overcome this problem we have now successfully developed a parallel tempering DMRG algorithm. Similar to parallel tempering in quantum Monte Carlo, this algorithm allows the systematic switching of DMRG states between different model parameters, which is very efficient for solving convergence problems. Using this method we have figured out the phase diagram of the xxz model on the anisotropic triangular lattice which can be realized by hardcore bosons in optical lattices.

15 min. break

TT 50.11 Wed 18:00 H18

Heisenberg antiferromagnets on the hexagonal bilayer with interlayer frustration — •Boris Celan and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig

Frustrated single layer Heisenberg antiferromagnets on the hexagonal lattice have seen an upsurge of interest. Recently also a bilayer system, i.e. $Bi_3Mn_4O_{12}(NO_3)$, with possibly interlayer frustration has come under scrutiny. For this material $S = 3/2$, rendering spin wave analysis a viable approach. We present results of a selfconsistent spin wave calculation for the hexagonal Heisenberg bilayer up to second order in $1/S$, explicitly taking into account the impact of interlayer frustration. Findings for the quantum phase diagram, the local moments, the ground state energies, and the magnon dispersions versus the exchange interactions will be discussed. Our results will be contrasted against those obtained from methods applied to the quantum limit $S = 1/2$.

TT 50.12 Wed 18:15 H18

Coulomb spin liquid on the honeycomb lattice — •Jorge Armando Rehn[1], Arnab Sen[2], Kedar Damle[3], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Indian Association for the Cultivation of Science, Kolkata, India — [3]Tata Institute of Fundamental Research, Mumbai, India

This talk will present a study of the maximally frustrated classical Heisenberg model on the honeycomb lattice which displays a Coulomb spin liquid phase of a new kind, where emergent gauge charges live on a triangular lattice, and, upon dilution with non-magnetic impurities, this model exhibits new fractionalized objects carrying 1/3 of the moment of the original spins. A zero temperature effective theory for these fractionalized, Coulomb vector charges, will be presented, which represents a new kind of Coulomb spin model presenting a glassy phase.

TT 50.13 Wed 18:30 H18

Kagome spin liquid: a deconfined critical phase driven by the gauge fluctuation — •Yin-Chen He[1], Fuji Yohei[1], and Subhro Bhattacharjee[2] — [1]Max-Planck-Institut fur Physik komplexer Systeme — [2]International Centre for Theoretical Sciences, Tata Institute of Fundamental Research

Recently, new insights emerge into the celebrated problem of spin liquids on the kagome lattice: The kagome spin liquid, the ground state of the nearest neighbor Heisenberg model, survives under the extreme easy-axis anisotropy, and it is neighboring a chiral spin liquid phase. Motivated by this, we study the kagome spin liquid problem in the easy-axis limit, and reformulate it to a lattice gauge model. In this framework, we propose a new theory that, the parent state of the kagome spin liquid is a deconfined critical point, which under the $U(1)$ gauge fluctuation gets extended into a critical phase. Besides the novelty, our theory also makes a vital connection between the seemly different subjects: topological order, critical spin liquid, symmetry protected topological phase, and deconfined criticality.

TT 50.14 Wed 18:45 H18

The transverse field Ising model on the three dimensional swedenborgite lattice: Disorder-by-disorder and an effective classical two dimensional dimer model — •Tycho Sikkenk[1], Lars Fritz[1], Kris Coester[2], and Kai Schmidt[2] — [1]Universiteit Utrecht, Institute for Theoretical Physics, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands — [2]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, Otto-Hahn-Str. 4, D-44221, Dortmund, Deutschland

Geometrical frustration in spin systems often results in a large number of degenerate ground states. In this work we study the antiferromagnetic Ising model on the swedenborgite lattice, a three-dimensional stacking of kagome and triangular layers. The model contains two exchange couplings, one within the kagome layer, another one in between kagome and triangular layers. We investigate the T=0 behaviour of the model in a transverse magnetic field and find a rich phase diagram with both degenerate and non-degenerate phases. Remarkably, for large ratios of out-of-plane coupling over field strength the problem reduces from a three-dimensional quantum model to a two-dimensional classical model at zero temperature.

TT 50.15 Wed 19:00 H18

1/d expansion for the transverse-field Ising model — •Darshan G. Joshi and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden

Analytic 1/d expansion method, previously developed for coupled-dimer magnets, is applied to the transverse-field Ising model ($d>1$) at zero temperature. We introduce auxiliary Bosons to map the spin Hamiltonian onto a Bosonic Hamiltonian. The hard-core constraint from the physical Hilbert space is implemented using the projection operator. The 1/d expansion is employed in both, the paramagnetic as well as the ferromagnetic, phases. We present 1/d expansion for static as well as dynamic observables, including the phase boundary. We thus have a consistent description of the entire phase diagram, including the quantum critical point.