



Numerical Methods in Strongly Correlated Quantum Systems

FOR 1807 Winter School 2018



Marburg, Feb. 19-23, 2018

Topics:

Machine learning applied to solid-state systems

Quantum dissipative systems

Quantum computation

Strongly correlated fermionic, bosonic, and magnetic systems

Methods:

Quantum Monte Carlo methods

Matrix-Product-State methods, DMRG

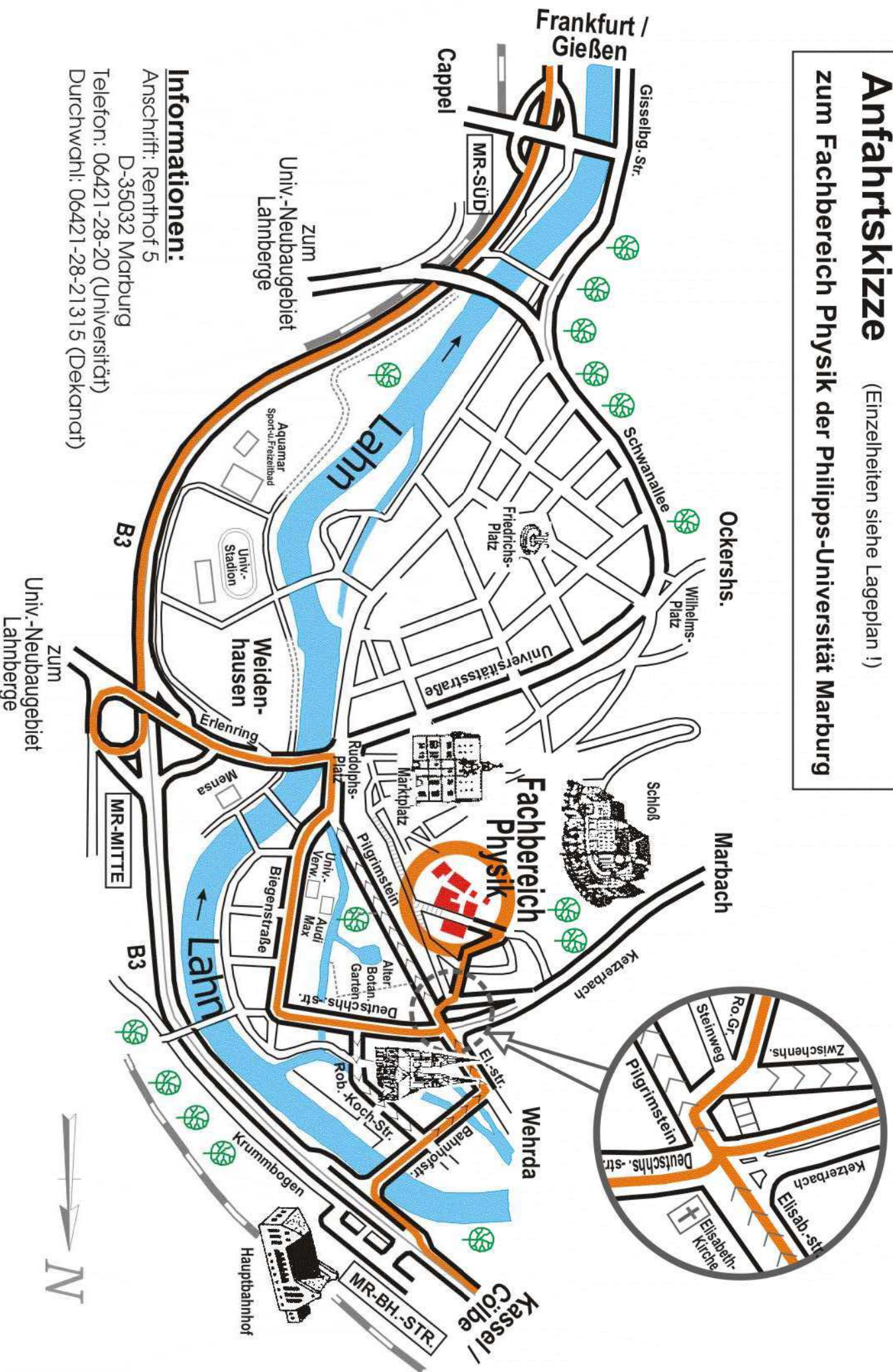
Tensor-Network-State methods

Machine Learning

Exact Diagonalization methods

Anfahrtskizze (Einzelheiten siehe Lageplan !)

zum Fachbereich Physik der Philipps-Universität Marburg



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Lecture Hall:
Großer Hörsaal

Fußweg zum
Marktplatz

MG 33 (R|02)

Laborbau II (R|03)

7b (R|04)



Registration, Posters
Coffee breaks

Labb. I

Lager

Anlieferung

Renthof 5 (R|01)

Gr.Hs.

Kl.Hs.

Tor

Renthof 7 (R|05)

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zur Wettergasse und zum Aufzug
Parkhaus Oberstadt

Fußgängerzone

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ABDELWAHAB, Anas
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 University of Innsbruck
 Philipps-Universität Marburg
 Max Planck Institute of Quantum Optics
 Sorbonne University
 El Manar University
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 Institute for Solid State Physics, University of Tokyo
 ETH Zurich
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università degli studi di Milano
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University of Minnesota
Institute of Physics
RWTH Aachen
Budapest University of Technology and Economics
RWTH Aachen
University of Innsbruck
Fudan
Fudan University
University of Tokyo
University of Tokyo

Speakers

Fakher Assaad (University of Würzburg)
 Martin Hohenadler (University of Würzburg)
 Andreas Honecker (University of Cergy-Pontoise)
 Corinna Kollath (University of Bonn)
 Salvatore Manmana (University of Göttingen)
 Frank Pollmann (Technical University of Munich)
 Robin Steinigeweg (University of Osnabrück)
 Lei Wang (Chinese Academy of Sciences, Beijing)
 Stefan Wessel (RWTH Aachen)

Auxiliary-field QMC (AFQMC)
 QMC for retarded interactions (CT-INT)
 Exact Diagonalization (ED)
 Quantum Dissipative Systems (QDS)
 DMRG at finite temp., time evolution (DMRG)
 Tensor Networks (TN)
 Quantum Dynamical Typicality (QDT)
 Machine Learning (ML)
 Stochastic Series Expansion (SSE)

Internet

WLAN via eduroam available in lecture hall and conference area.

Program

Registration: starting 7:30 am, Mon. Feb. 19

	Monday	Tuesday	Wednesday	Thursday	Friday
8:15-10:00	ML1 Wang	QMC2 (CT-INT) Hohenadler	TN1 Pollmann	TN2 Pollmann	QMC3 (AFQMC) Assaad
10:00-10:30	Coffee	Coffee	Coffee	Coffee	Coffee
10:30-12:15	QDS1 Kollath	ML2 Wang	ED1 Honecker	DMRG Manmana	ED2 Hands-On Honnecker/Wietek
12:15-14:30	Lunch	Lunch	Lunch	Lunch	Lunch
14:30-16:15	QMC1 (SSE) Wessel	QDS2 Kollath	ML3 Hands-On Wang	Social Program (Sightseeing)	QMC4 Hands-On (ALF) Hofmann/Goth/Assaad
16:15-16:45	Coffee	Coffee	Coffee	TN3 Hands-On Pollmann	End of school
16:45-17:30	Contributed Talks 1,2,3	Contributed Talks 4,5,6	QDT Steinigeweg		
17:30-18:15	Poster Session 1 (Open end, odd no.)	Poster Session 2 (Open end, even no.)			Banquet (from 19:00)

Posters with odd numbers will be presented on Monday, posters with even numbers on Tuesday.

Contributed Talks

1 Reverse engineering Hamiltonian from spectrum

Hiroyuki Fujita - Institute for Solid State Physics, University of Tokyo

Hiroyuki Fujita, Yuya O. Nakagawa, Sho Sugiura, and Masaki Oshikawa

Handling the large number of degrees of freedom with proper approximations, namely the construction of the effective Hamiltonians is at the heart of the condensed matter physics. Here we propose a simple scheme of constructing Hamiltonians from given energy spectra using the supervised learning algorithm. Taking the Hubbard model at the half-filling as an example, we show that we can optimize the parameters of a trial Hamiltonian and find the reduced description of the original model in a way that the estimation bias and error are well controlled. Using the ground states of the $S=1/2$ two-leg Heisenberg ladders, we also show that the same approach can be used to construct the entanglement Hamiltonian of a quantum many-body state from its entanglement spectrum.

2 Finding purifications with minimal entanglement

Johannes Hauschild - Technische Universität München

Johannes Hauschild, Eyal Leviatan, Jens H. Bardarson, Ehud Altman, Michael P. Zaletel, Frank Pollmann

Purification is a tool that allows to represent mixed quantum states as pure states on enlarged Hilbert spaces. A purification of a given state is not unique and its entanglement strongly depends on the particular choice made. Moreover, in one-dimensional systems, the amount of entanglement is linked to how efficiently the purified state can be represented using matrix-product states (MPS). We introduce an MPS based method that allows to find the minimally entangled representation by iteratively minimizing the second Rényi entropy [1]. First, we consider the thermofield double purification and show that its entanglement can be strongly reduced especially at low temperatures. Second, we show that a slowdown of the entanglement growth following a quench of an infinite temperature state is possible.

[1] J. Hauschild et al., arXiv:1711.01288

3 Fermion Bag Approach to Hamiltonian Lattice Field Theories

Emilie Huffman - Duke University

Emilie Huffman, Shailesh Chandrasekharan

We extend the idea of fermion bags to Hamiltonian lattice field theories in the continuous time formulation. Using a class of models we argue that the temperature is a parameter that splits the fermion dynamics into small spatial regions that can be used to identify fermion bags. Using this idea we construct Hamiltonian quantum Monte Carlo algorithms and compute critical exponents in the $3d$ Ising Gross-Neveu universality class using a single flavor of massless Hamiltonian staggered fermions. We argue that even sizes up to $N = 10,000$ sites should be accessible with supercomputers available today.

4 mVMC - Open-source software for many-variable variational Monte Carlo method

Takahiro Misawa - University of Tokyo

Takahiro Misawa (on behalf of mVMC developers)

mVMC (many-variable Variational Monte Carlo method) [1] is software for the highly-accurate variational Monte Carlo calculations with the simple and flexible user interfaces. mVMC also supports the large-scale parallelization. For widely studied models of strongly correlated electron systems such as the Hubbard model, the Heisenberg model, and the Kondo-lattice model, users can perform the calculation by preparing only one input files whose length is shorter than ten lines. By using the same input file, users can perform the exact diagonalization as well through H ϕ [2]. Thus, it is easy to test the accuracy of the variational calculation for small system sizes and then one can perform the calculations for large system sizes that can not be treated by the exact diagonalization. In this presentation, we will explain the basic usage of mVMC.

[1] <https://github.com/issp-center-dev/mVMC>

[2] <https://github.com/QLMS/Hphi>

5 The complex Langevin method for ultracold fermions

Lukas Rammelmüller - TU Darmstadt

Lukas Rammelmüller, Joaquin E. Drut, Jens Braun

A wide range of stochastic methods has been applied to approach the non-relativistic fermionic many-body problem. Despite the huge success of these approaches, the sign problem prohibits exploration of a large class of systems due to exponential scaling of computational effort. Recently the complex Langevin method, known from relativistic lattice models, was adapted to non-relativistic theories. With this method at hand, we are able to extract properties for spin-polarized Fermi mixtures of arbitrary masses in the ground state as well as at finite temperature. More specifically, we compute equations of state for Fermi mixtures of arbitrary mass and polarization as a function of interaction strength in one dimension as well as for the three-dimensional Fermi gas at unitarity. Additionally, we discuss pairing correlations in spin-polarized Fermi gases, ultimately aiming at a detection of the formation of an inhomogeneous superfluid condensate.

6 Weak Versus Strong Disorder Superfluid-Bose Glass Transition in One Dimension

Elmer Doggen - Karlsruhe Institute of Technology (KIT)

Elmer V. H. Doggen, Gabriel Lemarié, Sylvain Capponi, Nicolas Laflorencie

Using large-scale simulations based on matrix product state and quantum Monte Carlo techniques, we study the superfluid to Bose glass-transition for one-dimensional attractive hard-core bosons at zero temperature, across the full regime from weak to strong disorder. As a function of interaction and disorder strength, we identify a Berezinskii-Kosterlitz-Thouless critical line with two different regimes. At small attraction where critical disorder is weak compared to the bandwidth, the critical Luttinger parameter K_c takes its universal Giamarchi-Schulz value $K = 3/2$. Conversely, a non-universal $K > 3/2$ emerges for stronger attraction where weak-link physics is relevant. In this strong disorder regime, the transition is characterized by self-similar power-law distributed weak links with a continuously varying characteristic exponent α .

Poster Contributions

1 Ordered states in the Kitaev-Heisenberg model: from 1D chain to 2D honeycomb

Cliò Efthimia Agrapidis - IFW Dresden

Cliò Efthimia Agrapidis, Jeroen van den Brink, Satoshi Nishimoto

We study the ground state of the 1D Kitaev-Heisenberg (KH) model using the density-matrix renormalization group and Lanczos exact diagonalization methods. We obtain a rich ground-state phase diagram as a function of the ratio between Heisenberg ($J = \cos \phi$) and Kitaev ($K = \sin \phi$) interactions. Depending on the ratio, the system exhibits four long-range ordered states: ferromagnetic- z , ferromagnetic- xy , staggered- xy , Néel- z , and two liquid states: Tomonaga-Luttinger liquid and spiral- xy . The two Kitaev points $\phi = \frac{\pi}{2}$ and $\phi = \frac{3\pi}{2}$ are singular. The ϕ -dependent phase diagram is similar to that for the 2D honeycomb-lattice KH model. Remarkably, all the ordered states of the honeycomb-lattice KH model can be interpreted in terms of the coupled KH chains. We also discuss the magnetic structure of the K-intercalated RuCl_3 , a potential Kitaev material, in the framework of the 1D KH model. Furthermore, we demonstrate that the low-lying excitations of the 1D KH Hamiltonian can be explained within the combination of the known six-vertex model and spin-wave theory.

2 Dissipative quantum state engineering in topologically ordered dipolar systems

Durga B Rao Dasari - University of Stuttgart

Durga B Rao Dasari, S. Yang, K. Moelmer and J. Wrachtrup

We investigate the role of topology and decoherence for generating robust many body entanglement in a dipole-coupled Rydberg atomic system. Such decoherence assisted entanglement results only when the atoms are arranged on graph like structures with a preferred connectivity. Further, lattice structures that have maximum nearest neighbors of 2 in 1D, 4 in 2D and 6 in 3D always lead to such entanglement. Any defect arrangement that does not satisfy these geometrical constraints can destroy both entanglement and purity in the entire network. We further show how the topologically ordered state of Rydberg atoms can lead to

deterministic single photon emission without the requirement for the global Rydberg blockade. We further extend these ideas to dipolar coupled spin systems, in particular the NV centres in diamond to engineer the quantum spin state of a nuclear spin bath.

3 Understanding Chemical Bonding in Terms of Electronic Correlations

Gergely Barcza - Wigner Research Center for Physics

G. Barcza, Sz. Szalay, Ö. Legeza, T. Szilvási, L. Veis

Quantum information theory (QIT) emerged in physics as standard technique to investigate effective models of interacting quantum systems. The success of the method arises the question what we can learn from QIT applying it to molecules which are inherently quantum systems as well. By the rigorous analysis of the central quantities of standard QIT, which describes bonding purely in terms of two-orbital correlations, we identify covalent bond, donor-acceptor dative bond, multiple bond, charge-shift bond indicating unified picture of fundamental chemical models from *ab initio*. In order to give a better description of more complicated multiple bonds and aromaticity, we introduce the genuine multiorbital correlation theory, consisting of a framework for handling the structure of multiorbital correlations, a toolbox of true multiorbital correlation measures, and the formulation of the multiorbital correlation clustering, together with an algorithm for obtaining that. These make it possible to quantify the correctness of the associated "naive" bonding picture. As proof of concept, we apply the theory for the investigation of the bond structures of several molecules. We show that the non-existence of well-defined multiorbital correlation clustering provides a reason for debated bonding picture of the dicarbon.

4 Revisiting the Hybrid Quantum Monte Carlo Method for Hubbard and Electron-Phonon Models.

Stefan Beyl - Universität Würzburg

Stefan Beyl, Florian Goth, Fakhre Assaad

A unique feature of the Hybrid Quantum Monte Carlo (HQMC) method is the potential to simulate negative sign free lattice fermion models with sub-cubic scaling in system size. Here we will revisit the algorithm for various models. We will show that for the Hubbard model the HQMC suffers from ergodicity issues and unbounded forces in the effective action. Solutions to these issues can be found in terms of a complexification of the auxiliary fields, but nevertheless, the HQMC approach does not outperform single spin flip determinantal methods with cubic scaling. On the other hand we will argue that there is a set of models for which the HQMC is very efficient. This class is characterized by effective actions free of singularities. Using the Majorana representation, we show that models such as the Su-Schrieffer-Heeger Hamiltonian at half-filling and on a bipartite lattice belongs to this class. For this specific model sub-cubic scaling is achieved.

5 Interaction Driven Topological Magnetic Order in Frustrated Shastry-Sutherland Lattice

DHIMAN BHOWMICK - Nanyang Technological University

Dhiman Bhowmick and Pinaki Sengupta

The interplay between competing interactions, geometric frustration, enhanced quantum fluctuations due to reduced dimensionality and external magnetic fields results in low-lying magnetic excitations (magnons/triplons) with non-trivial topological character in the Shastry-Sutherland compound Strontium Copper Borate. Using a bond operator formalism, we investigate the evolution of topological character of the low-lying triplon excitations in the highly frustrated limit within the framework of a Heisenberg model supplemented by Dzyaloshinskii-Moriya(DM) interactions as the different Hamiltonian parameters are varied.

6 SU(N) spin chain and quantum Hall effect

Danu BIMLA - ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)

Bimla Danu, A.M.M. Pruisken and R.Shankar

7 Nonequilibrium dynamics of 1-D electron-phonon systems

Christoph Brockt - Leibniz Universität Hannover

Christoph Brockt, Eric Jeckelmann

We use a TEBD algorithm with a local basis optimization [1] for the phononic degrees of freedom to investigate the nonequilibrium dynamics of a Holstein chain with one electron [2]. Different relaxation regimes are found and the influence of dispersive phonons is studied. In a second setup the electron-phonon coupling is confined in a small structure between two tight-binding leads and the electron is initially in the left lead with momentum towards the structure [3]. We observe permanent energy transfer from the electron to the phonon system, different mechanisms that cause transient self-trapping of the electron in the electron-phonon coupled structure and transmission resonances, that depend on the adiabaticity ratio. Analytical results are provided for limiting cases and the advantages of the optimal basis are analyzed. Support from the DFG through the Research Unit FOR 1807 is gratefully acknowledged.

[1] C. Brockt et al., PRB 92, 241106(R) (2015)

[2] F. Dorfner et al., PRB 91, 104302 (2015)

[3] C. Brockt and E. Jeckelmann, PRB 95, 064309 (2017)

8 Quasi-One-Dimensional Topological Systems: Interactions and Edge States

Maximilian Buser - LMU Muenchen

Maximilian Buser

9 Exact diagonalization of SU(N) Heisenberg models

Ganahl Clemens - University of Innsbruck

Clemens Ganahl

I present a method to perform exact diagonalization of SU(N) Heisenberg models on various lattices. I show how storing parts of the Hamiltonian allow to achieve reasonable iteration times while keeping the memory usage at a feasible level.

10 A study of topological phases with iPEPS

Schelto Crone - University of Amsterdam

Schelto Crone and Philippe Corboz

The entanglement entropy of Kitaev's toric code on a finite cylinder is calculated using a combination of the iPEPS bulk-boundary correspondence and the corner transfer matrix renormalization group method. When applied on models which exhibit topologically ordered phases, this can be used to determine the topological entanglement entropy, allowing the method to be used as a way of determining the topological phase of the model. The scheme is first applied to the exact PEPS representation of the Kitaev's toric code model. Further, preliminary results of an unbiased optimization of the same model with a magnetic field are presented and used to determine the topological phase transition.

11 Quantum Monte Carlo Simulations of the Quantum Ising Model on the Pyrochlore Lattice

Patrick Emonts - Max Planck Institute of Quantum Optics

Patrick Emonts, Stefan Wessel

The highly frustrated transverse-field Ising model on the pyrochlore lattice shows a quantum phase transition from the low-field quantum spin ice phase to the high-field polarized phase. Recent field-theoretical analysis and series expansion results found this to be a first-order transition. Here, we examine this system using quantum Monte Carlo simulations in order to assess this scenario and access the thermal properties in the vicinity of the quantum phase transition. For this purpose, we consider several variants of cluster-update schemes for the transverse-field Ising model on frustrated lattices and compare their autocorrelation times to the conventional bond-based algorithm.

12 Nonmagnetic Impurities in Kagome Compounds

Karim Essafi - Sorbonne University

Karim Essafi, Bernard Bernu, Laura Messio

When compounds are synthesized impurities may appear in the material. For instance, in Herbertsmithite, a spin-1/2 kagome compound, it is known that a Cu/Zn substitution appears for 6-10% of the Zn ions. This leads to the presence of non-magnetic defects in the kagome structure. Motivated by these types of impurities we study their effect on the spin-1/2 kagome Heisenberg antiferromagnet using a high-temperature series expansion.

13 Spin dynamical structure factor: a variational Monte Carlo approach

Francesco Ferrari - SISSA - ISAS, Trieste

Francesco Ferrari

The spin dynamical structure factor is computed within a variational framework to study frustrated Heisenberg models in one and two dimensions. Within this approach, the relevant part of the spectrum is approximated by considering two-spinon excitations over the best variational Ansatz for the ground-state wave function [1]. A benchmark of this approach on the one-dimensional $J_1 - J_2$ model gives an excellent description of both the gapless and gapped (dimerized) phases, also describing the incommensurate structure for large frustrating ratios J_2/J_1 [2]. Preliminary results on the square lattice show signatures of the transition between the Neel ordered phase and the (gapless) spin-liquid phase that takes place for $J_2/J_1 \simeq 0.45$.

[1] T. Li, and F. Yang, Phys. Rev. B **81**, 214509 (2010)

[2] F. Ferrari et al., in preparation

14 Coexistence of d-wave superconductivity with antiferromagnetism in the Hubbard model for hole- and electron-doped cuprates

Alexandre Foley - Université de Sherbrooke

Alexandre Foley, Simon Verret, David Senechal

We obtained the zero temperature phase diagrams of one-band Hubbard models describing YBCO and NCCO for a few values of on-site interaction. We use Cluster Dynamical Mean Field theory at zero temperature with an exact diagonalization solver (ED-CDMFT) and the most general bath parametrization possible. The phase diagrams shows a region of homogeneous coexistence of antiferromagnetism (AFM) and superconductivity (SC) on the electron doped side. This region begins at a finite electron doping and ends with the complete suppression of AFM. On the hole doped side, when using YBCO hopping parameters and at intermediate coupling, no microscopic coexistence is observed. The two phases completely exclude one another, leaving a region of hole doping where no solution can be obtained with the channel of both phases are open. Macroscopic coexistence is then possible in this forbidden region. This contrast with previous work where a simpler form of the bath lead to a homogeneous coexistence appearing on both side of the phase diagrams.

15 Probing Exotic Tensor Spin Order with Supervised Machine Learning

Jonas Greitemann - Ludwig-Maximilians-Universität München

Jonas Greitemann and Ke Liu

We apply supervised machine learning to the identification of exotic spin phases with high-rank tensor order parameters. Following Ponte and Melko (PRB 96, 205146 (2017)), we find that the decision function of a support vector machine (SVM) produces the scalar order parameter. In addition to reproducing the order parameter curve, we are able to infer the analytic form of the tensor order parameter for a variety of symmetries with tensor order parameters of rank up to 6. This may prove useful in the exploration of exotic magnetic orders in spin liquid candidates.

16 Tree tensor networks in ab initio quantum chemistry

Klaas Gunst - UGent

Klaas Gunst

We present an efficient tree tensor network state ansatz (TTNS) for ab initio quantum chemistry. TTNS are a natural extension of the matrix product state ansatz (MPS) which is used in density matrix renormalization group theory (DMRG). While the MPS wave function can be depicted as a linear chain of tensors, the TTNS ansatz allows branching of the network. TTNS are the most general tensor networks without any loops. By using this ansatz, a better representation of the entanglement topology of the system is expected as compared to the MPS, while still avoiding loops and the complications introduced by them. In our TTNS implementation, we restrict ourselves to tensors with a maximum of 3 legs (3 virtual legs or 2 virtual and 1 physical leg). This has several advantages in comparison with a general TTNS, like the possibility to do two-site optimization without elevating the computational cost. Our current implementation has $U(1)$ symmetry but $SU(2)$ symmetry is not expected to prove more difficulty than with DMRG due to the restriction to 3-leg tensors.

17 Cavity-induced artificial gauge field in a Bose-Hubbard ladder

Catalin-Mihai Halati - University of Bonn

Catalin-Mihai Halati, Ameneh Sheikhan, and Corinna Kollath

We consider theoretically ultracold interacting bosonic atoms confined to quasi-one-dimensional ladder structures formed by optical lattices and coupled to the field of an optical cavity. The atoms can collect a spatial phase imprint during a cavity-assisted tunneling along a rung via Raman transitions employing a cavity mode and a transverse running wave pump beam. By adiabatic elimination of the cavity field we obtain an effective Hamiltonian for the bosonic atoms, with a self-consistency condition. Using the numerical density matrix renormalization group method, we obtain a rich steady state diagram of self-organized steady states. Transitions between superfluid to Mott-insulating states occur, on top of which we can have Meissner, vortex liquid, and vortex lattice phases.

18 Modelling magnetic anisotropy of single-chain magnets in $|d/J| \geq 1$ regime

Sumit Haldar - Indian Institute of Science

Sumit Haldar, Rajamani Raghunathan, Jean-Pascal Sutter, S. Ramasesha

Single molecule magnets (SMMs) are high nuclearity transition metal complexes (TMCs). The condition for SMM to exhibit slow relaxation behaviour below a certain characteristic blocking temperature (T_B) is that the molecule possesses simultaneously high-spin ground state and large uniaxial type molecular magnetic anisotropy (D_M). The grand challenge is to increase the blocking temperature. For that we need to model systems with large molecular anisotropy. Motivated by previous methodologies, here we develop a new theoretical framework based on a full Hamiltonian approach to compute the magnetic anisotropy parameters from single ion anisotropies, spin correlation and the orientations of the local ions. Our approach is very generic and can be applied in weak, as well as in strong anisotropy limit in which the ground state is mixed with the low lying excited states and previous perturbative approaches can not be applied. Using our methodology we study the role of single ion anisotropy, rotation of the local ions, dimerization and increase in the chain length on the anisotropy parameters. [S. Haldar, R. Raghunathan, J. P. Sutter, S. Ramasesha, Molecular Physics, 115, 2849-2859, (2017)]

19 Superconducting dome in doped organic mott insulators

Charles-David Hebert - Sherbrooke

Charles-David Hebert, Patrick Semon, Andre-Marie Tremblay

20 XXZ model in the Anderson basis

Lluís Hernández - Universität Innsbruck

L. Hernández, A. Läuchli

We show that working in the Anderson basis, the 2 and 3 particles sectors can be solved via a diagonalization of a matrix that grows linearly with the system size. We expect that these results hold for larger particle sectors.

21 Negative sign free auxiliary field algorithm for frustrated Kondo systems

Johannes Hofmann - Würzburg

Johannes Hofmann, Fakher Assaad, Tarun Grover

The absence of negative sign problem in quantum Monte Carlo simulations of spin and fermion systems has different origins. World-line based algorithms for spins require positivity of matrix elements whereas auxiliary field approaches for fermions depend on symmetries such as particle-hole. For negative-sign-free spin and fermionic systems, we show that one can formulate a negative-sign-free auxiliary field quantum Monte Carlo algorithm that allows Kondo coupling of fermions with the spins.

On this poster we will present preliminary results on the Kondo coupling between local moments participating in a \mathbb{Z}_2 spin liquid (based on Balents-Fisher-Girvin model) and conduction electrons on a honeycomb lattice. Our setup allows us to address the question of the relevance of the Kondo coupling at the quantum critical point corresponding to the destruction of the spin-liquid.

22 Identifying Quantum Phase Transitions with Adversarial Neural Networks

Patrick Huembeli - ICFO - Casteldefels

Patrick Huembeli, Alexandre Dauphin, Peter Wittek

The identification of phases of matter is a challenging task, especially in quantum mechanics, where the complexity of the ground state appears to grow exponentially with the size of the system. We address this problem with state-of-the-art deep learning techniques: adversarial domain adaptation. We derive the phase diagram of the whole parameter space starting from a fixed and known subspace using unsupervised learning. The input data set contains both labeled and unlabeled data instances. The first kind is a system that admits an accurate analytical or numerical solution, and one can recover its phase diagram. The second type is the physical system with an unknown phase diagram. Adversarial domain adaptation uses both types of data to create invariant feature extracting layers in a deep learning architecture. Once these layers are trained, we can attach an unsupervised learner to the network to find phase transitions. We show the success of this technique by applying it on several paradigmatic models: the Ising model with different temperatures, the Bose-Hubbard model, and the SSH model with disorder. The input is the ground state without any manual feature engineering, and the dimension of the parameter space is unrestricted. The method finds unknown transitions successfully and predicts transition points in close agreement with standard methods. This study opens the door to the classification of physical systems where the phases boundaries are complex such as the many-body localization problem or the Bose glass phase.

23 Ground State Properties of One Dimensional Spin-Half Antiferromagnetic Quantum Binary System

Ulvi KANBUR - Karabuk University

Ulvi Kanbur

A spin-1/2 quantum binary system in one dimension with antiferromagnetic exchange interactions will be studied by comparing exact and quantum Monte Carlo results. The simulations are based on a recent method called stochastic series expansion with operator loops. Ground state results of quantities spin-spin correlation and energy will be given by averaging over random realizations of the disorder system for different exchange and concentration parameters. Our sim-

ulation results reveal that both spin-spin correlations and energy of the system strongly depend on the considered value of the concentration and spin-spin coupling terms.

24 Spin transfer torques in interacting nano-wires

Hamidreza Kazemi - Technische Universität Kaiserslautern

Hamidreza Kazemi, Dr. Nicholas Sedlmayr, Dr. Imke Schneider, Dr. Axel Pelster, Dr. Sebastian Eggert

25 Observation of the Higgs mode in the superfluid BEC-BCS crossover in Fermi gases

Johannes Kombe - Uni Bonn

Johannes Kombe, Jean-Sébastien Bernier and Corinna Kollath

Thanks to recent advances, investigating the non-equilibrium dynamics of interacting systems is now possible. Using time-dependent perturbations, one can probe from a different angle the mechanisms responsible for the collective phenomena present in correlated systems. Taking advantage of this progress, we investigate both theoretically and experimentally the evolution of a three-dimensional Fermi gas while the interaction strength is effectively modulated. Our study, carried out on the BCS side, reveals various collective excitations. Interestingly, this approach highlights the presence of the Higgs mode.

26 Solving Quantum man-body problem with Feed-forward Neural Networks

Sheng-Hsuan Lin - Technische Universität München

Sheng-Hsuan Lin

Motivated by the successful result of studying quantum many-body problem with Restricted Boltzmann Machine, we show that it is possible to treat feedforward neural networks as variational wavefunctions for quantum spin models. We compare different optimization methods in terms of efficiency and convergence. The result of Variational Monte Carlo with neural network quantum states on 2 dimension J1J2 model suggests that it is a competitive method to study high dimensional frustrated problems.

27 The finite-temperature Lanczos method as solver for the variational cluster approach

Jan Lotze - University Stuttgart

Jan Lotze and Maria Daghofer

The variational cluster approximation (VCA) based on self-energy functional theory (SFT) [1] can be used to study correlated-electron Hamiltonians: Instead of the original systems self-energy, that of a 'reference system' is considered. While full diagonalisation suffices for small reference systems, larger systems require the Lanczos method or a quantum Monte Carlo method [2] to be tractable. Considering systems at finite temperature increases the numerical burden even further. Demanding on top of this the resolution of degenerate states in the reference system requires to switch from the regular Lanczos method to the Band Lanczos method. Here, thermodynamic and dynamical properties of the one- and two-dimensional Hubbard model at finite temperature are presented to illustrate the finite-temperature Lanczos and Band Lanczos method as solver of the reference system. The effect of degeneracies onto the results is discussed.

[1] M. Potthoff, 'Self-Energy-Functional Theory', in Strongly Correlated Systems – Theoretical Methods (Springer, 2012).

[2] G. Li, W. Hanke, A. N. Rubtsov, S. B  se and M. Potthoff, 'Accessing thermodynamics from dynamical cluster-embedding approaches', Phys. Rev. B 80, 195118 (2009).

28 Investigation of multipartite correlations in spin chains with matrix product state approach

Mih  ly M  t   - E  tv  s Lor  nd University

Mih  ly M  t  , Szil  rd Szalay,   rs Legeza

The simplest model showing the properties of the Haldane phase is the widely studied bilinear-biquadratic spin chain in a given range of the phase space. At a special point this model, known as AKLT model, is integrable and its ground state gives the simplest structure among matrix product states (MPS). In my poster, among other spin chains, the one-dimensional bilinear-biquadratic model is investigated using the density matrix renormalisation group method. This is the most powerful tool to study strongly correlated spin chains, based on the MPS representation of the wave function. Pair correlation and entanglement of spins are widely studied in strongly correlated systems, now we consider the multipartite correlations using bipartite as well as multipartite notions. The decay exponents for multipartite correlations are determined in the different intervals of phase spaces (e.g. critical-, dimerised-, Haldane phase) for various spin chains.

29 Effects of local approximations on topological phases

Thomas Mertz - Goethe-Universität

Thomas Mertz, Karim Zantout, Roser Valenti

We benchmark numerical methods with local approximations against methods including non-local effects to study possible inaccuracies of using local self-energies.

30 DSQSS – path-integral Monte Carlo solver based on worm algorithm

Yuichi Motoyama - The University of Tokyo

Yuichi Motoyama, Akiko Masaki-Kato, and Naoki Kawashima

DSQSS (Discrete Space Quantum Systems Solver) [1] is an open source software package for path-integral quantum Monte Carlo method based on single/multi worm algorithm. It can deal with arbitrary spin XXZ model under longitudinal and/or transverse magnetic field and hardcore/softcore Bose-Hubbard model on lattice with any dimension and shape. In this poster, we will show what DSQSS can do and how to use DSQSS.

[1] DSQSS on GitHub <https://github.com/qmc/dsqss>

31 Local hamiltonians for one dimensional critical models

Srivatsa N.S - Max-Planck-Institut für Physik komplexer Systeme

Dillip K. Nandy, N. S. Srivatsa, Anne E. B. Nielsen

Conformal field theory has turned out to be a powerful tool to derive interesting lattice models with analytical ground states. Here, we investigate a class of critical, one-dimensional lattice models of fermions and hardcore bosons related to the Laughlin states. The Hamiltonians of the exact models involve interactions over long distances, which is difficult to realize experimentally. This motivates us to study the properties of models with the same type of interactions, but now only between nearest and possibly next-nearest neighbor sites. Based on computations of wavefunction overlaps, entanglement entropies, and two-site correlation functions for systems of up to 32 sites, we find that the ground state is close to the ground state of the exact model. There is also a high overlap per site between the lowest excited states for the local and the exact models, although the energies of the low-lying excited states are modified to some extent for the system sizes considered. We also briefly discuss possibilities for realizing the local models in ultracold atoms in optical lattices.

32 A real-time quantum Monte Carlo approach to the master equation of open quantum systems

Alexandra Nagy - Ecole Polytechnique Federal de Lausanne

Alexandra Nagy, Vincenzo Savona

Many-body open quantum systems have attracted increasing attention in recent years. From a theoretical viewpoint, these systems call for new effective methods for the simulation of the dynamics and of the nonequilibrium steady state (NESS). In this contribution, we will discuss our recent progress in the development of a projector Monte Carlo approach to stochastically sample the time evolution of the density matrix – as dictated by the Liouville- von-Neumann equation – towards the NESS. For closed, Hamiltonian systems, various quantum Monte Carlo approaches have been the election tool to stochastically sample system properties, both at zero and finite temperature. Modeling the ground state properties at zero temperature in particular, is made possible by stochastically sampling the time evolution of the imaginary-time Schrödinger equation, with a class of methods generally known as projector Monte Carlo. The Liouvillian dynamics towards the steady state shares with the imaginary-time Schrödinger equation the fact that, in the long-time limit, the eigenstate with the smallest-real-part- eigenvalue will dominate. In the Liouvillian case, this corresponds to the NESS. It is therefore natural to attempt an extension of projector Monte Carlo techniques to the simulation of the NESS properties. However, the complex-valued density matrix follows an oscillatory dynamics which may easily result in the well known sign problem affecting most Monte Carlo algorithms. Recently, a new projector Monte Carlo approach – called Full Configuration Interaction Quantum Monte Carlo (FCIQMC) – has been developed for quantum chemistry simulations, and was found to alleviate significantly the sign problem. We present a proof of principle of the possibility to apply FCIQMC to the real-time evolution of the Liouville-von-Neumann equation towards the NESS. We study in particular the properties of the NESS of simple nonlinear arrays, where the FCIQMC results can be compared with exact numerical results obtained using quantum trajectories, and assess the accuracy and extent of the method. FCIQMC holds promise as a computationally effective tool to address open quantum system independently of their dimensionality.

33 Magnetic monopole supercurrent through a quantum spin ice tunnel junction

Sho NAKOSAI - RIKEN

Sho Nakosai, Shigeki Onoda

Quantum spin liquids are novel states of magnetic materials which exhibit a long-range quantum entanglement and the associated topological order, but no long-range symmetry-breaking order in many cases. Quasiparticles in quantum spin liquids are called spinons that carry fractionalized spin quanta and couple to emergent $U(1)$ gauge fields. Here, we theoretically demonstrate interference phenomena driven by a phase difference of spinon wavefunctions in an analogue of Josephson junction devices with superconductors. Two ferromagnetic phases, where spinons show a macroscopic phase coherence, are coupled through a thin film of a bulk $U(1)$ quantum spin liquid characterized by spin ice magnetic monopoles. There appears longitudinal spin supercurrent oscillation with the spinon phase difference. This unprecedented phenomena, if experimentally observed, confirm the emergence of magnetic monopole spinons and may open a new paradigm for spintronics application.

34 Spin-1 Heisenberg chain in a helical magnetic field

Ong Teng Siang, Ernest - Nanyang Technological University

Ong Teng Siang, Ernest and Pinaki Sengupta

We study the spin-1 Antiferromagnetic Heisenberg chain under the effects of a helical magnetic field. By varying the strength and helicity of the magnetic field, we identify several ground state phases. We use the density matrix renormalization group method to calculate the energy gaps, the string order parameter and the entanglement spectrum to characterise the different phases. Our preliminary results show that the topologically ordered Haldane phase at zero field is quenched by the magnetic field through closing of the energy gap and transition to a topologically trivial state. This gap closing is dependent on magnetic field strength and the helicity of the field. Interestingly, beyond a certain critical angle, the Haldane phase is destroyed without a gap closing.

35 Automated construction of $U(1)$ -invariant matrix-product operators from graph representations

Sebastian Paeckel - Georg-August-Universität Göttingen

S. Paeckel, T. Köhler, S. Manmana

We present an algorithmic construction scheme for matrix-product-operator (MPO) representations of arbitrary $U(1)$ -invariant operators whenever there is an expression of the local structure in terms of a finite-states machine (FSM). Given a set of local operators as building blocks, the method automatizes two major steps when constructing a $U(1)$ -invariant MPO representation: (i) the bookkeeping of auxiliary bond-index shifts arising from the application of operators changing the local quantum numbers and (ii) the appearance of phase factors due to particular commutation rules. The automatization is achieved by post-processing the operator strings generated by the FSM. Consequently, MPO representations of various types of $U(1)$ -invariant operators can be constructed generically in MPS algorithms reducing the necessity of expensive MPO arithmetics. This is demonstrated by generating arbitrary products of operators in terms of FSM, from which we obtain exact MPO representations for the variance of the Hamiltonian of a $S=1$ Heisenberg chain.

36 Flat bands in fractal-like geometry

Biplab Pal - Max Planck Institute for the Physics of Complex Systems (MPIPKS)

Biplab Pal and Kush Saha

We report the presence of multiple flat bands in a class of two-dimensional (2D) lattices formed by Sierpinski gasket (SPG) fractal geometries as the basic unit cells. Solving the tight-binding Hamiltonian for such lattices with different generations of a SPG network, we find multiple degenerate and non-degenerate completely flat bands, depending on the configuration of parameters of the Hamiltonian. Moreover, we find a generic formula to determine the number of such bands as a function of the generation index l of the fractal geometry. We show that the flat bands and their neighboring dispersive bands have remarkable features, the most interesting one being the spin-1 conical-type spectrum at the band center without any staggered magnetic flux, in contrast to the Kagome lattice. We furthermore investigate the effect of the magnetic flux in these lattice settings and show that different combinations of fluxes through such fractal unit cells lead to richer spectrum with a single isolated flat band or gapless electron- or hole-like flat bands. Finally, we discuss a possible experimental setup to engineer such fractal flat band network using single-mode laser-induced photonic waveguides.

37 Entanglement Hamiltonian of interacting fermionic models

Francesco Parisen Toldin - University of Würzburg

F. Parisen Toldin, F. F. Assaad

Recent numerical advances in the field of strongly correlated electron system have allowed the calculation of the correlations of the Entanglement Hamiltonian, and the associated entropies, for interacting fermionic systems [1]. On the other hand, an explicit determination of the Entanglement (modular) Hamiltonian has proven to be a considerably more difficult problem, where only a few results are available. We introduce a technique to directly determine the Entanglement Hamiltonian of interacting fermionic models by means of Auxiliary Field Quantum Monte Carlo simulations. We implement our method in the one-dimensional Hubbard chain model, partitioned into two segments, and in the two-legs Hubbard ladder model, partitioned into two chains.

[1] F. F. Assaad, T. C. Lang, F. Parisen Toldin, Phys. Rev. B 89, 125121 (2014)

38 Thorium Doping in Magnesium Fluoride

Martin Pimon - Technical University of Vienna

Martin Pimon

The thorium isotope ^{229}Th features a long-lived isomer state, $^{229\text{m}}\text{Th}$, which lies extremely close to the ground state at 7.8 eV. It is therefore proposed to be used as an atomic clock with extraordinary precision. Additionally, it might be used in studies of material properties by means of Mössbauer spectroscopy and it may be used for building a laser. Due to the scarcity of the material and the large density needed, it is suggested to be doped into a crystal. As a host crystal we investigated MgF_2 , that shows a band gap of 10.8 eV, with ab-initio calculations performed in VASP. It is shown that Th occupies a Mg site but considering that Th and Mg have a different valence of 4+ and 2+ respectively, two compensation charges must be present. We examined different possibilities for the atoms and positions of the compensation charges to determine if the band gap stays larger than the energy of $^{229\text{m}}\text{Th}$. The results presented include a comparison of the compensations investigated with their respective band gap.

39 Interplay between the edge-state magnetism and long-range Coulomb interaction in zigzag graphene nanoribbons

Marcin Raczkowski - Universität Würzburg

Marcin Raczkowski and Fakher F. Assaad

We perform projective quantum Monte Carlo simulations of zigzag graphene nanoribbons within a realistic model with long-range Coulomb interactions. Increasing the relative strength of nonlocal interactions with respect to the on-site repulsion does not generate a phase transition but has a number of nontrivial effects. At the single-particle level we observe a marked enhancement of the Fermi velocity at the Dirac points. At the two-particle level, spin- and charge-density-wave fluctuations compete. As a consequence, the edge magnetic moment is reduced but the edge dispersion relation increases in the sense that the single-particle gap at momentum $q = \pi/$ grows. We attribute this to nonlocal charge fluctuations which assist the spin fluctuations to generate the aforementioned gap. In contrast, the net result of the interaction-induced renormalization of different energy scales is a constant spin-wave velocity of the edge modes. However, since the particle-hole continuum is shifted to higher energies - due to the renormalization of the Fermi velocity - Landau damping is reduced. As a result, a roughly linear spin-wave-like mode at the edge spreads out through a larger part of the Brillouin zone.

40 Towards Real-Time Dynamics of Typical and Un-typical States in Non-Integrable Systems

Jonas Richter - University Osnabrück

Jonas Richter, Fengping Jin, Hans de Raedt, Kristel Michielsens, Jochen Gemmer, and Robin Steinigeweg

Due to controlled experiments with cold atomic gases and the development of sophisticated numerical methods, the study of non-equilibrium dynamics in many-body quantum systems has experienced an upsurge of interest. Particularly for closed systems, there has been immense theoretical effort to answer fundamental questions about equilibration and thermalization. Since such systems are isolated from their environment, out-of-equilibrium conditions can only be induced by the preparation of suitable initial states. In this context, we investigate the real-time dynamics for a class of non-equilibrium pure states in the spin-1/2 XXZ

chain. Such states have been recently studied for integrable models [1,2], and relying on the concept of typicality, allow a comparison with results from linear response theory. By introducing an additional next-to-nearest neighbor interaction, we discuss the effect of integrability vs. non-integrability on the dynamics. Furthermore, the role of the specific initial state realization is analyzed in terms of internal randomness, entanglement entropy, and local density of states.

[1] R. Steinigeweg et al., Phys. Rev. B 95, 035155 (2017)

[2] R. Steinigeweg et al., Phys. Rev. E 96, 020105(R) (2017)

[3] J. Richter et al., in preparation.

41 Photoinduced absorptions inside the Mott gap in the two-dimensional extended Hubbard model

Kazuya Shinjo - Tokyo University of Science

Kazuya Shinjo and Takami Tohyama

We theoretically investigate pump-probe optical responses in the two-dimensional extended Hubbard model describing cuprates by using a time-dependent Lanczos method. At half filling, pumping generates photoinduced absorptions inside the Mott gap. A part of low-energy absorptions is attributed to the independent propagation of photoinduced holons and doublons. The spectral weight just below the Mott gap increases with decreasing the on-site Coulomb interaction U . We find that the next-nearest-neighbor Coulomb interaction V_1 enhances this U dependence, indicating the presence of biexcitonic contributions formed by two holon-doublon pairs. Photopumping in hole-doped systems also induces spectral weights below remnant Mott-gap excitations, being consistent with recent experiments. The induced weights are less sensitive to V_1 and may be related to the formation of a biexcitonic state in the presence of hole carriers.

42 DFT+DMFT simulations of rare-earth hexaborides

Florian Sohn - Uni Göttingen

Florian Sohn, Steffen Backes, Salvatore R. Manmana, Roser Valentí, Peter E. Blöchl

Rare-earth hexaborides (REB6) are strongly correlated materials, where the strong Coulomb interaction between electrons in the rare earth's f -electron shell influence the electronic properties of the whole material decisively. REB6 exhibit a variety of low-temperature phenomena, including antiferromagnetic ordering for most partially filled f-shells, ferromagnetic ordering in EuB6, superconductivity for LuB6, topological insulating behavior in SmB6 and a complex phase diagram with Kondo behavior in CeB6. We present results of DFT+DMFT simulations performed on selected REB6, in particular for the spectral function. For the DFT calculations, the Wien2k code is applied, while for the DMFT we employ the continuous-time hybridization expansion quantum Monte Carlo (CT-HYB) matrix code of the ALPSCore project. Our goal is to compare with ARPES experiments. We gratefully acknowledge financial support by the DFG project PR298/19-1.

43 Influence of continuous spin symmetries on magnetic ordering in the Hubbard model with multiple spin and orbital components

Andrii Sotnikov - TU Wien

Andrii Sotnikov

We apply dynamical mean-field theory to study instabilities toward antiferromagnetic, ferromagnetic, and excitonic long-range ordered states in several realizations of the Hubbard-type models. It is shown that, while increase of spin components [SU(N) direction] usually suppresses magnetic phases, an increase of active orbitals (large-S direction) or lowering of spin-rotational symmetry leads to enhancement of long-range ordering. Other aspects as interplay with metal-insulator transitions, external magnetic fields and thermodynamic effects are discussed.

44 Interplay between topology and disorder in a two-dimensional semi-Dirac material

P.V. Sriluckshmy - Max-Planck Institute for Physics of Complex Systems

P.V. Sriluckshmy, Kush Saha and Roderich Moessner

We investigate the role of disorder in a two-dimensional semi-Dirac material characterized by a linear dispersion in one, and a parabolic dispersion in the orthogonal, direction. Using the self-consistent Born approximation, we show that disorder can drive a topological Lifshitz transition from an insulator to a semi-metal, as it generates a momentum independent off-diagonal contribution to the self-energy. Breaking time-reversal symmetry enriches the topological phase diagram with three distinct regimes— single-node trivial, two-node trivial and two-node Chern. We find that disorder can drive topological transitions from both the single- and two-node trivial to the two-node Chern regime. We further analyze these transitions in an appropriate tight-binding Hamiltonian of an anisotropic hexagonal lattice, by calculating the real-space Chern number. Additionally we compute the disorder-averaged entanglement entropy which signals both the topological Lifshitz and Chern transition as a function of the anisotropy of the hexagonal lattice. Finally, we discuss experimental aspects of our results.

45 Entanglement properties of lattice bosons from a variational wave function

Jérôme Thibaut - Laboratoire de physique de l'ENS Lyon

Jérôme Thibaut - Tommaso Roscilde

Entanglement is a defining characteristic of many-body quantum systems, expressing the degree of non-locality required by the description of the state of the system, and quantifying the amount of classical information demanded to faithfully reproduce the reduced state of any subsystem. The ground states of many-body Hamiltonians with short-range interactions are generically characterized by area-law scaling of entanglement entropies of a subsystem, implying that the classical information required to store the reduced density matrix is exponential in the surface of the subsystem itself this aspect impairs scalable simulations with methods based on the explicit reconstruction of reduced density matrix, such as DMRG, in dimensions higher than one. A viable alternative is based on variational ground states explicitly exhibiting an area-law scaling of entanglement. Here we explore the entanglement properties of entangled plaquette states (EPS) [1] representing a systematically improvable variational Ansatz for lattice boson models, and lending itself to an efficient optimization based on variational Monte Carlo. We evaluate the explicit dependence of the entanglement entropy on the number of coefficients in the variational Ansatz, and contrast the entanglement properties of local vs. nonlocal plaquettes in the EPS structure. Applying the EPS approach to a lattice boson model (the spatially anisotropic π -flux triangular lattice) which bridges 1d and 2d physics, we investigate how the entanglement scaling reveals the effective dimensionality of correlations.

[1] F. Mezzacapo et al, New Journal of Physics, 11, 083026 (2009).

46 Quantum Monte Carlo Simulation of Antiferromagnetic Binary Alloy System with Random Exchange Interactions

Erol Vatansever - Dokuz Eylul University

Erol Vatansever

Finite temperature properties of the 1D Antiferromagnetic Binary alloy of the type A_pB_{1-p} with random spin-spin interactions have been investigated by means of Quantum Monte Carlo (QMC) simulation based on stochastic series expansion method. First, thermal variations of heat capacity and susceptibility have been calculated for small system size, and the obtained data are compared with exact results. Next, influences of the finite-size on the thermodynamic variables have been discussed. Our QMC findings show that values of the spin-spin interaction terms and also concentration of the magnetic atoms have a crucial role on the system characteristic.

47 Finite size scaling of 1D topological model

Yuting Wang - University of Minnesota

Yuting Wang, Alex Kamenev

We investigate the scaling of ground state energy around topological quantum phase transition in one dimension. It is found that the finite-size correction to energy which is uniquely related to its central charge at criticality naturally extends into a scaling function when moving away from the critical point. The scaling function depends only on the ratio of the system size to the correlation length and shows universal behavior among non-interacting and interacting models.

48 Selective state spectroscopy and multifractality in disordered Bose-Einstein condensates: a numerical study

Miklos Antal Werner - Budapest University of Technology and Economics

Miklós Antal Werner, Eugene Demler, Alain Aspect, and Gergely Zaránd

We propose to use the method introduced by Volchkov et al., based on state dependent disordered ultracold bosons, to address the critical state at the mobility edge of the Anderson localization transition, and to observe its intriguing multifractal structure. An optimally designed external radio frequency pulse can be applied to generate transitions to eigenstates in a narrow energy window close to the mobility edge, where critical scaling and multifractality emerge. Two-photon laser scanning microscopy will be used to address individual localized states even close to the transition. The projected image of the cloud is shown to inherit multifractality and to display universal density correlations. Time of flight images of the excited states are predicted to show interference fringes in the localized phase, while they allow one to map equal energy surfaces deep in the metallic phase.

49 Exact QMC(SSE) for Quantum dimer models

Zheng YAN - Fudan University

Z.Yan,J.LOU,Y.Chen et al.

50 Analytical continuation of quantum Monte Carlo data using sparse modeling

Kazuyoshi Yoshimi - University of Tokyo

K. Yoshimi, J. Otsuki, H. Shinaoka and M. Ohzeki

In quantum Monte Carlo simulation, dynamic physical quantities such as single particle and magnetic excitation spectrum can be obtained by analytical continuation of imaginary-time data. However, analytical continuation is an ill-conditioned inverse problem and thus is sensitive to noise and statistical errors. To solve this problem, analysis using the maximum entropy method or statistical method, etc., has been proposed. But a definitive method has not yet been established. In this presentation, we propose a method of analytical continuation using sparse modeling[1]. In this method, analytical continuation becomes robust against noise since relevant basis unaffected by the noise is automatically selected. We also show that this compression basis gives a model-independent compact representation of imaginary-time data [2]. In addition, we will introduce the open source software “SpM” implementing the new method of analytical continuation [3].

[1] J. Otsuki, M. Ohzeki, H. Shinaoka, and K. Yoshimi, Phys. Rev. E 95 (2017), 061302(R)

[2] H. Shinaoka, J. Otsuki, M. Ohzeki, and K. Yoshimi, Phys. Rev. B 96 (2017), 035147

[3] <https://github.com/j-otsuki/SpM>

51 Learning Disordered Topological Phases by Statistical Recovery of Symmetry

Nobuyuki Yoshioka - University of Tokyo

Nobuyuki Yoshioka, Yutaka Akagi, and Hosho Katsura

A topological superconductor (TSC) is a superconductor (SC) with a bulk gap characterized by a nontrivial topological invariant, which reflects the global property of the wave functions. While the concrete expression of the topological number for the translationally invariant system is widely known, our understanding of the disordered SCs is limited. In this work, we investigate the phases of two-dimensional disordered TSC in the class DIII using the state-of-the-art machine

learning technique, i.e., the neural network (NN). With the surging development of experimental research, there is a growing demand for investigation in the class DIII system, or the spin-rotation-symmetry-breaking Bogoliubov de Gennes system with time reversal symmetry, since some candidate materials are believed to belong here (e.g. $\text{Cu}_x\text{Bi}_2\text{Se}_3$, FeTeSe). There are two valid ways to model such systems. One is so-called Chalker-Coddington network model, which phenomenologically formulates the propagation and the scattering of the electrons. The other method we consider in this work is the tight-binding model, whose parameters reflect the microscopic information and hence expected to be in a good connection with experimental works. The \mathbb{Z}_2 topological invariant exhibited in this class is reflected in the real-space distribution of the quasiparticle according to the bulk-edge correspondence. Hence, we give the machine the distribution as a "picture" with some label to learn the structure and perform the supervised learning. In our presentation, we compare the result to the phase diagram obtained by other methods, namely the transfer matrix and non-commutative geometry, and discuss the accuracy and the validity of the new technique.

52 Strongly-correlated photons in cavity arrays

Filippo Gaggioli - ETH Zürich

F. Gaggioli, M. Biondi, S. Schmidt, H. E. Türeci, J. W. Blatter

Quantum simulators of non-equilibrium many-body physics can be engineered using photonic lattices in various cavity QED architectures. These systems lie at the interface of condensed matter physics and quantum optics and are described by variants of the Bose-Hubbard model. In this project, we theoretically and numerically investigate strongly correlated photonic phases out of equilibrium in order to discover new phenomena and foster novel experiments on photonic arrays.

53 Single-magnon dynamics in a spin-1/2 XXZ chain coupled to phonons

Jan Stolpp - LMU München

J. Stolpp, F. Heidrich-Meisner, E. Jeckelmann

We study the real space and real time dynamics of single magnon excitations in a ferromagnetic background of an antiferromagnetic spin-1/2 chain where every spin can couple to phononic degrees of freedom. We scan a wide parameter regime of spin-phonon coupling, phonon energy and phonon band-width and find evidence for a transition from ballistic to diffusive dynamics. The numerical simulation of the time evolution for such a system is challenging because of the possibly large local dimension. Conventional matrix product state based methods will get stuck very soon because of the polynomial scaling with the local dimension. To overcome these limitations we implemented a TEBD algorithm with local basis optimization [1, 2]. We illustrate the performance of this algorithm in different parameter regimes and compare it to an implementation of conventional TEBD.

This research is supported by the DFG via Research Unit FOR 1807.

[1] C. Brockett, F. Dorfner, L. Vidmar, F. Heidrich-Meisner, and E. Jeckelmann. Matrix-product-state method with a dynamical local basis optimization for bosonic systems out of equilibrium. *Phys. Rev. B*, 92:241106, Dec 2015.

[2] Chunli Zhang, Eric Jeckelmann, and Steven R. White. Density matrix approach to local hilbert space reduction. *Phys. Rev. Lett.*, 80:2661–2664, Mar 1998.

A selection of Restaurants, pubs and bars

There are many restaurants, pubs, and cafes in the old town, near the market place, on the way from the market place to the Elisabeth church, from the market-place along Barfüßertor, and from the market place down Reitgasse back to the conference center. Restaurants are marked with an (R). Most other places offer a variety of small dishes.

Near the town center:

(R) "Bückingsgarten"	Landgraf-Philipp-Str. 6 35037 Marburg www.bueckingsgarten-marburg.de	Tel. 0 64 21/1657771
Weinstube "Weinlädele"	Schlosstreppe 1 35037 Marburg www.weinlaedele.com	Tel. 0 64 21/1 42 44
(R) Ratsschänke	Markt 3 35037 Marburg www.ratsschaenke-marburg.de	Tel. 06421-13834
Café am Markt	Markt 9 35037 Marburg www.cafe-am-markt.de	Tel. 06421-25522
(R) Edlunds	Markt 15 35037 Marburg www.edlunds.de	Tel. 06421-1669318
(R) "Zur Sonne"	Markt 14 35037 Marburg www.zur-sonne-marburg.de	Tel. 0 64 21 1 71 90
(R) Pizza Pasta Da Nella	Markt 17 35037 Marburg www.pizzeria-marburg.de	Tel. 06421-25822
(R) "Hostaria del Castello"	Markt 19 35037 Marburg www.del-castello.de	Tel. 0 64 21 2 58 84

Between town center and Elisabeth church:

Restaurant "Auflauf"	Steinweg 1 35037 Marburg www.auflauf-marburg.de	Tel. 06421 681343
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(R) Gartenlaube	Steinweg 40 35037 Marburg www.gartenlaube-marburg.de	Tel. 06421-617662
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Along Barfüßerstrasse:

(R) "KostBar"	Barfüßerstr. 7 35037 Marburg www.kostbar-marburg.de	Tel. 06421 161170
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Café 1900	Barfüßerstr. 27 35037 Marburg	Tel. 06421 27167
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Felix Café - Bar – Restaurant	Barfüßerstr. 28 35037 Marburg www.felix-marburg.de	Tel. 06421-307336
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Café Barfuß Studentenkneipe	Barfüßerstr. 33 35037 Marburg	Tel. 06421/ 25349
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MAXX Studentenrestaurant	Barfüßerstr. 55 35037 Marburg www.maxxbar.de	Tel. 06421/ 24266
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Between town center and conference site:

(R) Fionas"	Pilgrimstein 34 35037 Marburg www.fionas-marburg.de	Tel. 06421 6978837
5 Jahreszeiten Bar Restaurant	Reitgasse 5 35037 Marburg www.das5.de	Tel. 06421 8868988
Brasserie Café- Bar- Restaurant	Reitgasse 8 35037 Marburg www.brasserie-marburg.de	Tel. 06421-21992
Café Paprika Studentenkneipe	Reitgasse 12 35037 Marburg www.paprica-bar.de	Tel. 06421 3400808

Taxi Services

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City Taxi	06421 / 44411
EuroCar	06421 / 999995
Marburg City Taxi	06421 / 37777
Spar Car	06421 / 999988
Taxi Ayse	06421 / 44477
Taxi Gurhan	06421 / 44414
Taxi Kazim	06421 / 9488877
Taxi Sami Ali Saleh	06421 / 62222
Taxi Sorany	06421 / 484444
TAXI-RUF Wehrda	06421 / 880099
Telecar	06421 / 25100
Unicar	06421 / 65565
VIP Car	06421 / 66699

Pharmacy

A selection of pharmacies

Bahnhof-Apotheke Tel. +49 (6421) 66722	Bahnhofstr. 29, 35037 Marburg open: 08:00–19:00
Deutschhaus Apotheke Tel. +49 (6421) 65651	Biegenstraße 44, 35037 Marburg open 08:00–18:30
Einhorn Apotheke Tel. +49 (64 21) 88 90 90	Steinweg 39, 35037 Marburg, open 08:00 - 18:30 Uhr
Hirsch-Apotheke Tel. +49 (6421) 64078	Bahnhofstraße 9, 35037 Marburg, open 09:00–18:30
Lahn Apotheke Tel. +49 (6421) 12121,	Wilhelmstrasse 5-7, 35037 Marburg, open 08:00–20:00
Apotheke im Lahn-Center Tel. +49 (6421) 27806,	Biegenstraße 4, 35037 Marburg, open 08:00–19:00
Philipps Apotheke Tel. +49 (6421) 27711	Reitgasse 10, 35037 Marburg Open 8.30 - 19.00 Uhr
Rosenapotheke Tel. +49 (6421) 2 54 21	Schwanallee 1, 35037 Marburg, open 08:15–18:30
Schlossberg-Apotheke Tel. +49 (6421) 2 34 43	Universitätsstraße 15, 35037 Marburg, Open 8:00 - 19:00
Neue Universitäts-Apotheke Tel. +49 (6421) 22066	Universitätsstraße 41, 35037 Marburg, Open 08:00–18:30

Bank

A selection of banking possibilities

Commerzbank AG	Pilgrimstein 36 , 35037 Marburg, Tel. +49 (6421) 92710
Deutsche Bank	Biegenstr. 2, 35037 Marburg, Tel. +49 (6421) 99080
Postbank Data GmbH	Bahnhofstr. 6, 35037 Marburg, Tel. +49 (6421) 61014
Sparkasse Marburg	Universitätsstr. 10, 35037 Marburg, Tel. +49 (6421) 2060
Sparda-Bank Hessen eG	Krummbogen 15, 35039 Marburg, Fax +49 (6421) 6 85 09-29
Volksbank Mittelhessen eG	Bahnhofstr. 5 , 35037 Marburg, Tel. +49 (06421) 590860 Pilgrimstein 35, 35037 Marburg, Tel. +49 (6421) 2920
Santander Consumer Bank	Universitätsstraße 49, 35037 Marburg, Tel. +49 (6421) 804120

Zentrum für Notfallmedizin (central point of emergency medical aid)

Baldingerstraße, 35043 Marburg
Mail: znotmed@med.uni-marburg.de
Tel: +49 (6421) 58-61999, Fax:+49 (6421) 58-6699

	Monday	Tuesday	Wednesday	Thursday	Friday
8:15-10:00	ML1 Wang	QMC2 (CT-INT) Hohenadler	TN1 Pollmann	TN2 Pollmann	QMC3 (AFQMC) Assaad
10:00-10:30	Coffee	Coffee	Coffee	Coffee	Coffee
10:30-12:15	QDS1 Kollath	ML2 Wang	ED1 Honecker	DMRG Manmana	ED2 Hands-On Honnecker/Wietek
12:15-14:30	Lunch	Lunch	Lunch	Lunch	Lunch
14:30-16:15	QMC1 (SSE) Wessel	QDS2 Kollath	ML3 Hands-On Wang	Social Program (Sightseeing)	QMC4 Hands-On (ALF) Hofmann/Goth/Assaad
16:15-16:45	Coffee	Coffee	Coffee	TN3 Hands-On Pollmann	End of school
16:45-17:30	Contributed Talks 1,2,3	Contributed Talks 4,5,6	QDT Steinigeweg		
17:30-18:15	Poster Session 1 (Open end, odd no.)	Poster Session 2 (Open end, even no.)			