Trends in Quantum Magnetism

673. WE-Heraeus-Seminar

June 4 - 8, 2018
at the Physikzentrum Bad Honnef/Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Subject to alterations!

Introduction

The Wilhelm and Else Heraeus Foundation (Wilhelm und Else Heraeus-Stiftung) is a private foundation which supports research and education in science, especially in physics. A major activity is the organization of seminars. To German physicists the foundation is recognized as the most important private funding institution in their fields. Some activities of the foundation are carried out in cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft).

Scope of the 673. WE-Heraeus-Seminar:

Magnetism is an old subject: The material magnetite has been known for thousands of years. Yet, the richness of magnetic materials and phenomena continues to fascinate us with new ideas, problems, and concepts. The description of the interacting spins in magnetic insulators is a major challenge for theory, and the precise understanding involves ingenious theoretical tools and advanced numerical methods, like tensor networks and Monte-Carlo methods. Recently, concepts of topology are being used increasingly also in the field of magnetism to describe states and excitations in materials. The ideas developed for magnetic Mott insulators are also applied to cold atoms in optical lattices, a new fast growing field of physics.

The topics that we will address in this seminar include:

- Frustrated quantum Heisenberg systems: Theory and experiment
- Mott insulators with strong spin-orbit coupling and Kitaev spin liquids
- Numerical methods: Variational and quantum Monte Carlo methods, exact diagonalization, tensor networks, ab-initio methods
- Spin-orbital models, including SU(N) models
- Topological states of matter
- Dynamics at zero and finite temperature

Scientific Organizers:

Prof. Dr. Andreas Honecker	Université de Cergy-Pontoise E-mail andreas.honecker@u-cergy.fr
Dr. Karlo Penc	Wigner Research Centre for Physics, Budapest E-mail penc.karlo@wigner.mta.hu
Prof. Dr. Maria-Roser Valenti	Universität Frankfurt/Main E-mail valenti@th.physik.uni-frankfurt.de

Introduction

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Registration:

Jutta Lang (WE-Heraeus Foundation)
at the Physikzentrum, reception office
Sunday (17:00 h – 21:00 h) and
Monday morning

Door Code:

(Key symbol button) 2 6 7 3 #
For entering the Physikzentrum
during the whole seminar

Program

Program

Sunday, June 3, 2018

17:00 – 21:00	Registration
from 18:30	*BUFFET SUPPER / Informal get together*

Monday, June 4, 2018

08:00	*BREAKFAST*	

CHAIR: Maria-Roser Valentí

08:50 – 09:00	Scientific organizers	**Opening and welcome**
09:00 – 09:45	Frank Pollmann	**Efficient simulation of the dynamics in frustrated spin systems**
09:45 – 10:30	Frédéric Mila	**Generalization of the Haldane conjecture to SU(3)**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Andreas Läuchli	**Computational quantum field theory approaches to quantum magnetism**
11:45 – 12:30	Philippe Mendels	**Quantum kagome spin liquids: A local view**
12:30	**Conference Photo** (in the foyer of the lecture hall)	
12:40	*LUNCH*	

Program

Monday, June 4, 2018

CHAIR: Arnaud Ralko

14:30 – 15:15	Radu Coldea	**Spin dynamics of frustrated quantum pyrochlore magnets**
15:15 – 15:45	Yasir Iqbal	**Quantum and classical phases of the pyrochlore Heisenberg model with competing interactions**
15:45 – 16:15	Sasha Chernyshev	**Topography and mimicry of spin liquids on a triangular lattice**
16:15 – 16:45	*COFFEE BREAK*	

CHAIR: Jürgen Schnack

16:45 – 17:30	Christian Rüegg	**New phases and quantum criticality in spin- and spin-orbital singlet systems**
17:30 – 18:00	Ornella Vaccarelli	**Exotic phenomena in the new frustrated spin ladder $Li_2O(CuSO_4)_2$**
18:00 – 18:30	Toshihiro Sato	**Quantum Monte Carlo simulation of frustrated Kondo lattice models**
19:00	*DINNER*	

Program

Tuesday, June 5, 2018

08:00	*BREAKFAST*	

CHAIR: Johannes Richter

09:00 – 09:45	Natalia Perkins	**Evolution of intertwined orders in the Kitaev magnet β-Li_2IrO_3**
09:45 – 10:30	Stephen Winter	**Consequences of anisotropic magnetism in α-$RuCl_3$**
10:30 – 11:00	COFFEE BREAK	
11:00 – 11:45	Christian Hess	**Heat transport of the putative Kitaev quantum spin liquid α-$RuCl_3$**
11:45 – 12:30	Yukitoshi Motome	**Majorana fermions in Kitaev spin liquids**
12:30	*LUNCH*	

CHAIR: Andreas Honecker

14:30 – 15:15	Hidenori Takagi	**Spin-orbital entangled quantum liquid in $H_3LiIr_2O_6$**
15:15 – 16:00	Roderich Moessner	**Dynamics of two-dimensional quantum magnets**
16:00 – 16:30	**Poster flash presentations I**	
16:30 – 18:30	**Poster session I** and COFFEE	
19:00	*DINNER*	

Program

Wednesday, June 6, 2018

08:00	*BREAKFAST*	

CHAIR: Karlo Penc

09:00 – 09:45	Maria Daghofer	**Impact of Hund's rule on orbital and spin-orbital excitations**
09:45 – 10:30	George Jackeli	**Spin-orbital interplay in j=3/2 Mott insulators**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Bella Lake	**Experimental investigation of two new quantum spin liquids**
11:45 – 12:30	Salvatore Manmana	**Emergent structures in magnetic systems out-of-equilibrium**
12:30	*LUNCH*	

CHAIR: Karol Szałowski

14:30 – 15:15	Stefan Wessel	**Quantum Monte Carlo in the spin-dimer basis**
15:15 – 16:00	Frederico Becca	**Dynamical structure factor of frustrated spin models: A variational Monte Carlo approach**

16:00 – 18:30 **Excursion** (leisurely hike in the vicinity)

19:00 *HERAEUS DINNER at the Physikzentrum (cold & warm buffet, free beverages)*

Program

Thursday, June 7, 2018

08:00	*BREAKFAST*	

CHAIR: Kai Phillip Schmidt

09:00 – 09:45	Masaki Oshikawa	**Gauge invariance and stability of pi-flux critical phases**
09:45 – 10:30	Didier Poilblanc	**Approaching frustrated magnetism with tensor networks**
10:30 – 11:00	COFFEE BREAK	
11:00 – 11:45	Martin Hohenadler	**Antiferromagnet to valence-bond solid transition with Dirac fermions**
11:45 – 12:30	Chisa Hotta	**Thermodynamic properties of quantum spin systems**
12:30	*LUNCH*	

CHAIR: Gergely Szirmai

14:30 – 15:00	Natalia Chepiga	**DMRG investigation of quantum dimer ladders**
15:00 – 15:30	Götz Uhrig	**Electronic & nuclear spins in driven quantum dots: Paradigm for non-equilibrium states with induced coherence**
15:30 – 16:00	Jeffrey Rau	**Pseudo-Goldstone gaps and order-by-quantum-disorder in frustrated magnets**
16:00 – 16:30	**Poster flash presentations II**	
16:30 – 18:30	**Poster session II** and COFFEE	
19:00	*DINNER*	

Program

Friday, June 8, 2018

08:00	BREAKFAST	

CHAIR: Oleg Derzhko

09:00 – 09:45	Andreas Klümper	**Quantum impurity models as derivatives of the Hubbard model**
09:45 – 10:30	Laura Messio	**High temperature expansions for magnetic systems with impurities under a magnetic field**
10:30 – 11:00	COFFEE BREAK	
11:00 – 11:45	Corinna Kollath	**Finite temperature spectral functions in quasi-one-dimensional magnets**
11:45 – 12:30	Stefan Süllow	**Field induced phases in the low-dimensional frustrated quantum magnets linarite and atacamite**
12:30 – 12:45	Scientific organizers	**Poster awards, summary and closing remarks**
12:45	LUNCH	

End of the seminar and FAREWELL COFFEE **/ Departure**

Please note that there will be **no** dinner at the Physikzentrum on Friday evening for participants leaving the next morning.

Posters

Posters

1.	Jan Attig	**A SUSY-connection between classical spin spirals and free fermions**
2.	Péter Balla	**Directional dichroism of THz radiation in the high temperature phase of multiferroic $Sr_2CoSi_2O_7$**
3.	Jonas Becker	**Spin dynamics of a Z2 spin liquid on the kagome lattice**
4.	Tobias Biesner	**Detuning the Honeycomb of α-$RuCl_3$: Pressure-dependent optical studies reveal broken symmetry**
5.	Carolin Boos	**Chiral Mott phase of three-component fermions on the triangular lattice**
6.	Finn Lasse Buessen	**Competing magnetic orders and spin liquids in three-dimensional quantum magnets**
7.	Niklas Casper	**Alternating ferro- and antiferromagnetic Heisenberg chain: From dimer to Haldane limit**
8.	Ji-Yao Chen	**Topological Z2 resonating-valence-bond spin liquid on the square lattice**
9.	Agnieszka Cichy	**Breaking of SU(4) symmetry and interplay between strongly correlated phases in the Hubbard model**
10.	Jeanne Colbois	**Progressive lifting of the ground-state degeneracy of the long-range kagome Ising antiferromagnet**
11.	Oleg Derzhko	**Realization of flat-band physics in a highly frustrated quantum magnet $Ba_2CoSi_2O_6Cl_2$**
12.	Alexandar Donkov	**Heisenberg kagomé strip with two types of site spins**
13.	Satoshi Ejima	**Exotic criticality in the spin-1 XXZ chain with explicit bond dimerization**
14.	Tim Eschmann	**Thermodynamics of a gauge-frustrated Kitaev spin liquid**
15.	Virgile Favre	**A novel Kagome like Cu_2OSO_4 crystal**
16.	Teresa Feldmaier	**Excitonic magnetism in d_4 systems**
17.	Francesco Ferrari	**Variational Monte Carlo study of the frustrated spin-1/2 Heisenberg model on the honeycomb lattice**
18.	Matthias Gohlke	**Dynamical and topological properties of the Kitaev model in a [111] magnetic field**
19.	Samuel Gozel	**Asymptotic freedom in antiferromagnetic chains of large spin**

20.	Leonie Heinze	**Magnetic properties of the frustrated quantum magnet atacamite, $Cu_2Cl(OH)_3$**
21.	Max Hering	**Spinon band structures in quantum spin liquids from functional renormalization**
22.	Ciarán Hickey	**Complete phase diagram of the Kitaev honeycomb model in tilted magnetic fields: Gapless visons and emergent U(1) quantum spin liquid**
23.	Hajime Ishikawa	**Multipolar orders in $5d^1$ face centered cubic A_2TaCl_6 with $J_{eff} = 3/2$ state**
24.	David Jakab	**The bilinear–biquadratic model on the complete graph**
25.	Darshan Joshi	**Topological excitations in quantum spin systems with spin-orbit coupling**
26.	David Kaib	**Field-induced phase transitions in extended Kitaev models**
27.	Fatemeh Khastehdel Fumani	**Quantum correlations in frustrated isotropic Heisenberg model**
28.	Dominik Kiese	**Pseudofermion functional renormalization group for frustrated magnets: Stability of spin liquid phases from quantum to classical limit**
29.	Ekaterina Klyushina	**The critical phenomena in the S=1 honeycomb antiferromagnet $BaNi_2V_2O_8$**
30.	Miklós Lajkó	**Field theory approach for SU(N) symmetric spin chains**
31.	Thomas Lang	**Quantum Monte Carlo simulation of the O(4) chiral Heisenberg Gross-Neveux transition with a single Dirac cone**
32.	Maik Malki	**Topological properties of quantum magnets: Zak-Phase in $BiCu_2PO_6$ and Chern numbers in RE_5-Si_4F**
33.	Silvia Müllner	**Competing structural and electronic correlations in high temperature superconductors based on optical phonons and magnon scattering**
34.	Somayyeh Nemati	**Measures of correlation compatible with the principle of locality in the one-dimensional XX model**
35.	Arnaud Ralko	**Importance of virtual singlets in RVB theory of quantum spin liquids**

36.	Johannes Richter	**Finite-size realization of the sawtooth spin chain close to quantum criticality**
37.	Jonas Richter	**Real-time dynamics of typical and untypical states in non-integrable systems**
38.	Kira Riedl	**Impurities vs. criticality in the magnetic torque response of the charge transfer salt κ-$(ET)_2Cu_2(CN)_3$**
39.	Andreas Rückriegel	**Bulk and edge spin transport in topological magnon insulators**
40.	Kai Phillip Schmidt	**Mutually attracting spin waves in the square-lattice quantum antiferromagnet**
41.	Jürgen Schnack	**Influence of intermolecular interactions on magnetic observables**
42.	Andrew Smerald	**Spin-glass ordering due to orbital and lattice effects in spin-1 pyrochlores**
43.	PV Sriluckshmy	**Effect of electric field on breathing pyrochlores**
44.	Karol Szałowski	**Quantum entanglement in spin ladder-shaped nanomagnet**
45.	Gergely Szirmai	**Quanatum magnetism with four component fermions**
46.	Luc Testa	**A neutron scattering journey of a 2D chiral quantum magnet - A(Tio)$Cu_4(PO_4)_4$**
47.	Javad Vahedi	**Edge magnetic properties of black phosphorene nanoribbons**
48.	Laurens Vanderstraeten	**Quasiparticle excitations with tensor network states**
49.	Taras Verkholyak	**Fractional magnetization plateaux in the Shastry-Sutherland model: Effect of quantum XY interdimer interaction**
50.	Ruben Verresen	**Quantum dynamics of the square lattice Heisenberg model**
51.	Kyle Wamer	**Generalization of the Haldane conjecture to SU(3) chains**
52.	Zhenjiu Wang	**Spin and valence bond dynamics across a deconfined quantum critical point in a fermionic SU(3) model**
53.	Lukas Weber	**Critical edge states of two-dimensional quantum critical magnets**
54.	Yuan Yao	**Anomaly matching and symmetry-protected critical phases in SU(N) spin systems in 1+1 dimensions**

Abstracts of Lectures

(in alphabetical order)

Dynamical structure factor of frustrated spin models: a variational Monte Carlo approach

F. Becca

[1] *CNR and SISSA, Trieste, Italy*

The spin dynamical structure factor is computed within a variational framework to study frustrated Heisenberg models in one and two dimensions. Starting from Gutzwiller-projected fermionic wave functions, the low-energy spectrum is constructed by considering two-spinon excitations. A benchmark of this approach on the one-dimensional J1-J2 model is considered. Here, an excellent description of both the gapless and gapped (dimerized) phases is obtained, also describing the incommensurate structure for large frustrating ratios J2/J1>0.5[1]. In the square lattice, we are able to unveil the dynamical signatures of the transition between the Neel and the (gapless) spin-liquid phases that takes place for J2/J1~0.45. In particular, by increasing the frustration, the magnon excitation at q=(pi,0) and (0,pi) broadens, suggesting the tendency towards a spin fractionalization. In addition, its energy softens, indicating the presence of gapless states at the transition and within the spin-liquid phase. [2] Future applications will focus on the Heisenberg model on the Kagome lattice, as well as further benchmarks on the Kitaev model, where the exact calculation of the dynamical structure factor is possible [3].

References

[1] F. Ferrari, A. Parola, S. Sorella, and F. Becca, arXiv:1803.02359

[2] F. Ferrari and F. Bacca, in preparation

[3] J. Knolle, D. L. Kovrizhin, J. T. Chalker, and R. Moessner, Phys. Rev. Lett. **112**, 207203 (2014); Phys. Rev. B **92**, 115127 (2015).

DMRG investigation of Quantum Dimer Ladders

N. Chepiga[1] **and F.Mila**[2]

[1]University of California, Irvine, USA
[2] EPFL, Lausanne, Switzerland

We study quantum dimer model (QDM) on a two leg ladder using DMRG algorithm. While spin degrees of freedom are located in the nodes of the lattice, the dimer degrees of freedom are associated with the bonds. There is a local constraint associated with hard-core dimers: for any pair of corner sharing bonds no more than one can be occupied by a dimer. We will show how this constraint can be implemented in DMRG, so the Hilbert space of QDM grows slower than for spin model and one can reach the size of 3600 rungs. We use the method to study quantum phase transition in quantum dimer ladder and its generalization to hard-boson model. We were able to detect numerically critical incommensurate phase predicted by field theory in Ref.[1]. The proposed method is generic for any type of local constraints. Critical incommensurate phase also appears in the with two dimers per corner sharing bonds (equivalent to spin-1) on zig-zag ladder.

References

[1] Fendley, Sengupta, Sachdev, PRB 69, 075106 (2004)

Topography and mimicry of spin liquids on a triangular lattice

Zhenyue Zhu,[1] P. A. Maksimov,[1] Steven R. White,[1] and A. L. Chernyshev[1*]

[1]*Department of Physics and Astronomy, University of California, 92697, Irvine, California, USA*

There is a significant recent interest in spin systems with strongly-anisotropic frustrating spin interactions due to possible exotic ground states. We have explored an extended 3D phase diagram of a class of such models on an ideal triangular lattice using density-matrix renormalization group (DMRG) and quasiclassical approaches [1,2] and have mapped out the topography of the region that can harbor a spin liquid state. A 4D extension of this phase diagram naturally connects to a different spin liquid phase of the isotropic J_1-J_2 model. We find that spin-spin correlations are nearly identical between these two limits [2], making a strong case that their respective spin liquids are isomorphic to each other.

For $YbMgGaO_4$, a rare-earth-based triangular-lattice antiferromagnet with anisotropic spin-spin interactions, our analysis finds no transitions to a spin liquid near experimentally relevant range of parameters [1,2]. We have proposed that a randomization of the subleading pseudo-dipolar interactions due to spatially-fluctuating charge environment of the magnetic ions can successfully mimic a spin liquid by forming short-range stripe-ordered domains, producing the structure factor that is in agreement with experiment. This spin-liquid mimicry scenario is relevant to other quantum magnets with fragile ground states selected by an order-by-disorder fluctuations and random environments.

References

[1] Zhenyue Zhu, P. A. Maksimov, Steven R. White, and A. L. Chernyshev, Phys. Rev. Lett. **119**, 157201 (2017).

[2] Zhenyue Zhu, P. A. Maksimov, Steven R. White, and A. L. Chernyshev, arXiv:1801.01130 (accepted to Phys. Rev. Lett.).

Spin dynamics of frustrated quantum pyrochlore magnets

J.D. Thompson,[1] P.A. McClarty,[2,3] D. Prabhakaran,[1] J.G. Rau,[3] I. Cabrera,[1] T. Guidi,[2] D. Voneshen[2] and R. Coldea[1]

[1]*Clarendon Laboratory, University of Oxford, United Kingdom*
[2]*ISIS Facility, Rutherford Appleton Laboratory, Didcot, United Kingdom*
[3]*Max-Planck Institute for the Physics of Complex Systems, Dresden, Germany*

$Yb_2Ti_2O_7$ and $Er_2Ti_2O_7$ are effective spin-1/2 frustrated magnets on the three-dimensional pyrochlore lattice displaying distinct types of magnetic order in the ground state, ferromagnetic and XY antiferromagnetic order, respectively. Here we report results of single-crystal, high-resolution inelastic neutron scattering measurements to explore the interplay between sharp magnon modes and extended excitation continua, and the evolution of the spin dynamics in applied magnetic field.

References

[1] J.D. Thompson, P.A. McClarty, D. Prabhakaran, I. Cabrera, T. Guidi, D. Voneshen and R. Coldea, Phys. Rev. Lett. **119**, 057203 (2017).

Impact of Hund's rule on orbital and spin-orbital excitations

J. Heverhagen and M. Daghofer

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We study the impact of Hund's-rule coupling on orbital excitations, as e.g. measured in inelastic resonant x-ray scattering, with an emphasis on the regime of spin-orbit separation reported for one-dimensional Mott insulators. While the scenario of spin-orbit separation rests on a mapping that can only be derived for systems without Hund's rule, we find that an interpretation in terms of spinon and orbiton remains robust in its presence. Depending on whether or not the orbital excitation includes a spin flip, Hund's rule leads to an attractive or repulsive interaction between spinon and orbiton. Attraction and repulsion leave clear signatures through a transfer of spectral weight to the lower resp. upper edge of the spectrum.

References

[1] J. Heverhagen and M. Daghofer, arXiv:1804.04462

Heat transport of the putative Kitaev quantum spin liquid α-$RuCl_3$

Christian Hess[1]

[1]*IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany*

The honeycomb Kitaev-Heisenberg model is a source of a quantum spin liquid with Majorana fermions and gauge flux excitations as fractional quasiparticles. Here we unveil highly unusual low-temperature heat conductivity κ of α-$RuCl_3$, a prime candidate for realizing such physics: beyond a magnetic field of B>7.5T, the longitudinal component κ_{xx} increases by about one order of magnitude, both for in-plane as well as out-of-plane transport. This clarifies the unusual magnetic field dependence unambiguously to be the result of severe scattering of phonons off putative Kitaev-Heisenberg excitations in combination with a drastic field-induced change of the magnetic excitation spectrum. In particular, a large energy gap arises, which increases linearly with the magnetic field, reaching remarkable $\hbar\omega_0 / k_B \approx 50$K at 18T [1]. Interestingly, for fields perpendicular to the planes, where the magnetic ordering remains intact even up to 18T, the impact of the field on the longitudinal heat transport is more subtle: A small positive thermal magnetoresistance (in the order of 5%) occurs in the paramagnetic phase. Strikingly, in the same phase we observe a large positive transversal heat conductivity κ_{xy} which increases linearly with magnetic field B. Upon raising the temperature, κ_{xy} increases strongly, exhibits a broad maximum at around 30K, and eventually becomes negligible at T>125K [2]. These findings provide clear-cut evidence for longitudinal and transverse magnetic heat transport and underpin the unconventional nature of the quasiparticles in the paramagnetic phase of α-$RuCl_3$.

References

[1] R. Hentrich, A. U. B. Wolter, X. Zotos, W. Brenig, D. Nowak, A. Isaeva, T. Doert, A. Banerjee, P. Lampen-Kelley, D. G. Mandrus, S. E. Nagler, J. Sears, Y.-J. Kim, B. Büchner, C. Hess, Phys. Rev. Lett. **120**, 117204 (2018)

[2] R. Hentrich, M. Roslova, A. Isaeva, T. Doert, W. Brenig, B. Büchner, C. Hess, arXiv:1803.08162

Antiferromagnet to valence-bond solid transition with Dirac fermions

T. Sato, M. Hohenadler, F. F. Assaad

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We consider a model of Dirac fermions in 2+1 dimensions with dynamically generated, anticommuting SO(3) Néel and Z2 Kekulé mass terms that permits sign-free quantum Monte Carlo simulations. The phase diagram is obtained from finite-size scaling and includes a direct and continuous transition between the Néel and Kekulé phases. The fermions remain gapped across the transition, and our data support an emergent SO(4) symmetry unifying the two order parameters. While the bare symmetries of our model do not allow for spinon-carrying Z3 vortices in the Kekulé mass, the emergent SO(4) invariance permits an interpretation of the transition in terms of deconfined quantum criticality. The phase diagram also features a tricritical point at which Néel, Kekulé, and semimetallic phases meet. The present, sign-free approach can be generalized to a variety of other mass terms and thereby provides a new framework to study exotic critical phenomena.

References

[1] T. Sato, M. Hohenadler, F. F. Assaad, Phys. Rev. Lett. **119**, 197203 (2017)

Thermodynamic properties of quantum spin systems

C. Hotta[1] and K. Asano[2]

[1]*Department of Basic Science, University of Tokyo, Tokyo, Japan.*
[2] *Department of Physics, Osaka University, Osaka, Japan*

We develop a scheme to numerically obtain a uniform susceptibility and a specific heat of the quantum many body systems within a reasonable accuracy against the ones in the bulk limit without finite size scaling. The idea is based on the grand canonical analysis we proposed earlier [1,2]; by spatially varying the energy scale of the Hamiltonian from the ordinary scale at the center to zero on edges, we obtain local physical quantities of the ground state at the system center, which is found to give accurate evaluation of their corresponding bulk values[1,2]. We confirm that this holds also for excited states, by showing several demonstration for spin-1/2 Heisenberg models in one- and two-dimensions.

References

[1] C. Hotta and N. Shibata, Phys. Rev. B **86,** R041108 (2012).
[2] C. Hotta, S. Nishimoto and N. Shibata, Phys. Rev. B **87**, 115128 (2013).

Quantum and classical phases of the pyrochlore Heisenberg model with competing interactions

Y. Iqbal[1] , T. Müller[2] , P. Ghosh[3], M. J. P. Gingras[4,5,6], H. O. Jeschke[7], S. Rachel[8], J. Reuther[9,10], R. Thomale[2]

[1] Indian Institute of Technology Madras, Chennai, India
[2] University of Würzburg, Würzburg, Germany
[3] Jawaharlal Nehru University, New Delhi, India
[4] Perimeter Institute for Theoretical Physics, Waterloo, Canada
[5] University of Waterloo, Waterloo, Canada
[6] Canadian Institute for Advanced Research, Toronto, Canada
[7] Okayama University, Okayama, Japan
[8] The University of Melbourne, Parkville, Australia
[9] Free University of Berlin, Berlin, Germany
[10] Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

We investigate the quantum Heisenberg model on the pyrochlore lattice for a generic spin-S in the presence of nearest-neighbor J_1 and second-nearest-neighbor J_2 exchange interactions. By employing the pseudofermion functional renormalization group (PFFRG) method, we find, for S=1/2 and S=1, an extended quantum spin liquid phase centered around J_2=0, which is shown to be robust against the introduction of breathing anisotropy. The effects of temperature, quantum fluctuations, breathing anisotropies, and a J_2 coupling on the nature of the scattering profile, in particular, the pinch points are studied. For the magnetic phases of the J_1-J_2 model, quantum fluctuations are shown to strongly renormalize phase boundaries compared to the classical model and shift the ordering wave vectors of spiral magnetic states, however, no new magnetic orders are found to be stabilized [1].

References

[1] Y. Iqbal *et al.*, arXiv:1802.09546 (2018).

Spin-orbital interplay in j=3/2 Mott Insulators

G. Jackeli

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In d^1 Mott insulators, the spin-orbit coupling (SOC) stabilizes j=3/2 quartet of an effective total angular momentum thus allowing for the emergence of multi-orbital physics and related spin-orbital frustration. Considering molybdenum, and osmium oxides as examples, I discuss how resulting spin-orbital interplay can give rise to a host of novel quantum phases that includes multipolar order, non-collinear spin patterns, and nonmagnetic disordered valence bond states [1]. Finally, I present an example of the honeycomb lattice d^1 compound, such as zirconium trichloride, in which, paradoxically, the strong SOC enhances the symmetry of spin-orbital space to emergent SU(4) symmetric couplings [2] that in turn may lead to a spin-orbital liquid state.

References

[1] F. J. Romhányi, L. Balents, & G. Jackeli, Phys. Rev. Lett. **118**, 217202 (2017)
[2] A M. G. Yamada, M. Oshikawa, & G. Jackeli, arXiv:1709.05252 (2017)

Quantum impurity models as derivatives of the Hubbard model

A. Klümper[1] and **Y. Öz**[1]

[1] *University of Wuppertal, Gauss-Strasse 20, 42119 Wuppertal, Germany*

We derive the integrable Anderson Impurity Model (AIM) as a continuum limit of the Hubbard model with an integrable `transparent impurity'. This construction allows for an alternative derivation of the Bethe ansatz equations for the Hamiltonian, but also provides

i) an alternative treatment of the thermodynamics of the AIM on the basis of finitely many non-linear integral equations which is much more efficient than the thermodynamical Bethe ansatz (TBA),

ii) the host of the AIM can be manipulated yielding a vanishing density of states at the Fermi energy by keeping integrability. In this way an integrable Anderson impurity in a pseudo-gap system is realized.

Finite temperature spectral functions in quasi-one-dimensional magnets

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The properties of collective phases occuring in strongly correlated materials are often characterized by their two-time correlations and spectral functions. Many interesting excitations can be identified with the help of these quantities. The calculation of these properties at finite temperature and under the influence of dissipation in interacting many body systems is a great challenge. We present results which were obtained using the matrix product state formalism the calculation of these quantities in quasi-one-dimensional spin chains.

Experimental investigation of two new quantum spin liquids

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Unlike conventional magnets where the magnetic moments are partially or completely static in the ground state, in a quantum spin liquid they remain in collective motion down to the lowest temperatures. The importance of this state is that it is coherent and highly entangled without breaking local symmetries. The spin liquid state is expected to occur in highly frustrated magnets such as those consisting or triangular and tetrahedral arrangements of magnetic ions. This state is however very rare with only a few Hamiltonians known theoretically to support it and only a few experimental realizations in existence. This talk will discuss the discovery and investigation of two new compounds displaying spin liquid behaviour [1,2]. These compounds have two- and three-dimensional lattices respectively, and their magnetic Hamiltonians have not been investigated either experimentally or theoretically prior to this work. Neutron scattering and physical properties data will be presented alongside theoretical calculations which together provide strong evidence for the spin liquid state.

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Computational quantum field theory approaches to quantum magnetism

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Quantum field theories play an important role in many condensed matter systems for their description at low energies and long length scales. In 1+1 dimensional critical systems the energy spectrum and the spectrum of scaling dimensions are intimately related in the presence of conformal symmetry. In higher space-time dimensions this relation is more subtle and not well explored numerically. In this talk we motivate and review our recent effort to characterize 2+1 dimensional quantum field theories using computational techniques targeting the energy spectrum on a spatial torus. We discuss several examples ranging from the O(N) Wilson Fisher theories and Gross-Neveu-Yukawa theories to deconfinement-confinement transitions in the context of topological ordered systems. We advocate a phenomenological picture that provides insight into the operator content of the critical field theories. We close by discussing prospects of observing the critical energy spectrum in mesoscopic quantum magnets.

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Emergent structures in magnetic systems out-of-equilibrium

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The emergence of long-range order and the spontaneous breaking of symmetries is one of the hallmarks of magnetic systems. Recently, the question how to realize these in nonequilibrium set-ups has sparked a lot of interest. Here, I want to address both aspects in systems, which are either typical for the field of quantum magnetism, or in which the presence of magnetic structures is important for the behavior in time: in the first part, the spontaneous breaking of time translational symmetry (TTSB) in Floquet-driven Ising systems is considered, which in the past year has caused a lot of excitement as it realizes so-called 'time-crystals'. A combined approach using analytical and matrix product state techniques to compute the Loschmidt echo uncovers that a precursor region exists, in which the response happens at an arbitrary even multiple of the period of the driving. In the second part of my talk, I turn to the possibility to create periodic structures in space following a photoexcitation. This is realized in a one-dimensional toy-model for manganate systems, in which polarons cause a magnetic microstructure. In its presence a charge-density-wave-like pattern emerges in time for specific photoexcitations. An outlook to existing and possible future experimental realizations is given.

Quantum kagome spin liquids: a local view

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In my talk, I will present results on two kagome quantum spin liquids.

1- Herbertsmithite $ZnCu_3(OH)_6Cl_2$ has been known since 2005 as one of the best representative of spin liquid physics for the Heisenberg model on a quantum kagome antiferromagnetic lattice (KHAF). While some quasi-free Cu on Zn sites mask the signature of the kagome physics at low-T in most experimental techniques, typically T < J/10, one can take advantage of the strong coupling of O to the kagome Cu's to track this physics through ^{17}O NMR [1]. Recently, working on high quality single crystals considerably improved the accuracy of NMR measurements and its ability to address fundamental issues such as the existence of a gap and the class of models relevant to describe the ground state. However, the greatest challenge to reach firm conclusions about the low T kagome physics is still to discriminate between what belongs to kagome Cu's and what is the counterpart induced by defects. We have mapped out in detail the latter contribution and could then isolate the ^{17}O NMR spectral signature of kagome Cu's. Neither in our shift measurements nor in our relaxation studies, do we find any hint of a gap. On the contrary, we conclude that the susceptibility is finite and independent of the field in the range 2.6 - 12 Teslas [2]. Insights on the defect physics is also gained from recent high field ESR measurements on our samples [3].

2- In $[NH_4]_2[C_7H_{14}N][V_7O_6F_{18}]$, the V^{4+} ions (d^1) form a unique S = ½ breathing kagome lattice which consists of alternating equilateral triangles, preserving the full frustration of the isotropic model and the spin liquid ground state [4]. Combining NMR measurement of the local susceptibility and state-of-the-art series expansion analysis, we could evaluate the ratio $J_\Delta / J_\nabla \sim 0.55$ for the interactions of the two sets of triangles. In line with recent theoretical results from variational methods and DMRG, we found that the spinon excitations are gapless and lead to a metallic-like low T heat capacity in this strong insulator. This experimental study should trigger novel theory approaches of the kagome problem through a J'-> J limit.

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High temperature expansions for magnetic systems with impurities under a magnetic field.

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Many recently synthesized magnetic compounds display fascinating unconventional phases (gapped or un-gapped spin liquids, valence bond crystals,…). It is very difficult to extract the coupling constants from purely chemical and crystallographic considerations. A useful tool is the high temperature expansion, whose reliability has been proved on several compounds (Herbertsmithite[1], Kapellasite[2], breathing kagome[3]…).
It consists in an expansion of the partition function in the inverse temperature. From the resulting series, thermodynamic quantities are extrapolated (specific heat, magnetic susceptibility, ...). After a review of the last advances in this technique (notably the use of the entropy as a function of the energy to easily take into account sum rules constraining the result[4]), we will present our first results of series on Herbertsmithite in the presence of non magnetic impurities and under a magnetic field.

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Generalization of the Haldane conjecture to SU(3)

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In this talk, I will show how to study SU(3) chains in the symmetric representation using field theory methods [1], generalizing Haldane's semiclassical approach to SU(2) spin chains. I will show that the SU(3) chain with p boxes in the Young tableau can be mapped into a flag manifold non-linear σσ-model with a topological angle $\theta=2\pi p/3$. Combining Bethe ansatz results in the fundamental representation with a strong coupling analysis and Monte Carlo simulations of the σ-model, I will show why the SU(3) chain can be expected to be gapped for $p=3m$ but gapless for $p=3m\pm1$ (m integer), corresponding to a massless phase of the σ-model at $\theta=\pm2\pi/3$. I will also review the current efforts aimed at checking this conjecture with numerical simulations of the Heisenberg SU(3) model.

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Dynamics of two-dimensional quantum magnets

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Majorana fermions in Kitaev spin liquids

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Since the pioneering work by Kitaev [1], quantum spin liquids have gained renewed interest from both theoretical and experimental perspectives during the past decade. One of the most interesting aspects in the research of Kitaev spin liquids is the emergence of Majorana fermions as fractionalized excitations from the topological ground state. Stimulated by the argument by Jackeli and Khaliullin [2], there have been a lot of experimental efforts to materialize the Kitaev spin liquids and exotic excitations, but the clear identification remains elusive. In this talk, we will present our theoretical results for the experimentally-accessible fingerprints of Majorana fermions, in comparison with recent experimental data. We will discuss various thermodynamic properties [3,4], spin dynamics [5-9], and the effect of an applied magnetic field [10-12]. We will also make a remark on our recent efforts to extend the candidate materials for the Kitaev spin liquids [13,14].

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Gauge invariance and stability of pi-flux critical phases

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Evolution of intertwined orders in the Kitaev magnet β-Li2IrO3

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Recent scattering experiments in the 3D Kitaev magnet β-Li_2IrO_3 have shown that a relatively weak magnetic field along the crystallographic **b**-axis drives the system from its incommensurate counter-rotating order to a correlated paramagnet, with a significant uniform `zigzag' component superimposing the magnetization along the field. In our study we show that the zigzag order is not emerging from its linear coupling to the field (via a staggered, off-diagonal element of the **g**-tensor), but from its intertwining with the incommensurate order and the longitudinal magnetization. The emerging picture explains all qualitative experimental findings at zero and finite fields, including the rapid decline of the incommensurate order with field and the so-called intensity sum rule. The latter are shown to be independent signatures of the smallness of the Heisenberg exchange J, compared to the Kitaev coupling K and the off-diagonal anisotropy Γ. Remarkably, in the regime of interest, the field H' at which the incommensurate component vanishes, depends essentially only on J, which allows to extract an estimate of $J4K$ from reported measurements of H.

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Approaching frustrated magnetism with tensor networks

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In 2-dimensions, tensor networks such as Projected Entangled Pair States (PEPS) are elegant many-body wavefunctions which capture efficiently the quantum entanglement of ground states (or low-energy eigenstates) of local electronic or quantum spin Hamiltonians. In this talk, I will review recent progress to construct various spin liquids [1], including topological ones [2] and those carrying chiral edge modes described by simple CFTs [3]. (i) SU(2) symmetry can be implemented directly at the site tensor level [1] and (ii) tensor contraction can be performed directly in the thermodynamic limit using a Corner Transfer Matrix RG scheme. (i) and (ii) enable to attack difficult frustrated quantum spin models (examples of spin-1/2 [4] and spin-1 [5] models will be given) using an unbiased full energy minimization scheme.

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Efficient simulation of the dynamics in frustrated spin systems

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Dynamical response functions encode characteristic features of the emergent excitations in frustrated magnets. We introduce a matrix-product state based method to efficiently obtain these dynamical response functions for general two-dimensional lattice Hamiltonians. First, we apply this method to different phases of the Kitaev-Heisenberg model. Here we find significant broad high energy features beyond spin-wave theory even in the ordered phases proximate to spin liquids. This includes the phase with zig-zag order of the type observed in α-$RuCl_3$, where we find high energy features like those seen in inelastic neutron scattering experiments [1]. Second, we study the stability of magnon excitations in Heisenberg antiferromagnets.

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Pseudo-Goldstone gaps and order-by-quantum-disorder in frustrated magnets

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In systems with competing interactions, continuous degeneracies can appear which are accidental, in that they are not related to any symmetry of the Hamiltonian. Accordingly, the pseudo-Goldstone modes associated with these degeneracies are also unprotected. Indeed, through a process known as "order-by-quantum-disorder", quantum zero-point fluctuations can lift the degeneracy and induce a gap for these modes. We show that this gap can be exactly computed at leading order in $1/S$ in spin-wave theory from the mean curvature of the classical and quantum zero-point energies - without the need to consider any spin-wave interactions. We confirm this equivalence through direct calculations of the spin-wave spectrum to $O(1/S^2)$ in a wide variety of theoretically and experimentally relevant quantum spin models. We prove this equivalence through the use of an exact sum rule that provides the required mixing of different orders of $1/S$. Finally, we discuss some implications for several leading order-by-quantum-disorder candidate materials, clarifying the expected pseudo-Goldstone gap sizes in $Er_2Ti_2O_7$ and $Ca_3Fe_2Ge_3O_{12}$.

New Phases and Quantum Criticality in Spin- and Spin-Orbital Singlet Systems

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Materials made of arrays of magnetic ions forming well-defined lattices serve as model systems to study the phases of correlated magnetic quantum matter. We investigate elementary phases and quasi-particles and their stability under static multi-extreme conditions in temperature, magnetic field and pressure in frustrated and low-dimensional magnets. In one-dimensional ladder systems we observe single- and multi-particle excitations and their decay [1]. In the two-dimensional frustrated Shastry-Sutherland lattice, pressure is used to control directly the frustration and stability of quasi-particles resulting in novel quantum phases near (deconfined) quantum critical points [2]. Recently we extended these studies to systems with spin-orbit and spin-lattice coupling [3,4], with new degrees of freedom and new ways of probing them. The results will be discussed in the context of recent developments in computational physics and new opportunities that free electron lasers will offer to study out-of-equilibrium physics of such systems.

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Quantum Monte Carlo simulation of frustrated Kondo lattice models

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Our current focus is on emergent quantum phenomena when a spin system with a macroscopic degenerate ground state is coupled to fermions. For example, classically, frustration leads to a macroscopic degenerate ground state that violates the third law of thermodynamics. Turning on quantum effects is bound to generate exotic states of matter.

In our recent work [1], we have introduced a new class of coupled frustrated spin fermion models that can be simulated – free of the so called negative sign problem – in the realm of the auxiliary field quantum Monte Carlo method [2,3]. As a case study we present results for a half-filled Kondo lattice model on the honeycomb lattice supplemented by frustrating couplings between localized spins. The geometrical frustration adds a new competing energy scale in the generic Doniach phase diagram [4] which conventionally accounts only for the competition between the RKKY interaction and the Kondo screening. We provide evidence that this frustrating coupling term generates so called partial Kondo screened states of matter, where Kondo screening becomes site dependent so as to alleviate frustration effects and the lattice rotation symmetry is broken nematically [1].

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Field induced phases in the low-dimensional frustrated quantum magnets linarite and atacamite

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In recent years, low dimensional frustrated quantum spin systems have been the focus of extensive research efforts because of the observation of a multitude of exotic field induced phases. Both, the natural minerals linarite, $PbCuSO_4(OH)_2$, and atacamite, $Cu_2Cl(OH)_3$, are cases in point [1,2]. The former compound, linarite, has been established as a spin chain material, with a frustrated ferromagnetic nearest and antiferromagnetic next-nearest neighbor magnetic coupling. In result, the frustration induces complex magnetic phases in high magnetic fields, but where the microscopic nature of these phases remains a topic of dispute [3]. For the latter material, atacamite, from a recent combined experimental and theoretical study we propose that it represents the first clean example of the so-called saw-tooth or delta-chain, i.e., a chain of triangles with two different couplings on the triangle. Again, as result of the frustration, we find an unusual high-field behavior, with novel types of field-induced states. In my contribution, I will review the experimental cases of both linarite and atacamite, and in particular will present our efforts to (microscopically) characterize the field-induced states and phases.

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Spin-Orbital Entangled Quantum liquid in $H_3LiIr_2O_6$

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In 5d Ir4+ oxides, the spin-orbit coupling for 5d electrons is as large as ~0.5 eV and not small as compared with on-site Coulomb U. This often gives rise to a novel spin-orbital Mott state with J_{eff}=1/2 isospins, which was first identified in the layered perovskite Sr_2IrO_4 [1]. When J_{eff}=1/2 iso-spins interact with each other through 90° Ir-O2-Ir bonds, an Ising ferromagnetic coupling is expected [2]. In α-, β-, γ-Li_2IrO_3 with honeycomb based structure, J_{eff}=1/2 iso-spin are connected by the three competing 90° Ir-O_2-Ir bonds. These compounds were pointed out theoretically to be a materialization of Kiatev model [3], where S=1/2 spins on honeycomb lattice is connected by a bond dependent ferromagnetic interaction and a topological spin liquid with Majorana excitations is realized as the ground state. A long range magnetic ordering, however, was observed in α–, β–, γ-Li_2IrO_3, which is likely due to the presence of additional magnetic couplings not included in the original Kitaev model.

The exploration of Kitaev spin liquid state was recently extended. We found that a quantum spin liquid state is realized in $H_3LiIr_2O_6$ which can be viewed as "hydrogenated" α-Li_2IrO_3 [4]. This iridate does not show magnetic ordering down to 0.05 K, despite an energy scale of magnetic interaction ~ 100 K. Signature of energy symmetric, low-energy fermionic excitation is observed in the magnetization $M(T,B)$, NMR relaxation $1/T_1(T,B)$ and specific heat $C(B,T)$, which we ascribe to the presence of a small amount spin defects. All M, $1/T_1$ and C follows a scaling with B/T. After subtracting the scaled contribution originating from the defects, we observe dominant T^3-contribution in $C(T)$ below T = 5K independent B, likely originating from the lattice. This suggests the presence of gap in the spin excitations.

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Electronic & nuclear spins in driven quantum dots: Paradigm for non-equilibrium states with induced coherence

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The spin of localized electrons or holes in quantum dots is an interesting candidate for a quantum bit. Hence, one aims at keeping its coherence as long as possible. First, we discuss the main mechanism for the decoherence of the dynamics of the electronic spin and how one simulate them efficiently [1,2]. Second, we discuss the phenomenon of mode-locking observed in ensembles of quantum dots which leads to a coherent response of a large fraction of quantum dots [3]. This mode-locking is achieved by long trains of repeated laser pulses inducing a state far from equilibrium [4].

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Exotic phenomena in the new frustrated spin ladder $Li_2O(CuSO_4)_2$

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Despite decades of theoretical work devoted to the study of frustrated spin ladders (see, e.g., [1] and references therein), real material realizations of such systems still remain limited. In this work, we investigate the magnetic properties of the new compound $Li_2O(CuSO_4)_2$ [2], which appears as a very rare realization of a $S=1/2$ frustrated two-leg spin ladder in its high-temperature tetragonal structure, where magnetic frustration arises from competing interactions along the legs [3]. Moreover, the compound undergoes a structural transition at about 125K, involving a very weak distortion of the structure. Combining experimental and theoretical approaches, we demonstrate that the structural transition, while maintaining the global geometry of a ladder, induces the formation of a staggered dimer structure through a large magnetoelastic coupling, removing most of the magnetic frustration [4]. Furthermore, we present the first detailed investigation of the low-temperature magnetic excitations of $Li_2O(CuSO_4)_2$ combining magnetic susceptibility, infrared spectroscopy and inelastic neutron scattering measurements. Experimental observations are qualitatively explained by exact diagonalization and higher-order perturbation calculations carried out on the basis of the dimerized geometry derived from first principle calculations [5].

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Quantum Monte Carlo in the Spin-Dimer Basis

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We present a quantum Monte Carlo scheme for the simulation of frustrated dimerized quantum magnets that allows us to reduce or even eliminate the sign-problem for several specific dimerized spin systems [1,2]. We discuss in particular its application to the thermal properties of the spin-1/2 Heisenberg model on the fully frustrated 2-leg ladder and the fully frustrated square lattice bilayer model. At zero temperature for the later model, a discontinuous quantum phase transition separates an inter-layer singlet phase from an antiferromagnetic ground state forming from inter-layer triplet states. We show that this discontinuous transition extends towards finite temperatures, i.e., in the absence of long-range order. The thermodynamic behavior of this system furthermore exhibits similarities to the liquid-gas transition.

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Consequences of Anisotropic Magnetism in α-$RuCl_3$

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Intensive study of α-$RuCl_3$ has been motivated recently by signatures of strongly anisotropic and frustrated interactions reminiscent of the Kitaev honeycomb model [1]. Even though α-$RuCl_3$ orders magnetically in a zigzag ground state, it exhibits a broad continuum of magnetic excitations [2,3], which is inconsistent with conventional magnons. Many works have taken the breakdown of magnons as a signature of proximity to the Kitaev spin liquid. By analogy, the suppression of magnetic order at finite magnetic field has been discussed in terms of a field-induced spin-liquid state. In order to evaluate these proposals, we have considered the dynamical response and stability of magnons at zero and finite field with respect to the full range of realistic magnetic interactions suggested by recent ab-initio calculations [4,5]. Combining extensive exact diagonalization studies with semiclassical analysis, we will address the (i) relevant mechanisms for magnon breakdown, (ii) origin and robustness of the continuum, (iii) evolution of the spectra under applied field, and (iv) nature of the field-induced state.

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Abstracts of Posters

(in alphabetical order)

A SUSY-connection between Classical Spin Spirals and Free Fermions

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The formation of coplanar spin spirals is a common motif in the magnetic ordering of many frustrated magnets. For classical antiferromagnets, geometric frustration can lead to a massively degenerate ground state manifold of spirals whose propagation vectors can be described by points, lines or surfaces in momentum space.

On this poster we demonstrate an approach to describe the diversity of these manifolds by introducing a supersymmetry mapping to a free fermion system in which the degenerate spiral manifold maps to the nodal manifold of the fermion system, i.e. the Fermi surface. The mapping is goverened by an underlying lattice construction algorithm which allows the design of supersymmetrically related systems who share their ground states as well as their excitation spectra.

In a similar fashion, one can employ the SUSY mapping to connect the emergent Majorana fermions in honeycomb Kitaev systems to classical mechanical systems that are associated with the field of topological mechanics.

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Directional Dichroism of THz Radiation in the High Temperature Phase of Multiferroic $Sr_2CoSi_2O_7$

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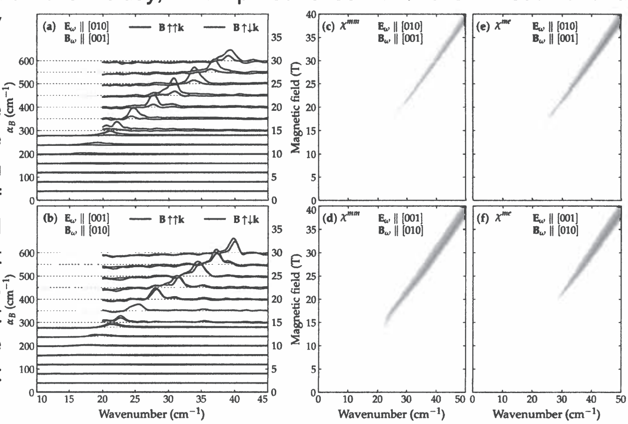
In multiferroic materials strongly coupled magnetic and electric (polarization) orders coexist in the low temperature ordered phase. This strong coupling manifests itself in the excitations (so called electromagnons), that are susceptible to both the electric and magnetic component of the exciting light field.

Directional dichroism is the phenomenon when counterpropagating lightbeams absorb differently, and is a hallmark of the presence of electromagnons. Here we present direction dependent absorption experiments on the multiferroic material $Sr_2CoSi_2O_7$ in the *high temperature paramagnetic* phase [1], where we found a peak showing directional dichroism. We examined the dependence of the absorption on the temperature, magnetic field and polarization (both electric and magnetic) on the exciting light field. We found simple explanations of these phenomena in a small cluster exact diagonalization study, a simplified effective one-ion model and a thorough symmetry analysis.



In panels (a), (b) we can see the measurement of the directional dichroism (the difference of the blue and red curves) for different polarizations (E_ω, B_ω). In the right panels there are the results of the exact diagonalization simulations of the magnetic (c), (d) and magnetoelectric (e), (f) suscptibilities (essentially the directional dichroism). Note the correct field dependence and sign of the excitation in panels (a)–(e) and (b)–(f).

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Spin dynamics of a Z2 spin liquid on the kagome lattice

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We study the spin dynamics of a spin-1/2 model on the kagome lattice of Balents, Fischer and Girvin type [1]. The model can be driven from a XY-ferromagnetic into a gapped Z2 spin liquid phase that can be described by the occurence of fractionalized excitations, namely spinons and visons. We calculate the dynamic spin structure factor via a combination of quantum Monte Carlo SSE simulations and the stochastic analytic continuation method. Within those spectra we then aim to find signatures of fractionalized excitations that were proposed earlier.

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Detuning the Honeycomb of α-$RuCl_3$: Pressure-Dependent Optical Studies Reveal Broken Symmetry

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The honeycomb Mott insulator α-$RuCl_3$ loses its low-temperature magnetic order by pressure. We report clear evidence for a dimerized structure at P > 1 GPa and observe the breakdown of the relativistic j_{eff} picture in this regime strongly affecting the electronic properties. A pressure-induced Kitaev quantum spin liquid cannot occur in this broken symmetry state. We shed light on the new phase by broad-band infrared spectroscopy of the low-temperature properties of α-$RuCl_3$ and *ab initio* density functional theory calculations, both under hydrostatic pressure.

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Chiral Mott phase of three-component fermions on the triangular lattice

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We provide numerical evidence in favor of spontaneous chiral symmetry breaking in the Mott phase of three-component fermions on the triangular lattice, that we describe by an SU(3) symmetric Hubbard model with hopping t and on-site interactions U. Our approach relies on effective models derived in the strong-coupling limit in powers of t/U for general SU(N) and arbitrary flux, which are studied using exact diagonalization and variational Monte Carlo simulations for N = 3. Up to third order in t/U, there is a large chiral phase that encompasses a range of real ring exchange where time-reversal is spontaneously broken. For the Hubbard model, this phase is stabilized below U/t~13, as revealed by including higher-order effects. How to realize it with ultra cold atoms without artificial gauge fields is briefly discussed.

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Competing magnetic orders and spin liquids in three-dimensional quantum magnets

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Quantum magnetism and the formation of quantum spin liquids remains one of the most intriguing aspects of contemporary solid-state physics, which is corroborated by the high research activity of experimentalists and theorists alike.

Candidate materials to host spin-liquid behavior include a variety of two-dimensional compounds, ranging from geometrically frustrated Heisenberg models to exchange-frustrated models of Kitaev type, but they also comprise three-dimensional structures. Only recently, interest was sparked by the discovery of spin liquid signatures in NiRh2O4, a three-dimensional material that realizes spin-1 moments on the diamond lattice with additional frustration mediated by next-nearest neighbor interactions.

To complement experimental findings with appropriate theoretical understanding, an efficient methodological framework is vital that is capable of capturing quantum magnetism in three dimensions -- a challenging regime, which is inaccessible to many conventional (both numerical and analytical) methods.

In this work, we report on recent methodological advances of the pseudofermion functional renormalization group (pf-FRG), which is suited to describe three-dimensional frustrated quantum magnetism even at finite temperatures, and leverage the method to model the interplay of magnetic order, quantum order-by-disorder, and spin liquids in NiRh2O4 as well as in other materials.

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Alternating ferro- and antiferromagnetic Heisenberg chain: from dimer to Haldane limit

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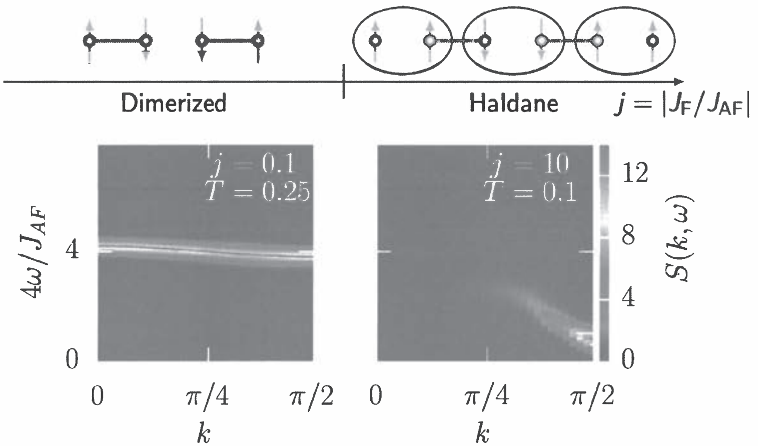
We present results of a study of the S = 1/2 Heisenberg chain with alternating ferro- and antiferromagnetic exchange, J_F and J_{AF} respectively. This system interpolates from a dimer to a Haldane chain as $j = |J_F/J_{AF}|$ varies from 0 to ∞. Using perturbation theory (PT) and quantum Monte Carlo based on the stochastic series expansion (SSE) method [1], we study elementary excitations, thermodynamic properties, and the dynamic structure factor S(k, ω). For $j \ll 1$ we find good agreement between PT and SSE. For arbitrary j we show that S(k, ω), obtained from SSE, scales between triplons at $j \ll 1$ and a Haldane chain spectrum at $j \gg 1$. Finally, we contrast our findings for the spin gap versus j against existing literature [2].



Spectra: Crossover between dimer and Haldane limit.

Financial support in part from “Niedersächsisches Vorab” through “Quantum- and Nano-Metrology (QUANOMET)” initiative within the project NP-2 is acknowledged.

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Topological Z_2 resonating-valence-bond spin liquid on the square lattice

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A one-parameter family of long-range resonating-valence-bond (RVB) state on the square lattice was previously proposed to describe a critical spin liquid (SL) phase of the spin-1/2 frustrated Heisenberg model. We provide evidence that this RVB state in fact also realizes a topological (long-range entangled) Z_2 SL, limited by two transitions to critical SL phases. The topological phase is naturally connected to the Z_2 gauge symmetry of the local tensor. This work shows that, on one hand, spin-1/2 topological SL with C_{4v} point-group symmetry and SU(2) spin rotation symmetry exists on the square lattice and, on the other hand, criticality and nonbipartiteness are compatible. We also point out that strong similarities between our phase diagram and the ones of classical interacting dimer models suggest both can be described by similar Kosterlitz-Thouless transitions. This scenario is further supported by the analysis of the one-dimensional boundary state. Forms of parent Hamiltonians hosting the Z_2 SL are suggested.

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Breaking of SU(4) symmetry and interplay between strongly correlated phases in the Hubbard model

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The impressive development of experimental techniques in ultracold quantum degenerate gases of alkaline-earth-like atoms in the last years has allowed investigation of strongly correlated systems. Long-lived metastable electronic states in combination with decoupled nuclear spin give the opportunity to study the Hamiltonians beyond the possibilities of current alkali-based experiments.

In [1] we study finite-temperature properties of ultracold four-component mixtures of alkaline-earth-metal-like atoms in optical lattices that can be effectively described by the two-band spin-1/2 Hubbard model including Hund's exchange coupling term. Our main goal is to investigate the effect of exchange interactions on finite-temperature magnetic phases for a wide range of lattice fillings. We use the dynamical mean-field theory approach and its real-space generalization to obtain finite-temperature phase diagrams including transitions to magnetically ordered phases. It allows to determine optimal experimental regimes for approaching long-range ferromagnetic ordering in ultracold gases.

In [2] we study the thermodynamic properties of four-component fermionic mixtures described by the Hubbard model using the dynamical mean-field-theory approach. Special attention is given to the system with SU(4)-symmetric interactions at half filling, where we analyze equilibrium many-body phases and their coexistence regions at nonzero temperature for the case of simple cubic lattice geometry. We also determine the evolution of observables in low-temperature phases while lowering the symmetry of the Hamiltonian towards the two-band Hubbard model. This is achieved by varying interflavor interactions or by introducing the spin-flip term (Hund's coupling). By calculating the entropy for different symmetries of the model, we determine the optimal regimes for approaching the studied phases in experiments with ultracold alkali and alkaline-earth-like atoms in optical lattices.

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Progressive lifting of the ground-state degeneracy of the long-range kagome Ising antiferromagnet

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The nearest-neighbour antiferromagnetic Ising model on the kagome lattice is well-known to be highly frustrated, and in particular to have a very large macroscopic ground-state degeneracy [1][2]. Recently, a candidate ground state for the model with dipolar couplings has been proposed [3]. In order to study the degeneracy lifting that leads to the ground state of the dipolar model, we implement a rejection-free dual worm algorithm [4] and use it to study the antiferromagnetic Ising model on the kagome lattice with up to fourth neighbour interactions. For the model with up to third neighbour interactions, we show that the ground state exhibits five different phases as a function of the ratio J3/J2, some of which still have a non-zero residual entropy. Surprisingly, for the model with dipolar couplings truncated at fourth neighbours, we find a ground state which is neither one of those of the J2 − J3 model, nor the one proposed for the full dipolar model [3]. This new state, however, is not the ground state for the model with full dipolar couplings, leading to the conclusion that further neighbours beyond the fourth one play an important role in the selection of the ground state of the dipolar model.

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Realization of flat-band physics in a highly frustrated quantum magnet $Ba_2CoSi_2O_6Cl_2$

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The search for flat-band solid-state realizations is a crucial issue to verify or to challenge theoretical predictions for quantum many-body flat-band systems. For frustrated quantum magnets flat bands lead to various unconventional properties related to the existence of localized many-magnon states, for a review see Ref. 1. The recently synthesized magnetic compound $Ba_2CoSi_2O_6Cl_2$ [2] seems to be an almost perfect candidate to observe these features in experiments. We develop a theory for $Ba_2CoSi_2O_6Cl_2$ by adapting the localized-magnon concept to this compound. We first show that our theory describes the known experimental facts and then we propose new experimental studies to detect a field-driven phase transition related to a Wigner-crystal-like ordering of localized magnons at low temperatures. Further details can be found in Ref. 3.

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Heisenberg kagomé strip with two types of site spins

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Using semiclassical spin-wave expansions as well as the Lanczos numerical diagonalization technique, we study the quantum phase diagram and the low-lying excited states of a Heisenberg kagomé strip (figure below) with two types of site spins $S = 1$, *and* $\sigma = 1/2$ and different exchange constants for the nearest-neighbor σS and $\sigma\sigma$ exchange bonds (J_1 and J_2, respectively). Geometrically, this system is a cut out from the kagomé lattice, so that a cluster of five spins repeats along the chain with the *S* spins placed on the central site of the cluster and σ spins placed on the remaining sites. Apart from the standard ferromagnetic and ferrimagnetic phases, the quantum phase diagram contains two Haldane-type phases with effective site spins *1* and *3*, as well as an exotic non-magnetic phase corresponding to a macroscopically degenerate classical canted phase*.

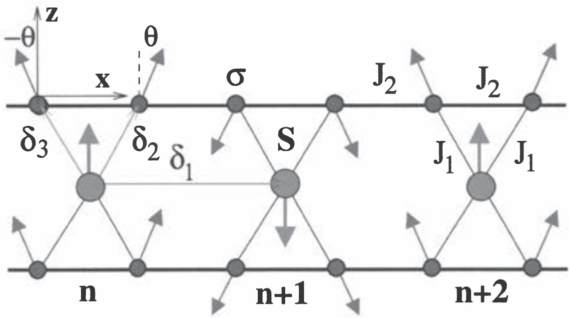

Figure One of the coplanar spin configurations stabilized on the kagomé strip in the macroscopically degenerate classical canted phase: $\cos(\theta) = -J_1 S/(2 J_2 \sigma)$, $J_2>0$.

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Exotic criticality in the spin-1 *XXZ* chain with explicit bond dimerization

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Applying the matrix-product-state based density-matrix renormalization group technique to the spin-1 *XXZ* chain with single-ion anisotropy, we demonstrate fascinating dynamic responses in the not only the Haldane, but also the large-*D* and Néel phases at zero and finite temperature [1]. Distinct thermally activated scattering processes make a significant contribution to the spectral weight in all cases.
Furthermore, at finite bond dimerization , we explore the criticality of the phase boundaries between large-*D*, Haldane and Néel phases at zero temperature [2]. The dimerization narrows the Haldane phase, and only dimerized and Néel states survive for large . The critical line between the latter two states exhibits a continuous Ising transition with central charge c=1/2, which terminates at a tricritical point, belonging to the universality class of the dilute Ising model with central charge c=7/10. Above this point, the quantum phase transition becomes first order. Simulating corresponding critical exponents β=1/8 (1/24) and ν=1 (5/9), we provide compelling evidence for the (tricritical) Ising quantum phase transition. This is demonstrated for the half-filled Hubbard model with alternating hopping dimerization [3,4].

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Thermodynamics of a gauge-frustrated Kitaev spin liquid

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Kitaev spin models are prototypical frustrated magnets in which the spin degrees of freedom fractionalize and the emergent spin liquid ground state can be described in terms of Majorana fermions coupled to a Z_2 gauge field. It is by now well known that varying the underlying lattice structure, these spin liquids can be described as Majorana metals with a topological band structure that includes the formation of Dirac or Weyl nodes, nodal lines, or entire Majorana Fermi surfaces.
Here our focus will be on the physics of the concurrently forming Z_2 gauge field. Typically, this (static) gauge field orders at low temperatures, with a finite-temperature (inverted Ising) transition occurring in three-dimensional settings. We will discuss an explicit example that goes beyond this paradigmatic situation where the gauge field is found to be subject to geometric frustration, the thermal ordering transition is suppressed, and a residual zero-temperature entropy arises. We discuss a variety of thermodynamic signatures of this physics obtained from large-scale, sign-free quantum Monte Carlo simulations of the underlying Kitaev model.

A novel Kagome like Cu2OSO4 crystal

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Low dimensional, geometrically frustrated antiferromagnets are at the forefront of condensed matter research.
Materials with antiferromagnetic interactions between spins on a triangle lattice inherently exhibit large frustration between similar energy ground states giving rise to new behavior.
Recently, experimental and theoretical results indicate that the kagome lattice can host spin liquid state[1].
The kagome lattice is an enticing example; however, various effects hinder its highly degenerate spin-liquid state and instead select a single magnetic ground state. It is therefore worthwhile to study nearly-kagomé compounds in an attempt to discern what precisely stops formation of the spin-liquid. We successfully synthesised a novel kagome like single crystal of Cu2OSO4 and report here its magnetism, since it has strong antiferromagnetic interactions on a diamond-kagomé lattice. Very little was previously published and the only experiment performed were always done on powder samples[2]. We studied the magnetic excitation spectra of Cu2OSO4 in order to help elucidate the mechanisms by which spin-liquid formation fails.
We will present thermodynamic measurements, such as specific heat and magnetisation results, as well as neutron and X-ray diffraction data. We also recently measured large swaths of reciprocal lattice, energy space thanks to time of flight, inelastic neutron scattering. We will thus present the latest results analysed on this compound and their interpretation, in order to explain why the spin-liquid state fails to form in this compound and understand better criteria for spin liquid formation on the kagome lattice.

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Excitonic magnetism in d^4 systems

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We use the variational cluster approximation [1] to investigate the phase diagram and one-particle spectral density of multi-band Hubbard models with strong spin-orbit coupling [2]. The approach includes quantum fluctuations on a small cluster exactly, where frustration can be treated without additional complications, and long-range order on a mean-field level.

We will in particular investigate systems with four electrons per site, where a local singlet competes with itinerant triplet excitations that can condense into magnetic order [3]. Further, the competition of Hund's rule and spin-orbit coupling with crystal-field splitting leads to various phases which are realized in some iridium and ruthenium compounds.

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Variational Monte Carlo study of the frustrated spin-1/2 Heisenberg model on the honeycomb lattice

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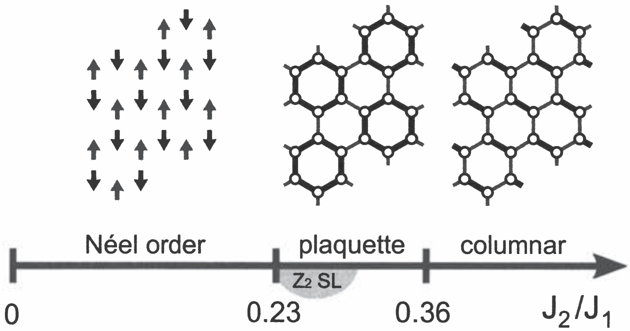
Using a variational Monte Carlo approach, we study the antiferromagnetic Heisenberg model with first- (J_1) and second-neighbor (J_2) couplings on the honeycomb lattice [1]. The phase diagram of the model is quite rich: the system undergoes two phase transitions, the first one (at $J_2/J_1 \approx 0.23$) from a Néel ordered phase to a plaquette valence-bond state, the second one (at $J_2/J_1 \approx 0.36$) from the plaquette to a columnar valence-bond solid. In the proximity of the first phase transition, a gapless Z_2 spin liquid with Dirac nodes has a very competitive energy, which outshines the one of the gapped spin liquid considered in previous works [2]. Finally, using the numerical approach described in Ref. [3,4], we compute the dynamical spin structure factor of the model for the different phases.



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Dynamical and Topological Properties of the Kitaev Model in a [111] Magnetic Field

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The Kitaev model exhibits a Quantum Spin Liquid hosting emergent fractionalized excitations.[1] We study the Kitaev model on the honeycomb lattice coupled to a magnetic field along [111]. Utilizing large scale matrix product based numerical models, we confirm three phases with transitions at different field strengths depending on the sign of the Kitaev exchange [2,3]: a non-abelian topological phase at low fields, an enigmatic intermediate regime only present for antiferromagnetic Kitaev exchange, and a field-polarized phase. For the topological phase, we numerically observe the expected cubic scaling of the gap and extract the quantum dimension of the non-abelian anyons. Furthermore, we investigate dynamical signatures of the topological and the field-polarized phase using a matrix product operator based time evolution method. The dynamical spin-structure factor in presence of a field behaves very differently compared to what is known for the three-spin exchange. The magnetic field causes the flux degrees of freedom to become mobile and as a consequence the low-energy spectrum contains more structure. Approaching the intermediate regime from the polarized phase, we observe a reduction in frequency and simultaneous flattening of the magnon modes.

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Asymptotic Freedom in Antiferromagnetic Chains of Large Spin

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It is well-known that Haldane's mapping of the spin-S Heisenberg antiferromagnetic chain onto the O(3) non-linear σ model with topological charge $\theta = 0, \pi$ for integer or half-odd integer S, respectively, was key to the solution of the so-called Haldane's conjecture [1,2]. For $\theta = 0$ the field theory exhibits a gap Δ between the singlet ground state and the triplet first excited state, leading to exponentially decaying two-point functions at large distance (wrt the correlation length $\xi \sim 1/\Delta$) [3]. For $\theta = \pi$ however the field theory is massless, leading to power-law decay of two-point functions at large distance [4]. Besides these results the O(n) non-linear σ model was shown to be asymptotically free for $n > 2$ [5]. Based on the β-function one can derive an expression for the correlation-length of the integer-spin chain $\xi_S \simeq e^{\pi S}/S$. This result actually extends to half-odd integer spin because the topological term is irrelevant in perturbation theory. It thus defines a crossover lengthscale beyond which perturbation theory fails. For large values of the spin this lengthscale becomes very large and the perturbative regime is expected to be the main observable feature in experiments.

There is one issue however which *a priori* prevents us from doing perturbation theory at large energy: Mermin-Wagner-Coleman theorem forbids spontaneous breaking of continuous symmetries in (1+1)-dimension. This theorem manifests itself under the form of infrared divergences in the perturbative expansion. However infrared divergences were shown to cancel to all orders in perturbation theory when computing O(3)-invariant quantities in the field theory, opening the door to a possible perturbative treatment of the antiferromagnetic Heisenberg spin chain [6-7].

In this project we proceed to such an analysis. We compute perturbatively the O(3)-invariant spin-spin correlation function to second order in $1/S$ on the lattice an show that it is infrared-finite, that it corresponds to the field theory result and that it describes accurately the behavior of the spin chain by comparing to Quantum Monte-Carlo simulations with spin $2, 5/2, 3$. In particular a characteristic logarithmic behavior at distances below the crossover lengthscale is observed in the spin chain. In order to provide complete information to experimentalists we also compute the dynamical spin structure factor. Finally we extend all our calculations to finite temperature.

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Magnetic properties of the frustrated quantum magnet atacamite, $Cu_2Cl(OH)_3$

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The natural mineral atacamite, $Cu_2Cl(OH)_3$, exhibits magnetic behavior characteristic of a frustrated quantum magnet [1-3]. From temperature and field dependent magnetization measurements in low and intermediate magnetic fields, together with an elastic neutron scattering study, it can be inferred that long-range magnetic order is present below T_N = 9 K and is described by a magnetic propagation vector $\boldsymbol{q}$ = (1/2 0 1/2).
The long-range magnetic order is suppressed in fields of ~15-20 T (for $H \parallel b$ and c axis) whereas saturation is attained beyond ~70 T. In this situation, we have carried out a high magnetic field magnetostriction experiment in fields up to 60 T applied along the three principal crystallographic axes. We find rich magnetic phase diagrams which we discuss in terms of possible magnetic models accounting for the properties of atacamite.

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Spinon band structures in quantum spin liquids from functional renormalization

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We develop a numerical technique based on the pseudofermion functional renormalization group (PFFRG) to calculate hopping and pairing amplitudes of emergent spinon quasiparticles in spin-1/2 quantum spin liquids. Within this approach, we first formulate a self-consistent Fock-like equation for these amplitudes where instead of the bare propagators and couplings we use the fully renormalized ones from PFFRG. We solve these equations using different ansätze for the hoppings and pairings which we take from a projective symmetry group (PSG) classification. From the overall size of these amplitudes we identify which of the PSGs are preferably realized in the system. We apply this approach to the antiferromagnetic J1-J2 Heisenberg model on the square lattice and to the antiferromagnetic nearest neighbor Heisenberg model on the kagome lattice. For the J1-J2 model, we find that in the regime of maximal frustration (J2~J1/2) the largest amplitudes are obtained for a SU(2) pi-flux state with a Dirac cone spinon dispersion. In the case of the kagome model, we identify a gapless Z2 pi-flux state where the bands show a Dirac-cone-like structure at finite energies but also feature a small circular Fermi surface at zero energy. We discuss our findings and benchmark them against variational Monte Carlo results.

Complete Phase Diagram of the Kitaev Honeycomb Model in Tilted Magnetic Fields: Gapless Visons and Emergent U(1) Quantum Spin Liquid

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In the field of quantum magnetism, the exactly solvable Kitaev honeycomb model with its bond-directional spin interactions serves as a paradigm for the fractionalization of spin degrees of freedom and the formation of Z_2 spin liquid ground states. An intense experimental search has led to the discovery of a number of spin-orbit entangled Mott insulators that realize its characteristic bond-directional spin interactions. In one of these materials, $RuCl_3$, the application of a strong external magnetic field can fully suppress the long-range magnetic order, potentially leading to a disordered quantum spin liquid state. Such results serve as motivation to exploring Kitaev physics in the presence of a magnetic field.

Here, we map out the complete phase diagram of the pure Kitaev model in tilted magnetic fields and report the emergence of a distinct gapless quantum spin liquid at intermediate field strengths. Analyzing a number of static, dynamical and finite temperature quantities using numerical exact diagonalization techniques, we find strong evidence that this phase exhibits gapless fermions coupled to a massless gauge field resulting in a plethora of low-energy states. We also discuss its stability in the presence of perturbations, Heisenberg and off-diagonal symmetric exchange interactions, that naturally arise in Kitaev materials.

Multipolar orders in $5d^1$ face centered cubic A_2TaCl_6 with J_{eff} =3/2 state

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In d^1 ion in cubic octahedral crystal field, cancellation of spin angular momentum S = 1/2 and effective orbital angular momentum L_{eff} = 1 by the spin-orbit coupling is expected and nonmagnetic J_{eff} = 3/2 quartet is formed in the strong spin-orbit coupling limit [1]. Theoretically, localized J_{eff} = 3/2 electron system with face centered cubic lattice is predicted to show various phases such as multipolar orders and dimer singlet state instead of conventional magnetic dipolar orders [2,3]. We have experimentally studied structural and magnetic properties of A_2TaCl_6 (A = K, Rb, Cs), where Ta^{4+} ($5d^1$) ions form face centered cubic lattice. We have revealed that almost ideal J_{eff} = 3/2 state with tiny magnetic dipolar moment is formed. In Cs_2TaCl_6, structural and magnetic transitions are observed at low temperatures. We discuss that they are the electric quadrupolar and magnetic octupolar orders of the J_{eff} = 3/2 quartet. We also discuss the ionic size effect on the structural and magnetic properties in comparison with Rb_2TaCl_6 and K_2TaCl_6.

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The bilinear-biquadratic model on the complete graph

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We study the spin-1 bilinear-biquadratic model on the complete graph on N sites i.e., when each spin is interacting with every other spin with the same strength. Because of its complete permutation invariance, this Hamiltonian can be rewritten as the linear combination of the quadratic Casimir operators of SU(3) and SU(2). Using group representation theory, we explicitly diagonalize the Hamiltonian and map out the ground-state phase diagram of the model. Furthermore, the complete energy spectrum, with degeneracies, is obtained analytically for any number of sites.

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Topological excitations in quantum spin systems with spin-orbit coupling

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Many frustrated magnets host exotic states of matter with non-trivial ground states. We show that in certain systems even if the ground-state is trivial, one can realize exotic states by the virtue of non-trivial topological excitations. These topological excitations are in a way analogs of the fermionic topological states of matter, albeit with many differences. We shall show that the paramagnetic phase of coupled-dimer systems on a ladder [1] as well as a honeycomb bilayer support topological excitations in the presence of spin-orbit coupling. These excitations are localized at the edges and in case of the ladder they are even fractionalized. We discuss relevant observables, topological invariants, and possible experimental set-up [2] to detect these non-trivial excitations. Another important example, namely the Kitaev-Heisenberg model, will be shown to host chiral edge states [3]. In this case, we will discuss interplay between external magnetic field and spin-asymmetric interaction. In all the cases, we shall show that there is a well-defined tuning parameter (eq. field, pressure) which can be used to also study a topological quantum phase transition.

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Field-induced phase transitions in extended Kitaev models

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Kitaev's exactly solvable honeycomb model hosts a gapless Z2 spin liquid (KSL) with itinerant Majorana fermions. Candidate materials (Na2IrO3, Li2IrO3, α-RuCl3) however show magnetic order at low temperatures due to additional magnetic interactions (Heisenberg, offdiagonal exchange, long range couplings, ...).
In this work, we investigate the behaviour of ferro- and antiferromagnetic Kitaev models under field in the presence of various additional interaction terms. Within our exact diagonalization calculations and the studied parameter space, we do not find a substantial region where a field-induced transition from an ordered state to the KSL is possible. The extended antiferromagnetic Kitaev models display richer phase diagrams due to the presence of an enigmatic field-induced phase in the pure antiferromagnetic Kitaev model that is separate from the B=0 KSL phase [1,2].

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Quantum correlations in frustrated isotropic Heisenberg model

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In this work the ground state phase diagram of a one-dimensional Spin-1/2 frustrated isotropic Heisenberge model with ferromagnetic nearest-neighbor ($J_1<0$) and antiferromagnetic next-nearest neighbor interactions ($J_2>0$) has been studied. It is known that the ground state has ferromagnetic order in the region $0\leq\alpha=J_2/|J_1|<0.25$ and at $\alpha_{c1}=0.25$ the ferromagnetic state is degenerate with the singlet state and a quantum phase transition is happened. Chubukov [1] studied this model by using a bosonization technique. Based on his idea, there is another phase transition at a critical value of $\alpha_{c2}=0.38$. In 2002, Liqun Sun et al [2] solved this model by using the Fermionization approach. We intend to investigate whether it is possible to recognize different phases especially in the region $\alpha>0.25$ by entanglement? Moreover, we want to find a clearer picture of the properties of different phases. We diagonalized the Hamiltonian by Fermionization approach. After diagonalization, energy spectrum is plotted. It has been found that in region $0\leq\alpha<0.25$, two Fermi points exist, but when α increases to values larger than 0.38, four Fermi points are observed. It is an evidence for existence of a critical point at $\alpha_{c2}=0.38$. By calculating $\langle S^z(n)S^z(n+r)\rangle$ correlation function and observation of the power-law decay of this spin-spin correlations in region with two Femi point, it is proved that this phase is a lattinger liquid phase. Computing the last correlation function in the region with four Fermi points, is obtained a function with different power decay which shows a new Lattinger Liquid. Moreover, we calculated concurrence. The concurrence is plotted as a function of frustrated parameter. The plot is clearly showing that there is a region between $0<\alpha<0.25$ in which the spins are not entangled, indicates a ferromagnetic phase. Increasing α we observe a new entangled region. This is the Lattinger Liquid I. This area commences at $\alpha_{c2}=0.25$. Concurrence reaches to a maximum and when increasing α has been continued, entanglement becomes zero again and a new phase, the Lattinger Liquid II, appears. In search of Quantum phase transitions, Quantum Discord (QD) is also calculated. Three separate areas are recognizable by QD, too. It should be noted that, in addition to entanglement and QD between the nearest neighbors, we calculated entanglement and QD between the second, third and fourth nearest neighbor pair spins.

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Pseudofermion functional renormalization group for frustrated magnets: stability of spin liquid phases from quantum to classical limit

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One of the most fascinating phenomena in frustrated quantum magnets is the formation of quantum spin liquids (QSL) -- states of matter that give rise to unconventional behavior, such as macroscopic entanglement and fractionalization of quantum numbers.

Conceptual progress has been driven by the analytic works of Kitaev and Wen, revealing the lattice gauge theory nature of QSLs. In the meantime, the effective description of frustrated magnetism remains challenging for many numerical methods, especially in three spatial dimensions. Quantum Monte-Carlo simulations tend to suffer from the sign problem and density matrix renormalization group techniques perform well only in one- and two-dimensional models. In recent years however, the pseudofermion functional renormalization group (pf-FRG) has become a valuable member in the family of numerical tools aiming to discriminate spin liquid phases from conventionally ordered ground states.

State-of-the-art pf-FRG has been generalized to models with arbitrary spin length S, allowing us to study the emergence of spin liquid phases as we systematically approach the quantum-limit at spin-1/2, where quantum fluctuations are strongest. At the same time, we can benchmark the results against the more accessible classical phase diagram. We apply the generalized pf-FRG framework to frustrated Heisenberg models e.g. on the square lattice or the kagome lattice, and map out the phase diagrams in the quantum-to-classical crossover.

The critical phenomena in the S=1 honeycomb antiferromagnet $BaNi_2V_2O_8$

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We investigate the critical phenomena in the S=1 honeycomb antiferromagnet $BaNi_2V_2O_8$. To solve the Hamiltonian of $BaNi_2V_2O_8$ we measure and analyze the magnetic excitation spectrum at T=4K using the inelastic neutron scattering technique [1]. After that, we explore both temperature regions below and above ordering temperature T_N~48K using the technique of neutron diffraction. The critical exponent of the order parameter was extracted and the thermal decay of the correlation length was analyzed within power-law and Kosterlitz-Thouless approaches. We found that $BaNi_2V_2O_8$ is a quasi-two dimensional (2D) antiferromagnet which displays the crossover from 2D Ising like to 2D XY and then to 2D Heisenberg system with increasing temperature. Our results predict the presence of the decoupled spin vortex-antivortex pairs just above T_N where the system behaves as a 2D XY-magnet and the results are compared to Monte-Carlo simulations.

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Field theory approach for SU(*N*) symmetric spin chains

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We present a spin-coherent state path integral approach to SU(*N*) symmetric spin chains with spins in the fully symmetric representation. Based on symmetry considerations we will discuss the possible terms appearing in the resulting nonlinear sigma model. For larger *N*, an increasing number of topological and other unusual imaginary terms can appear. Based on numerical results and analytic calculations in the strong coupling limit a phase diagram can be drawn out for the nonlinear sigma model which gives an insight to the ground state properties of the SU(*N*) spin chains as well. We will present the phase diagrams of the SU(3) and SU(4) cases and also discuss the structure for general *N*.

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Quantum Monte Carlo simulation of the O(4) chiral Heisenberg Gross-Neveux transition with a single Dirac cone

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We present the first quantum Monte Carlo simulations for the chiral Heisenberg Gross Neveu quantum phase transition of $N_f = 2$, O(4) fermions subject to a repulsive, local four fermion interaction. Here we employ a low energy effective lattice Hamiltonian with a single Dirac cone, which in the absence of interactions exactly reproduces a perfectly linear energy-momentum relation for all finite size lattice momenta. This allows one to significantly reduce finite size corrections compared to honeycomb and π-flux lattices. We extract a self-consistent set of critical exponents and compare them to analytical predictions.

Topological Properties of Quantum Magnets: Zak-Phase in BiCu_2PO_6 and Chern numbers in RE_5-Si_4F

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There is an increasing interest in finding topological one-particle excitations in quantum magnets. The combination of geometrical frustration and Dzyaloshinskii–Moriya interactions is prone to make topological properties emerge in magnetic systems. Thus, we present the compounds BiCu_2PO_6 and RE_5-Si_4 as promising topological materials. BiCu2PO6 is a quasi-one-dimensional dimerized quantum antiferromagnet displaying a non-trivial quantized Zak phase, but no edge states occur. In contrast, RE_5-Si_4 is a layered three-dimensional material realizing a ferromagnetic Shastry-Sutherland model in each layer. The magnon bands show non-trivial Chern numbers.

Competing structural and electronic correlations in high temperature superconductors based on optical phonons and magnon scattering

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Using inelastic light scattering experiments the interplay between lattice and electronic degrees of freedom are studied in $REBa_2Cu_2O_{6+\delta}$ (RE123, RE: Y, Dy, Gd, Sm, Nd). Lattice parameters, hopping matrix elements and the geometry of the exchange path are tuned by the radius of the RE-ion $r_{\mathrm{RE\text{-}ion}}$. The charge doping within the CuO_2 planes and the coherence of the spin system are controlled by the oxygen stoichiometry. Using phonon frequencies, as well as two-magnon scattering and its linewidth and intensity, very detailed and systematic relations between these parameters are found. Our data shows that oxygen doping within the region $\delta \approx 0.1$-0.3 has little effect on the antiferromagnetic (AFM) coupling strength J despite its fundamental effect on the Neel and superconducting temperature. In contrast, J and the spin coherence length ξ_0 appear to be influenced by lattice parameters. Previously obtained controversial results concerning the relation between J and the maximum transition temperature $T_{c,\,max}$ are also discussed [1, 2].

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Measures of correlation compatible with the principle of locality in the one-dimensional XX model

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Quantum discord and entanglement both are the criteria for distinguishing quantum correlations in a quantum system. The difference between them leads us to study a measure of quantum correlations compatible with the principle of locality which is called *"compatible correlation"*. Here, we have studied the effect of the transverse magnetic field on the compatible correlations of the one-dimensional spin-1/2 XX model. This study has focused on pair of spins at different distances. We show that in some situations quantum discord and compatible correlation are equal. In addition, relying on our calculations, we show that the derivatives of quantum discord can be used to identify the border between entangled and separable regions in the Luttinger liquid phase.

Importance of virtual singlets in RVB theory of quantum spin liquids

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It is well known that the low-energy sector of quantum spin liquids and other magnetically disordered systems is governed by short-ranged resonating-valence bonds. Here, we will show that the standard minimal truncation to the nearest neighbor valence-bond basis fails completely even for systems where it should work the most, according to received wisdom. This paradigm shift is demonstrated for both the quantum spin-1/2 square-kagome [1] and kagome [2] lattices, where the strong geometric frustration prevents magnetic ordering down to zero temperature. In the former, the shortest tunneling events bear the strongest longer- range fluctuations, leading to amplitudes that do not drop exponentially with the length of the loop, and to an unexpected loop-six valence-bond crystal, which is otherwise very high in energy at the minimal truncation level. In the latter, we will show from preliminary results [3] how the virtual singlets help in understanding the complex structure of the spin liquid of the RVB description of spin-1/2 kagome antiferromagnets by evidencing the proximity of a diamond-like crystal and making comparison with other numerical methods such as DMRG.

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Finite-size realization of the sawtooth spin chain close to quantum criticality

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The quatum Heisenberg model on the sawtooth chain is an example for a frustrated quantum spin system with a flat one-magnon band leading to a massively degenerate ground state and an unconventional low-temperature thermodynamics. For the well-studied sawtooth chain with antiferromagnetic (AFM) nearest-neighbor (NN) zigzag bonds J1 and AFM next-nearest-neighbor (NNN) basal bonds J2 [1-3] the flat band-physics emerges for J2=J1/2 near the saturation field, which, as a rule, is not easily accessible in experiments. By contrast, for the sawtooth chain with ferromagnetic (FM) J1 and AFM J2 [4,5] a zero-temperature transition between a ferro- and a ferrimagnetic ground state takes place at J2=-J1/2 and the flat band-physics is present at this point for zero magnetic field. At the transition point a class of exact many-body ground states formed by localized magnons can be found and the ground state is macroscopically degenerate with a large residual entropy per spin $s_0=(\ln 2)/2$. Another important feature is a sharp decrease of the gaps for excited states with an increase of the number of magnons. These excitations give an essential contribution to the low-temperature thermodynamics. In the recently synthesized magnetic molecule $[Fe_{10}Gd_{10}(Me\text{-}tea)_{10}(Me\text{-}teaH)_{10}(NO_3)_{10}]20MeCN$ (Fe10Gd10) the magnetic ions Fe ($S_{Fe}=5/2$) and Gd ($S_{Gd}=7/2$) form a sawtooth chain with a FM NN Fe-Gd coupling J1 and an AFM NNN Fe-Fe coupling J2, where the ratio of J2/J1 is close to the transition point [6]. As a consequence, the low-temperature physics of Fe10Gd10 is strongly influenced by the unusually high density of low-lying excitations stemming from the huge manifold of states becoming macroscopically degenerate at the transition point. Since these low-lying excitations belong to different magnetizations there is a strong impact of the magnetic field on the low-temperature properties of Fe10Gd10 [6].

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Real-Time Dynamics of Typical and Untypical States in Non-Integrable Systems

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Understanding (i) the emergence of diffusion from truly microscopic principles continues to be a major challenge in experimental and theoretical physics. At the same time, isolated quantum many-body systems have experienced an upsurge of interest in recent years. Since in such systems the realization of a proper initial state is the only possibility to induce a nonequilibrium process, understanding (ii) the largely unexplored role of the specific realization is vitally important. Our work reports a substantial step forward and tackles the two issues (i) and (ii) in the context of typicality, entanglement as well as integrability and nonintegrability. Specifically, we consider the spin-1/2 XXZ chain, where integrability can be broken due to an additional next-nearest neighbor interaction, and study the real-time and real-space dynamics of non-equilibrium magnetization profiles for a class of pure states. Summarizing our main results, we show that signatures of diffusion for strong interactions are equally pronounced for the integrable and nonintegrable case. In both cases, we further find a clear difference between the dynamics of states with and without internal randomness. We provide an explanation of this difference by a detailed analysis of the local density of states.

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Impurities vs. criticality in the magnetic torque response of the charge transfer salt κ-$(ET)_2Cu_2(CN)_3$

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The geometrically frustrated organic charge transfer salts have proven to host a number of promising quantum spin liquid (QSL) candidate materials, with κ-$(ET)_2Cu_2(CN)_3$ (κ-Cu) being the most well-studied[1]. Recently, magnetic torque measurements[2] on κ-Cu found a diverging torque susceptibility (τ/H^2) with respect to magnetic field and temperature, which was interpreted in terms of field-induced (quantum) criticality. Motivated by this experiment, we theoretically analyze the behavior of (τ/H^2) within several possible scenarios.

We first consider whether the observed response can stem from bulk criticality. We previously[3] suggested that spin-orbit coupling (SOC) effects can play an important role in the organics. In κ-Cu, these introduce a staggered *g*-tensor and a finite Dzyaloshinskii-Moriya (DM) interaction, which lead to a (τ/H^2) contribution from a staggered (π,π) susceptibility. This contribution may naturally diverge near a critical point between a QSL and a Néel phase. However, we show that the experimental angle and temperature dependence of the torque is inconsistent with this scenario.

We next consider inhomogeneous impurity-induced effects. After consideration of both SOC and weak interactions between impurities, we conclude that the temperature, field, and angle dependence of the experimental torque is well reproduced by a small impurity concentration. These conclusions are connected with the observation of inhomogeneity in the NMR relaxation at low temperature[4].

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Bulk and edge spin transport in topological magnon insulators

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We investigate the spin transport properties of a topological magnon insulator, a magnetic insulator characterized by topologically nontrivial bulk magnon bands and protected magnon edge modes located in the bulk band gaps. Employing the Landau-Lifshitz-Gilbert phenomenology, we calculate the spin current driven through a normal metal | topological magnon insulator | normal metal heterostructure by a spin accumulation imbalance between the metals, with and without random lattice defects. We show that bulk and edge transport are characterized by different length scales. This results in a characteristic system size where the magnon transport crosses over from being bulk-dominated for small systems to edge-dominated for larger systems. These findings are generic and relevant for topological transport in systems of nonconserved bosons.

Mutually attracting spin waves in the square-lattice quantum antiferromagnet

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The Heisenberg model for S=1/2 describes the interacting spins of electrons localized on lattice sites due to strong repulsion. It is the simplest strong-coupling model in condensed matter physics with wide-spread applications. Its relevance has been boosted further by the discovery of curate high-temperature superconductors. In leading order, their undoped parent compounds realize the Heisenberg model on square-lattices. Much is known about the model, but mostly at small wave vectors, i.e., for long-range processes, where the physics is governed by spin waves (magnons), the Goldstone bosons of the long-range ordered antiferromagnetic phase. Much less, however, is known for short-range processes, i.e., at large wave vectors. Yet these processes are decisive for understanding high-temperature superconductivity. Recent reports suggest that one has to resort to qualitatively different fractional excitations, spinons. By contrast, we present a comprehensive picture in terms of dressed magnons with strong mutual attraction on short length scales. The resulting spectral signatures agree strikingly with experimental data.

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Influence of intermolecular interactions on magnetic observables

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Very often it is an implied paradigm of molecular magnetism that magnetic molecules in a crystal interact so weakly that measurements of dc magnetic observables reflect ensemble properties of single molecules. But the number of cases where the assumption of virtually noninteracting molecules does not hold grows steadily. A deviation from the noninteracting case can be clearly seen in clusters with antiferromagnetic couplings, where steps of the low-temperature magnetization curve are smeared out with increasing intermolecular interaction. We demonstrate with examples in one, two, and three space dimensions how intermolecular interactions influence typical magnetic observables such as magnetization, susceptibility, and specific heat.

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Spin-glass ordering due to orbital and lattice effects in spin-1 pyrochlores

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We consider the range of behaviour that can occur in spin-1 pyrochlores with active orbital degrees of freedom. In particular we show how a combination of spin-orbit coupling and lattice distortion can result in a low-temperature, spin-glass state, even in the absence of impurities. We compare these results to experiments on $Y_2Mo_2O_7$ [1,2] and $Lu_2Mo_2O_7$ [3].

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Effect of Electric field on Breathing Pyrochlores

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The coupling between conventional (Maxwell) and emergent electrodynamics in quantum spin ice has been studied by Lantagne-Hurtubise et al. [1] where they find that a uniform electric field can be used to tune the properties of both the ground state and excitations of the spin liquid. Extending the study to the case of breathing pyrochlores, we find a sufficiently strong electric field triggers a quantum phase transition into new U (1) quantum spin liquid phases along a direction that did not show a phase transition in the isotropic limit. We also analyse the phase diagram of breathing pyrochlores in the presence of Electric field using gauge mean field theory. Finally, we discuss experimental aspects of our results.

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Quantum entanglement in spin ladder-shaped nanomagnet

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Quantum nanomagnets attract both theoretical and experimental attention as highly promising systems for a variety of applications. In particular, they have been demonstrated experimentally to serve as a basis for the classical memory devices [1,2] as well as to possess a high potential for applications in quantum computing [3]. The paper presents a theoretical study of quantum entanglement within spin pairs in a model nanomagnet. The system of interest is a two-legged spin ladder of finite length [4-6], consisting of 12 spins S = 1/2, modeled with a quantum Heisenberg Hamiltonian, mainly with antiferromagnetic intraleg and interleg (rung) couplings. The entanglement between spins in the system is quantified by means of Wootters concurrence [7,8]. This entanglement measure is thoroughly studied, both in the ground state and at finite temperatures, as a function of interaction parameters and magnetic field. The calculations are based on the exact diagonalization approach and canonical ensemble formalism, providing rigorous results in a whole range of the model parameters. The conditions in which various spin pairs exhibit entanglement are identified and discussed. In particular, the critical temperatures below which the entanglement is present are discussed. Moreover, a non-monotonic behavior of the concurrence as a function of the magnetic field is predicted. The importance of non-uniformity of entanglement in a finite system is emphasized, as the detailed behavior of entanglement vitally depends on the position of a considered pair in the ladder.

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Quanatum Magnetism with four component fermions

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We investigate magnetic properties of strongly interacting four component spin-3/2 ultracold fermionic atoms in the Mott insulator limit with one particle per site in an optical lattice. In this limit, atomic tunneling is virtual, and only the atomic spins can exchange. We find a competition between symmetry-breaking and liquidlike disordered phases. Particularly interesting are valence bond states with bond centered magnetizations, situated between the ferromagnetic and conventional valence bond phases. In the framework of a mean-field theory, we calculate the phase diagram and identify an experimentally relevant parameter region where a homogeneous SU(4) symmetric Affleck-Kennedy-Lieb-Tasaki–like valence bond state is present.

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A neutron scattering journey of a 2D chiral quantum magnet - $A(TiO)Cu_4(PO_4)_4$

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The chiral quantum magnet family $A(TiO)Cu_4(PO_4)_4$, where *A* = Ba, Pb, Sr, is an exciting series of compounds to study quantum effects in a magnetoelectric chiral system. Indeed, substitution of A^{2+} cation allows quantitative control of the degree of chirality in this family, which leads to concomitant changes in the magnetic interactions. These compounds are composed of layers of Cu_4O_{12} square cupola stacked along the *c* axis.
In this poster, I will present how a toy model is being derived thanks to Inelastic Neutron Scattering (INS) measurements and Linear Flavour Wave Theory (LFWT). I will also show how Spherical Neutron Polarimetry (SNP) has been used to solve the complex magnetic structure of some members of this family. Another interesting feature of this series of compound is the competition between a plaquette like ground state and a long range ordered one, due to its complex crystallographic structure. I will briefly explain why solving its ground state properties could help us filling the theoretical phase diagram of the modified *J-J'* model on the square lattice with trustful experimental values.

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Edge magnetic properties of black phosphorene nanoribbons

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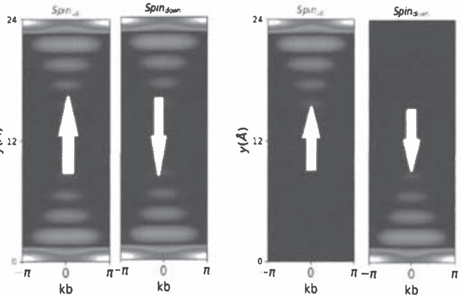
Recently, a promising 2D material phosphorene has attracted attentions owing to the unusual anisotropic band structure [1-2]. It is a bilayer puckered hexagonal lattice of black phosphorus exhibiting both the linear and quadratic energy dispersion in the bulk, depending on the direction of the quasi-particle's momentum. Apart from the bulk, zigzag phosphorene nanoribbon (ZPNR) can possess two quasi-state edge modes which are completely isolated from the conduction and valence bands [8-10]. This is in complete contrast to the case of other existing 2D hexagonal lattice structures like graphene [3] and silicene [4] etc. where the edge modes merge into the bulk at the two Dirac points. In this work, edge-state magnetic properties of ZPNR are investigated using tight-binding model with electron-electron interaction at the level of mean-field Hubbard model. Comparing to the edge-state magnetism in graphene nanoribbons, BPN displays some interesting characteristics: (i) only edges exhibit prominent magnetism and the insulating bulks remain nonmagnetic. (ii) The edge-state magnetism is almost independent on the width of nanoribbons. (iii) Two magnetic configurations are found: inter-edge antiferromagnetism, intra-edge antiferromagnetism and inter-edge antiferromagnetism. The two mentioned magnetic configurations phase are separated by an unstable magnetic phase.



Contour map of the valance-band wave function $|\Psi_{k\sigma}(y)|^2$ for spin up and spin down in non-magnetic phase(left panel) and in magnetic phase (right panel)

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Quasiparticle Excitations with Tensor Network States

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In the last decade tensor networks have become one of the main variational methods for studying strongly-correlated quantum lattice systems in low dimensions. In particular, they provide an efficient parametrization for the ground state of these systems directly in the thermodynamic limit. We show that the tensor-network language can be extended to describe the quasiparticle excitations on top of these ground states as well.

In one dimension, this method has been used to compute dispersion relations, bound states and spectral functions of generic spin chains to very high precision [1]. We show that the method can be extended to two dimensions, where the tensor-network toolbox is typically less developed [2]. This extension allows us to compute the spectrum of generic two-dimensional spin systems, and provides the first method to simulate dynamical properties using projected entangled-pair states.

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Fractional magnetization plateaux in the Shastry-Sutherland model: effect of quantum *XY* interdimer interaction

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The Heisenberg model on Shastry-Sutherland lattice is treated within the perturbative approach based on the exact solution for the hybrid Ising-Heisenberg model with the Heisenberg intradimer and Ising interdimer interactions [1]. The former fully quantum Heisenberg model on Shastry-Sutherland lattice is characterized at a rather strong intradimer coupling by the singlet-dimer ground state and a series of fractional magnetization plateaux, observed in its magnetic representative $SrCu_2(BO_3)_2$, at 1/8, 2/15, 1/6, 1/4, 1/3, 1/2 of the saturation magnetization [2,3]. The exact ground state of the latter hybrid Ising-Heisenberg model on Shastry-Sutherland lattice indicates that the Ising part of the interdimer interaction is responsible for rather wide 1/3 and 1/2 plateaux, and their boundaries are quite close to the results for the Heisenberg model on the same lattice [1]. Thus, it can be supposed that the smaller plateaux below 1/3 of the saturation magnetization are caused by the quantum (*XY*) part of the interdimer interaction. Using the perturbation theory, developed from the exact solution for the corresponding Ising-Heisenberg model [1], we find the effective models of interacting triplons with the hard-core repulsion. Such results can be used for the description of the intermediate plateaux in the magnetic compound $SrCu_2(BO_3)_2$. The method was tested on the orthogonal-dimer chain, which is a one-dimensional counterpart of the Shastry-Sutherland model, and it showed a good agreement with the results of the numerical methods [4].

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Quantum Dynamics of the Square Lattice Heisenberg Model

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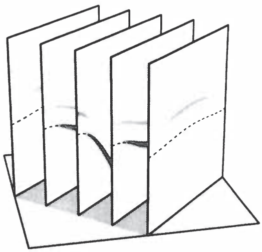
We revisit the dynamical properties above the ground state of the S = 1/2 Heisenberg model on the square lattice – a paradigmatic model of quantum magnetism. Despite the apparent simplicity of the model, spin wave theory fails to capture certain salient features of its excitations. Opposing descriptions – strongly-interacting magnons and emergent spinons – have been proposed. Here we use a time-dependent density matrix renormalization group (DMRG) method to obtain the dynamical structure factor. In particular, we investigate its features by continuously tracking the spectral function as a function of a tuning parameter around the soluble Ising limit. This offers new insights into both the nature of the so-called roton mode as well as the relevance of many-particle excitations. We also analyze peculiar entanglement properties of these excitations.



Generalization of the Haldane Conjecture to SU(3) Chains

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We apply field theory methods to SU(3) chains in the symmetric representation, with p boxes in the Young tableau, mapping them into a flag manifold nonlinear σ-model with a topological angle $\theta = 2\pi p/3$. Generalizing the Haldane conjecture, we argue that the models are gapped for $p = 3m$ but gapless for $p = 3m \pm 1$ (for integer m), corresponding to a massless phase of the σ-model at $\theta = \pm 2\pi/3$. We confirm this with Monte Carlo calculations on the σ-model. [1]

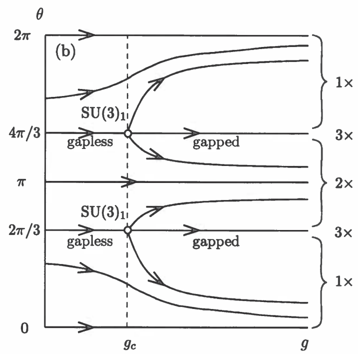

Figure 1: Proposed renormalization group flow diagram for the SU(3)/[U(1) × U(1)] nonlinear σ-model in the special case where the two topological angles are equal and opposite,.

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Spin and valence bond dynamics across a deconfined quantum critical point in a fermionic SU(3) model

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We consider a model of SU(3) fermions coupled to a transverse Ising field that harbors deconfined phases and phase transitions between antiferromagnetic (AFM) and valence bond solid (VBS) states [1]. Here, we supplement the model with a flux term and use the auxiliary field quantum Monte Carlo algorithm [2] to map out the phase diagram as a function of the transverse field and the flux. We find a phase transition between AFM and VBS is continuous, which belongs to a deconfined quantum critical points (DQCP) of the noncompact CP^2 field theory. A systematic finite size scaling analysis of the correlation length exponent and anomalous dimension at the DQCP point shows a large deviation with previous study on quantum spin models with SU(3) symmetry [4,5].

Special emphasis is placed on the VBS and AFM dynamics across the phase transition. Using a recent improved method of stochastic analytic continuation of imaginary-time correlation functions [3], we successfully locate the lowest excitation spin gap in both singlet and triplet sector. With approaching the DQCP point, a triplet spin excitation gap with broad spectral-weight continuum around $(\pi, 0)$ reduces as well as the singlet spin excitation around (π, π) and this is attributed to deconfined spinons.

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Critical Edge States of Two-Dimensional Quantum Critical Magnets

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Based on large-scale quantum Monte Carlo simulations, we examine the correlations along the edges of two-dimensional semi-infinite quantum critical Heisenberg spin-1/2 systems. In particular, we consider coupled quantum spin-dimer systems at their bulk quantum critical points, including the columnar-dimer model and the plaquette-square lattice. The alignment of the edge spins strongly affects these correlations and the corresponding scaling exponents, with remarkably similar values obtained for various quantum spin-dimer systems. We furthermore observe subtle effects on the scaling behavior from perturbing the edge spins that exhibit the genuine quantum nature of these edge states. Our observations furthermore challenge recent attempts that relate the edge spin criticality to the presence of symmetry-protected topological phases in such quantum spin systems.

Anomaly matching and symmetry-protected critical phases in SU(N) spin systems in 1+1 dimensions

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We apply the idea of 't Hooft anomaly matching to study generic (1+1)-dimensional SU(N) spin systems in the presence of spin-rotation and translation symmetries. By matching the anomaly of the PSU(N)×Z symmetry in the continuum limit, we identify a topological quantity for an SU(N) lattice spin model, evaluated as the total number of Young-tableaux boxes of spins per unit cell modulo N, which characterizes the "ingappability" of the system. Such a quantity, if nontrivial, implies the nonexistence of a unique gapped ground state as well as a restriction on the ground-state degeneracy. In addition, it also imposes constraints on possible critical phases. Therefore, our result can be thought of as a generalization of the Lieb-Schultz-Mattis-Affleck theorem[1]. Furthermore, anomaly matching among SU(N) Wess-Zumino-Witten models[2] shows a Z_N classification of these symmetry-protected critical (SPC) phases[3], and each spin system can only realize one class at criticality. It implies a no-go theorem that an RG flow is possible between two critical points only if they belong to the same SPC class, as long as the underlying lattice spin models respect the imposed symmetries.

*These two authors contributed equally to this work.

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Notes