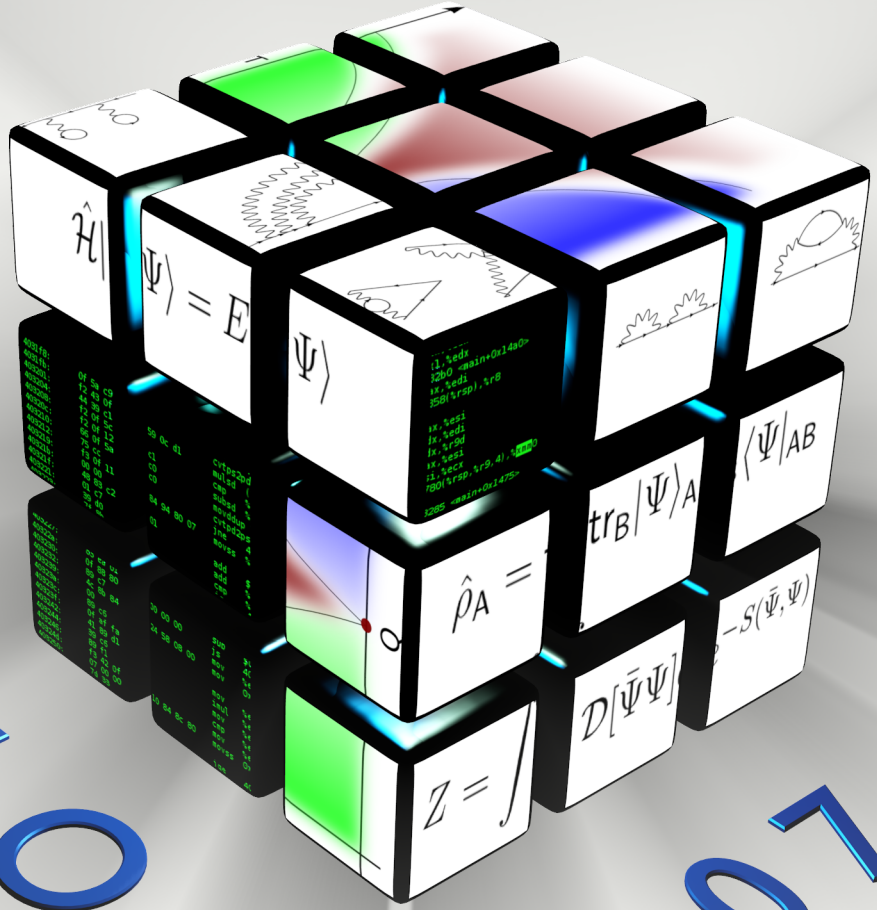
Advanced Numerical Algorithms for Strongly Correlated Quantum Systems



FOR 1807

Würzburg, February 23 - 26 2015

Conference Program at a Glance

	Sunday	Monday	Tuesday	Wednesday	Thursday
08:30-09:00		Welcome/Registration			
09:00-09:40		O1 Schultheiss	O2 Polkonikov	O3 Prokof'ev	O4 Verstraete
09:40-10:10		I1 Alvermann	I6 Pollmann	F3 Osorio	F6 Weber
10:10-10:30		C1 Weichselbaum	C5 Zotos	C9 Vairinhos	C14 Beach
10:30-11:00		Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00-11:30		F1 Wietek	I7 Stoudenmire	I13 Daghofer	F7 Kerkdyk
11:30-12:00		I2 Luitz	I8 Chan	I14 Manmana	C15 Adam
12:00-12:20		C2 Baker	C6 Rizzi	C10 Capponi	F8 Wessel
12:25-12:30				Group Photo	
until 14:00		Lunch Break	Lunch Break	Lunch Break	Lunch Break/End
14:00-14:30		I3 Kollath	I9 Chandrasekharan	F4 Wolf	Internal Meeting of FOR 1807
14:30-15:00		I4 Vidmar	I10 Lähde	F5 Ehlers	
15:00-15:20		C3 Mierzejewski	C7 Pollet	C11 Möller	
15:20-16:00		Coffee break	Coffee break	Coffee break	
16:00-16:30		I5 Rigol	I11 Sorella	C12 Schmidt	16:00-16:20
16:30-17:00		F2 Jeckelmann	I12 Lang	C13 Bröcker	16:20-16:40
17:00-17:20		C4 Arrigoni	C8 Buividovich		
17:20-19:30	Reception/Registration	Poster Session I	Poster Session II	Guided Tour (17:30) Dinner (19:00)	

Colour coding: Overview talk | Invited talk | Contributed talk | FOR 1807 talk

Monday Sessions at a Glance

Monday 1

Chair: G. Sangiovanni

09:00–09:40	**TBA**
O1	*Thomas Schulthess (ETH Zurich)*
09:40–10:10	**Polynomial expansions in quantum physics computations**
I1	*Andreas Alvermann (University of Greifswald)*
10:10–10:30	**QSpace – a generic framework for non-abelian symmetries in tensor networks**
C1	*Andreas Weichselbaum (LMU Munich)*

Monday 2

Chair: J. Schnack

11:00–11:30	**Exact Diagonalization Techniques on Distributed Memory Machines and the Quest for Identifying Spin Liquid Phases**
F1	*Alexander Wietek (University of Innsbruck)*
11:30–12:00	**Many-body localization edge in the random-field Heisenberg chain**
I2	*David J. Luitz (Université Paul Sabatier Toulouse)*
12:00–12:20	**Probing the Failures of DFT with Computationally Efficient Interactions and DMRG**
C2	*Thomas E. Baker (UC Irvine)*

Monday 3

Chair: J. von Delft

14:00–14:30	**Unconventional dynamics in dissipative ultracold atomic gases**
I3	*Corinna Kollath (University of Bonn)*
14:30-15:00	**Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in the cuprates**
I4	*Lev Vidmar (LMU Munich)*
15:00–15:20	**Local and Quasilocal Conserved Quantities in Integrable Systems**
C3	*Marcin Mierzejewski (University of Silesia)*

Monday 4

Chair: TBA

16:00–16:30	**Numerical Linked Cluster Expansions for Quantum Quenches in the Thermodynamic Limit**
I5	*Marcos Rigol (Pennsylvania State University)*
16:30-17:00	**Numerical methods for nonequilibrium polarons**
F2	*Eric Jeckelmann (University of Hanover)*
17:00–17:20	**Auxiliary master equation approach for correlated quantum impurities out of equilibrium**
C4	*Enrico Arrigoni (Graz University of Technology)*

Poster I

Chair: M. Hohenadler

17:20–19:30	**Oral poster presentation (one minute per poster), followed by Poster Session I**

09:00–09:40 **TBA**
O1 *Thomas Schulthess (ETH Zurich)*

09:40–10:10 **Polynomial expansions in quantum physics computations**
I1 *Andreas Alvermann (University of Greifswald)*

Polynomial expansions can play an important role in numerical quantum physics, especially for few particle problems or continuous degrees of freedom. They can be used for two complementary purposes: First, to set up the matrix representation of the physical Hamiltonian, using polynomials as the building blocks of the computational Hilbert space. Second, to compute the properties of interest, e.g., with time-propagation techniques based on Chebyshev and Faber polynomials. The talk will discuss specific aspects of these two purposes: First, how to use polynomials on sparse grids for continuous degrees of freedom. Second, how three key algorithms for quantum physics computations (Kernel Polynomial Method, Chebyshev time propagation, Krylov eigensolvers) can be developed and understood in terms of the underlying polynomial approximations. Using the spin-boson model as the motivating example, I will show how such techniques allow for the computation of phase transitions and dynamics in the presence of strong bosonic correlations.

Computations of the above kind rely heavily on sparse linear numerics, with sparse matrix vector multiplication as the core operation that determines performance. To address this issue I will shortly report on a new initiative towards up-to-date implementations of quantum physics algorithms on modern hardware architectures.

10:10–10:30 **QSpace – a generic framework for non-abelian symmetries in tensor networks**
C1 *Andreas Weichselbaum (LMU Munich)*

Non-abelian symmetries can be implemented generically into tensor networks. I will briefly discuss the framework developed in that respect which has already been successfully applied in numerous effective one-dimensional model calculations (primarily the numerical renormalizaton group (NRG)). There in particular for SU(3) [Sp(6)] symmetric three-channel calculations, the exploitation of these larger non-abelian symmetries was quintessential for reliable converged results to start with. After pointing out recent advances in the treatment of generalized Clebsch-Gordan coefficient tensors, finally I will also discuss preliminary results on the symmetry fractionalization in SU(2n) antiferromagnetic Heisenberg chains. There we explore generalizations of the Affleck-Kennedy-Lieb-Tasaki (AKLT, 1987) model for spin-1 antiferromagnetic Heisenberg chains to higher-rank SU(2n) symmetries. In particular we show that by proper tuning of higher order spin interactions there also exist exact low-dimensional matrix-product ground states with fractionalized edge states. These states are adiabatically connected to the ground state of the plain SU(2n) Heisenberg model as demonstrated by density matrix renormalization group (DMRG) calculations.

11:00–11:30 **Exact Diagonalization Techniques on Distributed Memory Machines and the Quest for Identifying Spin Liquid Phases**

F1 *Alexander Wietek (University of Innsbruck)*

In the field of strongly correlated electron systems a major numerical technique is Exact Diagonalization. It is capable of calculating exact and unbiased properties of Quantum many-body systems excitation energies, correlation functions, time-evolution and many more. The main drawback of this method is that the computational effort scales exponentially in the system sizes. We present methods how to efficiently design a modern Exact Diagonalization code for distributed memory machines in order to further push the limits of attainable system sizes and show benchmarks of our implementation. Since Exact Diagonalization is also capable of calculating the groundstate many-body wavefunction it is possible to compare groundstates to variational wavefunctions such as Gutzwiller Projected spinliquid wavefunctions. Thereby we are able to identify spin liquid phases in Quantum Phase diagrams. We will show how we applied this method to identifying a Chiral Spin Liquid phase in the phase diagram of the J_1-J_2-J_3 Heisenberg model on the kagome lattice.

11:30–12:00 **Many-body localization edge in the random-field Heisenberg chain**

I2 *David J. Luitz (Université Paul Sabatier Toulouse)*

We present a large scale exact diagonalization study of the one dimensional spin-$1/2$ Heisenberg model in a random magnetic field. In order to access properties at varying energy densities across the entire spectrum for system sizes up to L=22 spins, we use a spectral transformation which can be applied in a massively parallel fashion. Our results allow for an energy-resolved interpretation of the many body localization transition including the existence of an extensive many-body mobility edge. The ergodic phase is well characterized by Gaussian orthogonal ensemble statistics, volume-law entanglement, and a full delocalization in the Hilbert space. Conversely, the localized regime displays Poisson statistics, area-law entanglement and non ergodicity in the Hilbert space where a true localization never occurs. We perform finite size scaling to extract the critical edge and exponent of the localization length divergence.

12:00–12:20 **Probing the Failures of DFT with Computationally Efficient Interactions and DMRG**

C2 *Thomas E. Baker (UC Irvine)*

We examine the exact properties of Density Functional Theory (DFT) in one dimension and compare it with the numerically exact answer provided by Density Matrix Renormalization Group. Using the exact answers, we can compare exact DFT quantities against commonly used approximations. In order to explore the structure of DFT, we have generated an efficient one dimensional system that mimics the more commonly used soft-Coulomb interaction's energetics. The computational efficiency in both DFT and DMRG is much lower in this modified system and may be useful in other research efforts. We then use this system to explore fundamental issues in DFT.

14:00–14:30 **Unconventional dynamics in dissipative ultracold atomic gases**
I3 *Corinna Kollath (University of Bonn)*

Atomic gases cooled to Nanokelvin temperatures are a new exciting tool to study a broad range of quantum phenomena. The outstanding tunability of cold gases allows to rapidly change the system parameters and to observe the subsequent quantum evolution. This ability is unmatched in conventional solid state samples and poses new challenges for the understanding of quantum dynamics in correlated many-body systems. I will report on recent progress on the dynamics of quantum gases under the influence of controlled dissipative coupling. One focus will be the occurrence of critical dynamics and ageing behaviour in bosonic gases and the creation of pair correlations in fermionic gases.

14:30-15:00 **Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in the cuprates**
I4 *Lev Vidmar (LMU Munich)*

The substantial increase of the time-resolution and versatility of ultrafast techniques is paving the way to directly access the timescale of the fastest electron scattering processes in correlated materials. We made a joint experimental/theoretical effort to measure and model the ultrafast dynamics of photo-excited holes with the surrounding short-range antiferromagnetic background in doped cuprates on their relevant timescale (≈ 10 fs), that has been hitherto inaccessible [1]. This allows us to address one of the pivotal questions in the physics of high-temperature superconductors, i.e., whether the low-energy dynamics of the charge carriers is mediated by bosons with a characteristic timescale. In the experimental context, a novel time-domain approach was developed that allowed us to measure, for the first time, the dynamics of the optical properties of a hole-doped cuprate over an extremely broad energy range (0.75–2.4 eV) and with < 20 fs resolution over the entire spectrum. This has been the key to demonstrate the effectiveness of the boson-mediated description on a timescale that is on the order of few times $1/2J$, where J is the exchange coupling constant originated by the electronic interactions. Fundamental insight into the microscopic processes responsible for the ultrafast relaxation process of the photo-excited holes is provided by state of the art numerical simulations within the out-of-equilibrium t-J model [2]. We show that the key relaxation mechanism at very short times corresponds to the creation of high-energy antiferromagnetic excitations in the close proximity of the photo-excited holes. Such a mechanism enables an energy transfer of more than 1 eV on a 10 femtosecond time scale.

[1] S. Dal Conte, L. Vidmar, *et al.*, (accepted by Nature Physics, 2015).

[2] D. Golež, J. Bonča, M. Mierzejewski, and L. Vidmar, Phys. Rev. B **89**, 165118 (2014).

15:00–15:20 **Local and Quasilocal Conserved Quantities in Integrable Systems**
C3 *Marcin Mierzejewski (University of Silesia)*

We outline a numerical procedure for counting and identifying a complete set of local and quasilocal conserved operators in integrable lattice systems. The method yields a systematic generation of all independent, conserved quasilocal operators related to time-average of local operators with a support on up to M consecutive sites. As an example we study the anisotropic Heisenberg spin-$1/2$ chain and show that the number of independent conserved operators grows linearly with M. Besides the known local operators there exist novel quasilocal conserved quantities in all the parity sectors. The existence of quasilocal conserved operators is shown also for the isotropic Heisenberg model. Implications for the anomalous relaxation of quenched systems are discussed as well.

16:00–16:30 **Numerical Linked Cluster Expansions for Quantum Quenches in the Thermodynamic Limit**
I5 *Marcos Rigol (Pennsylvania State University)*

16:30-17:00 **Numerical methods for nonequilibrium polarons**
F2 *Eric Jeckelmann (University of Hanover)*

17:00–17:20 **Auxiliary master equation approach for correlated quantum impurities out of equilibrium**
C4 *Enrico Arrigoni (Graz University of Technology)*

The auxiliary master equation approach [1,2] allows for a direct and efficient calculation of steady state properties of correlated impurities out of equilibrium, as is needed, e.g., for non-equilibrium dynamical mean field theory (DMFT). It is based upon a mapping onto an auxiliary open quantum system in which the impurity is coupled to bath orbitals as well as to a Markovian environment. The dynamics of this auxiliary system are controlled by a Lindblad master equation whose parameters are used to optimize the mapping, which quickly becomes exact upon increasing the number of bath orbitals. Steady state and Green's functions of the auxiliary system are evaluated by (non-hermitian) Lanczos exact diagonalization or by matrix-product states (MPS). Dissipation is taken into account already with a small number of bath orbitals. We discuss steady-state transport properties and spectrum of the Anderson impurity model in the presence of a voltage bias. The splitting of the Kondo peak as function of voltage is discussed. The approach can be regarded as the non-equilibrium steady-state extension of the exact-diagonalization or MPS-based DMFT, and introduces appropriate absorbing boundary conditions for a many-body system.

[1] E. Arrigoni *et al.*, Phys. Rev. Lett. **110**, 086403 (2013).

[2] A. Dorda *et al.*, Phys. Rev. B **89** 165105 (2014).

Monday Posters at a Glance

P1 **Advanced finite-temperature Lanczos method for anisotropic spin systems**
Jürgen Schnack (Bielefeld University)

P2 **Coulombic liquid phases of bosonic cluster Mott insulators on pyrochlore lattice**
Zi Yang Meng (Chinese Academy of Sciences)

P3 **Unusual vortex matter in rotating Bose-Einstein condensates with SU(2) broken symmetry**
Peder Galteland (Norwegian University of Science and Technology)

P4 **A dual-fermion analysis of the Anderson-Hubbard model**
Patrick Haase (Georg-August Universität Göttingen)

P5 **Real-time decay of a highly excited charge carrier in the one-dimensional Holstein model**
Florian Dorfner (LMU Munich)

P6 **Matrix-product-state method with local basis optimization for bosonic systems out of equilibrium**
Christoph Brockt (Leibniz Universität Hannover)

P7 **A Strictly Single-Site DMRG Algorithm with Subspace Expansion**
Claudius Hubig (LMU München)

P8 **Fermionic quantum criticality in honeycomb and π-flux Hubbard models**
Francesco Parisen Toldin (University of Würzburg)

P9 **Cluster Techniques for Spin Systems**
Benjamin Lenz (Georg-August-Universität Göttingen)

P10 **Matrix product state formulation of frequency-space dynamics at finite temperatures**
Alexander Clemens Tiegel (Georg-August-Universität Göttingen)

P11 **Relaxation dynamics of a Fermi gas in an optical superlattice**
Ameneh Sheikhan Soudani (University of Bonn)

P12 **Partial Separability Revisited: Necessary and Sufficient Criteria**
Szilard Szalay (Wigner Research Centre for Physics Budapest)

P13 **Symmetry Breaking and the Geometry of Reduced Density Matrices**
Valentin Zauner (University of Vienna)

P14 **Dynamics of Heisenberg spin chains at finite temperatures using hardware-independent parallelization of matrix product state codes**
Thomas Köhler (Universität Göttingen)

P15 **Hybrid Monte Carlo simulations of graphene in external magnetic field**
Ulybyshev Maksim (Regensburg University)

P16 **Zero temperature dynamics of the Hubbard model in infinite dimensions: A local moment approach**
Himadri Barman (Tata Institute of Fundamental Research)

P17 **Collective density excitations in mass-symmetric and asymmetric dipolar bosonic bilayers**
Alexey Filinov (Institut für Theoretische Physik und Astrophysik, CAU Kiel)

P18 **Localization length and non-adiabaticity braiding errors in Majorana quantum wires**
Mikheil Sekania (Universität Augsburg)

P19 **Identifying a bath-induced Bose liquid in interacting spin-boson models**
Zi Cai (Institut für Quantenoptik und Quanteninformation, Österr. Akademie der Wissenschaften)

P1 **Advanced finite-temperature Lanczos method for anisotropic spin systems**
Jürgen Schnack (Bielefeld University)

It is virtually impossible to evaluate the magnetic properties of large anisotropic magnetic molecules numerically exactly due to the huge Hilbert space dimensions as well as due to the absence of symmetries. Here we propose to advance the finite-temperature Lanczos method (FTLM) to the case of single-ion anisotropy. The main obstacle, namely the loss of the spin rotational symmetry about the field axis, can be overcome by choosing symmetry related random vectors for the approximate evaluation of the partition function. We demonstrate that now thermodynamic functions for anisotropic magnetic molecules of unprecedented size can be evaluated.

P2 **Coulombic liquid phases of bosonic cluster Mott insulators on pyrochlore lattice**
Zi Yang Meng (Chinese Academy of Sciences)

Employing large-scale quantum Monte Carlo simulations, we reveal the full phase diagram of hard-core boson model on the pyrochlore lattice with fractional fillings, considering the boson hopping as well as repulsion between nearest neighbour sites. Due to the partial boson filling, the system is in a cluster Mott insulator (Coulombic liquid) phase with bosons localized inside the tetrahedral units of the pyrochlore lattice when the inter-site repulsion is dominant. We show that the full phase diagram contains three Coulombic liquid phases in the Mott regime at 1/4, 1/2 and 3/4 boson fillings, all of which are described by the emergent compact U(1) quantum electrodynamics (QED). Besides measuring the specific heat and entropy of the cluster Mott insulator phases, we further investigate the boson density-density correlation function and find it is consistent with the electric field correlation of the compact U(1) QED. Our results shed lights on magnetic properties of various pyrochlore systems as well as the charge physics of the cluster magnets.

P3 **Unusual vortex matter in rotating Bose-Einstein condensates with SU(2) broken symmetry**
Peder Galteland (Norwegian University of Science and Technology)

We consider a Ginzburg-Landau model of a rotating two-component Bose-Einstein condensate with SU(2) broken symmetry through the use of numerical Monte Carlo techniques. We include the full spectrum of thermal amplitude- and phase-fluctuations. The model exhibits an unusual state of global phase coherence with no accompanying vortex line lattice. This state has no counterpart in single-component condensates. The conditions for such a state are experimentally realizable in, e.g., homonuclear mixes of atomic gases in separate hyperfine states, tuned to the SU(2) point with Feshbach resonance techniques.

P4 **A dual-fermion analysis of the Anderson-Hubbard model**
Patrick Haase (Georg-August Universität Göttingen)

We apply the recently developed dual-fermion method for disordered interacting systems to the Anderson Hubbard model. This method treats both disorder and interactions on an equal footing, takes into account non-local correlations systematically, and thus represents a significant extension of the single-site mean-field description. We analyze the metal-insulator transition as well as the antiferromagnetic transition of the three-dimensional lattice, by looking at both one- and two-particle quantities, such as the local Green function and the conductivity.

P5 **Real-time decay of a highly excited charge carrier in the one-dimensional Holstein model**
Florian Dorfner (LMU Munich)

We study the real-time dynamics of a highly excited charge carrier coupled to quantum phonons via a Holstein-type electron-phonon coupling [1]. This is a prototypical example for the non-equilibrium dynamics in an interacting many-body system where excess energy is transferred from electronic to phononic degrees of freedom. We use an efficient numerical method, i.e., diagonalization in a limited functional space, to study the non-equilibrium dynamics on a finite one-dimensional chain. We perform a comprehensive analysis of the time evolution in different parameter regimes by calculating the electron, phonon and electron-phonon coupling energies, and the electronic momentum distribution function. For example, we demonstrate that in the weak coupling regime, the relaxation dynamics obtained from the Boltzmann equation agrees very well with the numerical data. We also study the time dependence of the eigenstates of the single-site reduced density matrix, the so-called optimal phonon modes, unveiling that their structure in non-equilibrium contains very useful information for the interpretation of the numerical data. Support from the DFG through FOR 1807 is gratefully acknowledged.

[1] Dorfner *et al.*, arXiv:1411.5074 (2014).

P6 **Matrix-product-state method with local basis optimization for bosonic systems out of equilibrium**

Christoph Brockt (Leibniz Universität Hannover)

We present a method for simulating the time evolution of quasi-one-dimensional correlated systems with bosonic degrees of freedom using matrix product states. Our goal is the accurate description of systems with large bosonic fluctuations for long periods of time. For this purpose we combine the time-evolving block decimation (TEBD) algorithm [1] with a local basis optimization approach which yields so-called optimal boson states [2]. We discuss the performance of this approach in comparison to TEBD with a bare boson basis, exact diagonalizations, and diagonalizations in a limited functional space. First, we test our method for the non-equilibrium dynamics of a Holstein polaron [3] and show that it allows us to study the regime of strong electron-phonon coupling. Second, the method is applied to the scattering and self-trapping of an electronic Gaussian wave packet travelling through a quantum wire with electron-phonon coupling.

[1] G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004).

[2] C. Zhang, E. Jeckelmann, and S.R. White, Phys. Rev. Lett. **80**, 2661 (1998).

[3] F. Dorfner *et al.*, arXiv:1411.5074.

P7 **A Strictly Single-Site DMRG Algorithm with Subspace Expansion**

Claudius Hubig (LMU München)

We introduce a strictly single-site DMRG algorithm based on the subspace expansion of the Alternating Minimal Energy (AMEn) method. The proposed new MPS basis enrichment method is sufficient to avoid local minima during the optimisation, similarly to the density matrix perturbation method, but computationally cheaper. Each application of the Hamiltonian to the variational state in the central eigensolver is reduced in cost for a speedup of approximately $(d+1)/2$, with d the physical site dimension. Further speedups result from cheaper auxiliary calculations and an often improved convergence rate per DMRG sweep. Runtime to convergence improves by up to a factor of 4 in the Fermi-Hubbard model. The method is compatible with real-space parallelisation and non-abelian symmetries.

P8 **Fermionic quantum criticality in honeycomb and π-flux Hubbard models**

Francesco Parisen Toldin (University of Würzburg)

We numerically investigate the critical behaviour of the Hubbard model on the honeycomb and the π-flux lattice, which exhibits a direct transition from a Dirac semimetal to an antiferromagnetically ordered Mott insulator. We use projective auxiliary-field quantum Monte Carlo simulations and a careful finite-size scaling analysis that exploits improved renormalization-group invariant observables. This approach, which is successfully verified for the 3D XY transition of the Kane-Mele-Hubbard model, allows us to extract estimates for the critical couplings and the critical exponents. The results confirm that the critical behaviour for the semimetal to Mott insulator transition in the Hubbard model belongs to the Gross-Neveu-Heisenberg universality class on both lattices.

[1] F. Parisen Toldin, M. Hohenadler, F. F. Assaad, I. F. Herbut, arXiv:1411.2502.

P9 **Cluster Techniques for Spin Systems**

Benjamin Lenz (Georg-August-Universität Göttingen)

Quantum cluster methods such as Cluster Perturbation Theory (CPT) or Variational Cluster Approximation (VCA) have been broadly applied to electron systems, but there are just very few applications to spin systems so far. Using Larkin's equations, a first order perturbation theory in cluster-cluster interactions can be constructed for spin systems and in a first attempt, dimerized Heisenberg chains have been addressed within CPT [1]. Here, we present CPT studies on Heisenberg zig-zag-ladders, which possess intriguing properties at high magnetic fields. When extending Potthoff's self-energy functional theory (SFT) to spin systems with non-local interactions one encounters severe problems [2]. However, lattices with local spin interactions like the Kondo lattice model can be treated. We explore the possibility to address superconductivity at finite doping in this model, motivated by findings for heavy fermion systems and dynamical mean-field theory (DMFT) [3].

[1] Ovchinnikov, Bostrem, and Sinitsyn, Theor. Math. Phys. **162**, 179 (2010).

[2] Filor and Pruschke, New J. Phys. **16**, 063059 (2014).

[3] Bodensiek, Zitko, Vojta, Jarrell, and Pruschke, Phys. Rev. Lett. **110**, 146406 (2013).

P10 **Matrix product state formulation of frequency-space dynamics at finite temperatures**
Alexander Clemens Tiegel (Georg-August-Universität Göttingen)

We present an approach to compute finite-temperature spectral functions of one-dimensional strongly correlated quantum systems [1]. The method is based on a purification of the finite-temperature density operator and works directly in the frequency domain by exploiting a Liouville space formulation of the dynamics. Our implementation is a Chebyshev expansion of the Green's function in a density-matrix renormalization group (DMRG) framework using matrix product states (MPS). We apply the method to study experimentally relevant spectral functions of one-dimensional quantum magnets.

[1] Tiegel *et al.*, Phys. Rev. B **90**, 060406(R) (2014).

P11 **Relaxation dynamics of a Fermi gas in an optical superlattice**
Ameneh Sheikhan Soudani (University of Bonn)

The question of how a closed quantum system out of equilibrium evolves and relaxes, is still not well understood. A specific setting of coherent quantum dynamics can be provided by quenches when one starts from the ground state of an initial Hamiltonian and suddenly changes the Hamiltonians parameters. After this change the system is highly excited with respect to the new Hamiltonian and evolves in time. Ultracold quantum gases in optical lattice are good candidates to study such non-equilibrium situations, since these gases are approximately isolated from their environment. Here we present an experimental and theoretical investigation of the time evolution of a Fermi gas following fast and slow quenches of a one-dimensional double-well superlattice potential. We probe both the local tunnelling in the double wells and the global dynamics towards a steady state. The local observables in the steady state resemble those of a thermal equilibrium state, whereas the global properties indicate a strong non-equilibrium situation. The experimental results are compared to the numerical studies based on the exact diagonalization of the Hamiltonian in the continuum considering the loading procedure of the three-dimensional Fermionic cloud into the one-dimensional optical superlattice and the measurement sequences.

P12 **Partial Separability Revisited: Necessary and Sufficient Criteria**
Szilard Szalay (Wigner Research Centre for Physics Budapest)

We extend the classification of mixed states of quantum systems composed of arbitrary numbers of subsystems of arbitrary dimensions [1]. This extended classification is complete in the sense of partial separability and gives $1+18+1$ partial separability classes in the tripartite case contrary to the formerly used $1+8+1$ [2,3]. Then we give necessary and sufficient criteria for these classes, which make it possible to determine to which class a mixed state belongs. These criteria are given by convex roof extensions of functions defined on pure states. These functions can be defined so as to be entanglement-monotones. In the special case of three-qubit systems [4], we define a different set of such functions with the help of the Freudenthal triple system approach of three-qubit entanglement [5].

[1] Sz. Szalay, Z. Kökényesi, Phys. Rev. A **86**, 032341 (2012).

[2] M. Seevinck and J. Uffink, Phys. Rev. A **78**, 032101 (2008).

[3] W. Dür and J. I. Cirac, Phys. Rev. A **61**, 042314 (2000).

[4] A. Acín, D. Bruß, M. Lewenstein, and A. Sanpera, Phys. Rev. Lett. **87**, 040401 (2001).

[5] L. Borsten, D. Dahanayake, M. J. Duff, W. Rubens, and H. Ebrahim, Phys. Rev. A **80**, 032326 (2009).

P13 **Symmetry Breaking and the Geometry of Reduced Density Matrices**
Valentin Zauner (University of Vienna)

The concept of symmetry breaking and the emergence of a local order parameter form the pillars of modern day quantum many body physics and of the theory of quantum phase transitions. We illustrate that the existence of symmetry breaking can be understood as a consequence of the geometry of the convex set of reduced density matrices of all possible many body wavefunctions. We show a three-dimensional projection of the convex set of the nearest neighbour reduced density matrices of all translational invariant states of a chain of qubits in the thermodynamic limit and see the emergence of ruled surfaces. Because extreme points of this set correspond to ground states of Hamiltonians with nearest neighbour interactions and because surfaces of equal energy are represented by planes, these ruled surfaces are defining signatures for the emergence of symmetry breaking and of an associated order parameter. We also show that similar pictures arise in the context of (1+1)-dimensional field theories and classical statistical physics, which we illustrate by drawing the corresponding convex sets for a Lieb-Liniger type model as well as for the classical 2D Ising model respectively.

P14 **Dynamics of Heisenberg spin chains at finite temperatures using hardware-independent parallelization of matrix product state codes**

Thomas Köhler (Universität Göttingen)

We compute dynamical spectral functions for Heisenberg systems at finite temperatures using matrix product state (MPS) approaches. This is achieved by parallelizing the time evolution on GPUs, and via a linear prediction ansatz on the time evolution results. The code is based on the linear algebra environment SciPAL [1] which implements expression templates for BLAS operations. Because SciPAL's expression templates are hardware-independent we can provide an objective comparison of the performance of CPU- or GPU-based computations and hybrid forms thereof.

[1] S. C. Kramer and J. Hagemann, ACM TOPC (accepted).

P15 **Hybrid Monte Carlo simulations of graphene in external magnetic field**

Ulybyshev Maksim (Regensburg University)

Recent experiments revealed that graphene turns into insulating phase in sufficiently strong external magnetic field perpendicular to graphene plane. Nevertheless, the precise nature of this phase remains unclear. Presumable candidates are spin-density and charge-density wave and Kekule distortion. We performed Hybrid Monte Carlo simulations of graphene in strong magnetic field to calculate order parameters corresponding to different types of insulating phases and to measure mass gap.

P16 **Zero temperature dynamics of the Hubbard model in infinite dimensions: A local moment approach**

Himadri Barman (Tata Institute of Fundamental Research)

The local moment approach (LMA) has presented itself as a powerful semi-analytical quantum impurity solver (QIS) in the context of the dynamical mean-field theory (DMFT) for the periodic Anderson model and it correctly captures the low energy Kondo scale for the single impurity model, having excellent agreement with the Bethe ansatz and numerical renormalization group results. However, the most common correlated lattice model, the Hubbard model, has not been explored well within the LMA+DMFT framework beyond the insulating phase. Here in our work, within the framework we attempt to complete the phase diagram of the single band Hubbard model at zero temperature. Our formalism is generic to any particle filling and can be extended to finite temperature. We contrast our results with another QIS, namely the iterated perturbation theory (IPT) and show that the second spectral moment sum-rule improves better as the Hubbard interaction strength grows stronger in LMA, whereas it severely breaks down after the Mott transition in IPT. We also show that, in the metallic phase, the low-energy scaling of the spectral density leads to universality which extends to infinite frequency range at infinite correlation strength (strong-coupling). At large interaction strength, the off half-filling spectral density forms a pseudogap near the Fermi level and filling-controlled Mott transition occurs as one approaches the half-filling. Finally we study optical properties and find universal features such as absorption peak position governed by the low-energy scale and a doping independent crossing point, often dubbed as the isosbestic point in experiments. This has been published in arXiv:1412.4434.

P17 **Collective density excitations in mass-symmetric and asymmetric dipolar bosonic bilayers**

Alexey Filinov (Institut für Theoretische Physik und Astrophysik, CAU Kiel)

We consider a two-component 2D dipolar bosonic system in the bilayer geometry. The system is translationally invariant in the plane (no optical lattice). By performing quantum Monte Carlo simulations [1] we analyze in detail static distribution functions, kinetic and interaction energies as a function of the interlayer distance. By reducing the layer distance and a continuous increase of the interlayer coupling we, finally, observe formation of the dimer states. This transition is accompanied by pronounced changes in the static properties, the off-diagonal (quasi)long-range order (superfluid response), as well as in the spectrum of collective density modes. The diagonal and off-diagonal components of the dynamic structure factor are reconstructed from the imaginary time density response functions via the stochastic optimization method [1]. The excitation spectrum undergoes a gradual transition between three regimes: i) for large layer separations two independent single layer spectra, ii) for intermediate distances a strongly hybridized spectrum with two characteristic in-phase and out-of-phase modes, iii) single-layer-like spectrum of quasiparticles (double mass and dipole moment) when a strongly bound dimer states are formed. The dispersion law for the in-phase and out-of-phase collective modes during this crossover is studied in detail and compared with the predictions based on the sum rules formalism [2]. We repeat our analysis for mass-asymmetric bilayers and observe some additional effects which are peculiar for mixtures of light and heavy bosonic species.

[1] A. Filinov and M. Bonitz, Phys. Rev. A **86**, 043628 (2012)

[2] K. I. Golden, G. J. Kalman, Phys. Rev. E **88**, 033107 (2013).

P18 **Localization length and non-adiabaticity braiding errors in Majorana quantum wires**
Mikheil Sekania (Universität Augsburg)

Majorana fermions have been attracting substantial interest in recent years. Several experimental groups have already reported tentative observation of Majorana zero modes in quantum nanowires that are proximity-coupled to a bulk superconductor. The unambiguous detection of Majorana quasi-particles, however, has so far remained elusive. One of the ultimate experimental checks for the existence of Majorana zero modes would be a braiding experiment, that reveals the non-trivial braiding statistics of the Majorana fermions. We present numerical studies of the braiding of Majorana bound states (MBS) in presence of a quasi-particle background, and show braiding errors due to non-adiabaticity - which is a realistic scenario for experiments - and due to system sizes which are comparable to the localization length of the MBS. The latter seems to be the case for certain experimental realizations reported recently. We further address the influence of finite-range interactions on the braiding process.

P19 **Identifying a bath-induced Bose liquid in interacting spin-boson models**
Zi Cai (Institut für Quantenoptik und Quanteninformation, Österr. Akademie der Wissenschaften)

We study the ground state phase diagram of a one-dimensional hard-core bosonic model with nearest-neighbour interactions (XXZ model) where every site is coupled Ohmically to an independent but identical reservoir, hereby generalizing spin-boson models to interacting spin-boson systems. We show that a bath-induced Bose metal phase can occur in the ground state phase diagram away from half filling. This phase is compressible, gapless, and conducting but not superfluid. At haf-filling, only a Luttinger liquid and a charge density wave are found. The phase transition between them is of Kosterlitz-Thouless type where the Luttinger parameter takes a non-universal value. The applied quantum Monte Carlo method can be used for all open bosonic and non-frustrated spin systems, regardless of their dimension, filling factor and spectrum of the dissipation as long as the quantum system couples to the bath via the density operators.

Tuesday Sessions at a Glance

Tuesday 1 — Chair: U. Schollwöck

09:00–09:40	**TBA**
O2	*Anatoli Polkonikov (Boston University)*
09:40–10:10	**Detecting topological orders in quantum matter**
I6	*Frank Pollmann (Max-Planck-Institut für Physik komplexer Systeme)*
10:10–10:30	**Light induced magnetisation in an $S = 1$ antiferromagnet**
C5	*Xenophon Zotos (University of Crete)*

Tuesday 2 — Chair: R. Noack

11:00–11:30	**Uncovering the Fibonacci Phase in Z3 Parafermion Systems with DMRG**
I7	*Miles Stoudenmire (Perimeter Institute)*
11:30–12:00	**TBA**
I8	*Garnet Chan (Princeton University)*
12:00–12:20	**Optimal Persistent Currents for Interacting Bosons on a Ring with a Gauge Field**
C6	*Matteo Rizzi (University of Mainz)*

Tuesday 3 — Chair: M. Ulybyshev

14:00–14:30	**An Exotic Quantum Phase Transition with Staggered Dirac Fermions**
I9	*Shailesh Chandrasekharan (Duke University)*
14:30-15:00	**Lattice Monte Carlo for carbon nanostructures**
I10	*Timo Lähde (Forschungszentrum Jülich)*
15:00–15:20	**Superphenomena in solid Helium-4**
C7	*Lode Pollet (LMU Munich)*

Tuesday 4 — Chair: F. Parisen Toldin

16:00–16:30	**The metal-insulator transition for two-dimensional interacting Dirac electrons**
I11	*Sandro Sorella (SISSA)*
16:30-17:00	**Dimensionless ratios for SU(N) symmetric Hubbard models and their critical points**
I12	*Thomas C. Lang (University of Würzburg)*
17:00–17:20	**Anomalous transport phenomena in lattice field theory**
C8	*Pavel Buividovich (University of Regensburg)*

Poster II — Chair: M. Hohenadler

17:20–19:30	**Oral poster presentation (one minute per poster), followed by Poster Session II**

09:00–09:40 **TBA**
O2 *Anatoli Polkonikov (Boston University)*

09:40–10:10 **Detecting topological orders in quantum matter**
I6 *Frank Pollmann (Max-Planck-Institut für Physik komplexer Systeme)*

Matter occurs in various phases that are usually characterized in terms of symmetry breaking. A major discovery in the 1980s were the quantum Hall effects which exhibit a new kind of "topological" order. This order represents a class of exotic phases which cannot be described by spontaneous symmetry breaking. The lack of symmetry breaking order parameters makes it difficult to characterize these phases. In this talk, I will show that numerical investigations of a many-body wavefunction can yield a remarkably complete characterization of different types of topological orders. A central tool is the ground state entanglement which encodes many of the essential features. First, I will show how characteristic properties of the topological excitations in spin liquids and fractional quantum Hall states can be extracted directly from the ground state wave functions. Second, I will consider symmetry protected topological phases in one-dimensional systems for which a complete classification can be derived from the entanglement.

10:10–10:30 **Light induced magnetisation in an $S = 1$ antiferromagnet**
C5 *Xenophon Zotos (University of Crete)*

We present a study of circularly polarised light induced magnetisation in the spin S=1 easy plane antiferromagnetic chain DTN. The thermodynamic and dynamic properties of this compound are well understood as they have been extensively studied experimentally as well as theoretically [1,2]. We will present extensive numerical simulation results on the model describing DTN. Furthermore, we will use an effective 2-level system, to understand the main features of the time evolution of the system and propose the most appropriate protocol to optimally induce a magnetisation.

[1] C. Psaroudaki, S. A. Zvyagin, J. Krzystek, A. Paduan-Filho, X. Zotos, and N. Papanicolaou, Phys. Rev. B **85**, 014412 (2012).

[2] C. Psaroudaki, J. Herbrych, J. Karadamoglou, P. Prelovsek, X. Zotos, and N. Papanicolaou, Phys. Rev. B **89**, 224418 (2014).

11:00–11:30 **Uncovering the Fibonacci Phase in Z3 Parafermion Systems with DMRG**
I7 *Miles Stoudenmire (Perimeter Institute)*

Recently there has been great progress in realizing platforms for topological quantum computation, with mounting evidence of the experimental observation of Ising anyons (Majorana zero modes). However, Ising anyons do not have sufficiently rich braiding statistics to perform universal, fault tolerant computation. One way forward is to engineer systems realizing Z3 parafermion zero modes, which generalize Majorana zero modes. Hybridizing Z3 parafermions could yield a phase with bulk Fibonacci anyons, a type of non-Abelian anyon that has universal braiding statistics.

Using the density matrix renormalization group (DMRG), we study a two-dimensional model of coupled Z3 parafermions. By working close to the weakly-coupled chain limit, we are able to identify the Fibonacci phase on cylinders as small as four sites in circumference, then track its evolution, finding it survives even to the isotropic limit of our model on larger cylinders. We examine the extent of this phase and the fuller phase diagram of our model, which turns out to harbour a second topological phase.

11:30–12:00 **TBA**
I8 *Garnet Chan (Princeton University)*

12:00–12:20 **Optimal Persistent Currents for Interacting Bosons on a Ring with a Gauge Field**
C6 *Matteo Rizzi (University of Mainz)*

We study persistent currents for interacting 1D bosons on a tight ring trap, subjected to a rotating barrier potential, which induces an artificial U(1) gauge field. By combining analytical as well as numerical techniques suited for the different regimes of the 1D problem, we show that the current amplitude is a non-monotonous function of the interaction strength and displays a pronounced maximum in all regimes of barrier height. The presence of an optimal regime illustrates the highly non-trivial combination of correlations, quantum fluctuations and barrier effects. Our results demonstrate that, in a large range of interaction strengths, unwanted impurities or imperfections on the ring affect only weakly the system properties. For the application to quantum state manipulation, the regimes of choice should be either very weak or very strong interactions, where the response to a localized external probe is stronger. Our predictions are readily amenable to experimental testing with quasi-1D ultracold atomic gases confined in mesoscopic uniform and lattice rings.

[1] M. Cominotti, D. Rossini, M. Rizzi, F. Hekking, and A. Minguzzi, Phys. Rev. Lett. **113**, 025301 (2014).

14:00–14:30 **An Exotic Quantum Phase Transition with Staggered Dirac Fermions**
I9 *Shailesh Chandrasekharan (Duke University)*

Using the fermion bag approach, we study a simple lattice field theory model with two flavors of staggered Dirac fermions with a four-fermion coupling. In three dimensions we show evidence that the model contains a single exotic quantum phase transition between a massless and a massive fermion phase where fermion bilinear condensates vanish on both sides. There is no local order parameter that distinguishes the two phases. We suggest that the transition is the same as the one recently proposed in a bilayer system of fermions on a honeycomb lattice.

14:30-15:00 **Lattice Monte Carlo for carbon nanostructures**
I10 *Timo Lähde (Forschungszentrum Jülich)*

I will discuss how Lattice Monte Carlo simulations can be applied to graphene and other carbon nanostructures in order to compute the properties of strongly correlated electrons in such systems. I will focus on the Dirac and tight-binding theories of the graphene monolayer, and discuss preliminary results from the latter for graphene bilayers and carbon nanotubes.

15:00–15:20 **Superphenomena in solid Helium-4**
C7 *Lode Pollet (LMU Munich)*

The ground state of Helium-4 confined in a system with the topology of a cylinder can display properties of a solid, superfluid and liquid crystal. This phase, which we call compactified supersolid (CSS), originates from wrapping the basal planes of the bulk hcp solid into concentric cylindrical shells, with several central shells exhibiting superfluidity along the axial direction. Its main feature is the presence of a topological defect which can be viewed as a disclination with Frank index n=1 observed in liquid crystals, and which, in addition, has a superfluid core. The CSS as well as its transition to an insulating compactified solid with a very wide hysteresis loop are found by ab initio Monte Carlo simulations. We also review experimental evidence for mass supertransport, anomalous isochoric compressibility (syringe effect), and giant plasticity in bulk Helium-4, and argue the quantum nature of these effects.

16:00–16:30 **The metal-insulator transition for two-dimensional interacting Dirac electrons**
I11 *Sandro Sorella (SISSA)*

In this study we extend our previous work [1] by considering electrons with massless Dirac-like dispersion on several two-dimensional lattices, and perform numerically exact calculations on unprecedentedly large systems, allowing us to explore the quantum critical behaviour in the vicinity of the interaction-driven metal-insulator transition. We find thereby that the transition is continuous and determine the quantum criticality for the corresponding universality class, which is described in the continuous limit by the Gross-Neveu model, a model extensively studied in quantum field theory. We furthermore establish a highly non-trivial fluctuation-driven scenario for the Mott metal-insulator transition in the Dirac fermions, by showing that it is triggered only by the vanishing of the quasiparticle weight and not by the Dirac Fermi velocity, which instead remains finite across the transition. This is in sharp contrast with simple mean-field or Gutzwiller-type approximate pictures where both quasiparticle weight and Dirac velocity vanish at the transition.

[1] S. Sorella, Y. Otsuka and S. Yunoki, Sci. Rep. **2**, 992 (2012).

16:30-17:00 **Dimensionless ratios for SU(N) symmetric Hubbard models and their critical points**
I12 *Thomas C. Lang (University of Würzburg)*

Using unbiased quantum Monte Carlo simulations we investigate the quantum phase transitions in SU(N) Hubbard models on square and honeycomb lattices. We construct and measure dimensionless fermionic correlation and order parameter ratios, which provide precise and independent estimates for the couplings at which a mass gap opens in the single particle spectrum and at which the order sets in. Furthermore these correlation ratios prove to be highly sensitive to weak order and render the need of pinning fields unnecessary. In particular, we study the nature and location of the phase transition between the semi-metal and Mott insulating antiferromagnetic state in the SU(2) Hubbard model on the honeycomb as well as the potentially deconfined Neel to valence bond solid phase transition in the SU(6) Hubbard model on the square lattice.

17:00–17:20 **Anomalous transport phenomena in lattice field theory**
C8 *Pavel Buividovich (University of Regensburg)*

We consider the implementation of the non-dissipative anomaly-driven quantum transport phenomena, such as the Chiral Magnetic and the Chiral Separation effects, in lattice quantum field theories which are relevant both for the description of Weyl semimetals and for lattice QCD simulations. We discuss the disagreement between anomalous transport coefficients obtained from the consistent lattice regularization and from the continuum kinetic theory, which has important effect on the dispersion relation of collective excitations in the plasma of chiral fermions. We also demonstrate that repulsive interactions strongly enhance anomalous transport coefficients, at least at the mean-field level. We also introduce the lattice Dirac operators at finite chiral density and demonstrate that they are free of the fermionic sign problem, regardless of whether the chiral symmetry is preserved on the lattice by virtue of the Ginsparg-Wilson relations. Finally, we point out that tight-binding models of parity-breaking Weyl semimetals can be efficiently simulated using the Rational Hybrid Monte-Carlo algorithm. On the other hand, simulations of time-reversal breaking Weyl semimetals are hindered by the fermionic sign problem. anomalies, such as the Chiral Magnetic and the Chiral Separation effects, in lattice field theories.

P20 **The spin-1 kagome Heisenberg antiferromagnet: an SU(2) PEPS study**
Wei Li (LMU Munich)

P21 **Truncating an exact Matrix Product State for the XY model: correlations and the transfer matrix**
Marek Rams (Jagiellonian University)

P22 **Coherence-incoherence crossover in Hund's metals – Insights into the normal state of iron pnictide superconductors from a Numerical Renormalization Group study**
Katharina Stadler (LMU München)

P23 **Combining Projector Quantum Monte Carlo with Tensor Network methods**
Brecht Verstichel (Ghent University)

P24 **Berezinskii-Kosterlitz-Thouless phase transition of spin-orbit coupled Fermi gas in optical lattice**
Tang Ho Kin (National University of Singapore)

P25 **Composite boson mean field for strongly correlated systems**
Daniel Huerga (Universitï Stuttgart)

P26 **SYMETTS - Symmetric Minimally Entangled Typical Thermal States**
Benedikt Bruognolo (LMU Munich)

P27 **Calculating Conserved Currents and Fermionic Force for the Lanczos Approximation to the Overlap Dirac Operator**
Matthias Puhr (Universität Regensburg)

P28 **Towards a Matrix Product State based description of steady-state non-equilibrium physics in 1D correlated quantum systems using Lindblad driving**
Frauke Schwarz (Ludwig-Maximilians-Universität München)

P29 **Measurement-driven dynamics of large quantum spin systems**
Hebenstreit Florian (Bern)

P30 **An integrability-based class of non-orthogonal geminal wavefunctions for the description of strongly-correlated systems**
Pieter Claeys (Ghent University)

P31 **Effective spin models for edge magnetism in graphene zigzag ribbons**
Cornelie Koop (RWTH Aachen)

P32 **Spin and charge dynamics of a quasi-one-dimensional antiferromagnetic metal**
Marcin Raczkowski (LMU Munich)

P33 **Linear to zigzag transition in dipolar chains**
Florian Cartarius (Universität des Saarlandes)

P34 **Quantum Monte Carlo Study of Long-Range Transverse-Field Ising Models on the Triangular Lattice**
Stephan Humeniuk (Universität Stuttgart)

P35 **Localized excitations on top of a PEPS ground state**
Laurens Vanderstraeten (University of Ghent)

P36 **Extended density-density interactions in auxiliary field QMC**
Michael Golor (RWTH Aachen University)

P37 **Néel transition temperatures for the Hubbard model on layered honeycomb lattice**
Jakub Imriska (ETH Zurich)

P38 **Strongly Correlated Phases and Ferromagnetic Phases of Fermions in an Optical Flux Lattice Model**
Simon Davenport (University of Cambridge)

P20 **The spin-1 kagome Heisenberg antiferromagnet: an SU(2) PEPS study**
Wei Li (LMU Munich)

We have implemented non-abelian symmetries in the projected entangled-pair state (PEPS) and its related tensor network algorithms, in an uniform, transparent, and practical framework called QSpace. By exploiting the symmetries, i.e., keeping track of symmetry multiplets instead of individual state on each bond of the tensor, we achieve great numerical gain (both in time and memory), and are thus able to explore larger bond dimensions than before. As an illustrative (nontrivial) application, we apply our SU(2) PEPS code to study the spin-1 kagome Heisenberg antiferromagnetic (KHAF) model. We show that the hexagon-singlet solid state, a trial wavefunction of the spin-1 KHAF model, has a compact SU(2)-invariant PEPS representation [with only two multiplets $(0+1)$ on each bond, i.e., a bond dimension of $D=4$], and the variational energy can be determined very accurately ($e_0=-1.3599$) through SU(2) iPEPS contractions. Furthermore, we enlarge the bond dimension to include more multiplets on the bonds, optimizing the PEPS with imaginary-time evolution, and reveal that the ground state of spin-1 KHAF model is an inversion-symmetry-breaking state with a simplex valence bond crystal order; the ground state energy estimate is as low as $e_0=-1.41035$, obtained by retaining seven multiplets on each bond ($D=20$).

P21 **Truncating an exact Matrix Product State for the XY model: correlations and the transfer matrix**
Marek Rams (Jagiellonian University)

We discuss how to analytically obtain an – essentially infinite – Matrix Product State (MPS) representation of the ground state of the XY model. On the one hand this allows to illustrate how the algebraic part of the correlation function emerges in the exact case using standard MPS language. On the other hand we study the consequences of truncating the bond dimension of the exact MPS which is also part of many tensor network algorithms and we focus on how well the truncated MPS transfer matrix reproduces the dominant part of the exact quantum transfer matrix. In the gapped phase we observe that the correlation length obtained from a truncated MPS approaches the exact value following a power law in effective bond dimension. In the gapless phase we find a good match between a state obtained numerically from standard MPS techniques with finite bond dimension, and a state obtained by effective finite imaginary time evolution in our framework. This provides a direct hint for a geometric interpretation of Finite Entanglement Scaling at the critical point.

[1] M. M. Rams, V. Zauner, J. Haegeman, F. Verstraete, arXiv:1411.2607.

P22 **Coherence-incoherence crossover in Hund's metals – Insights into the normal state of iron pnictide superconductors from a Numerical Renormalization Group study**
Katharina Stadler (LMU München)

In 2008, the iron pnictides were discovered as a new class of strongly correlated high-temperature superconductors [Takahashi *et al.*, Nature **453** (2008)]. The normal state of these itinerant multi-band materials shows characteristic anomalous properties, which are assigned to a coherence-incoherence crossover at very low temperatures, mediated by Hund's rule coupling. We study a N-channel Anderson impurity model with Hund's coupling and a filling of N-1, together with the corresponding Kondo model, for the cases N=2 and 3, using the full density-matrix Numerical Renormalization Group (fdmNRG) with non-abelian symmetries [A. Weichselbaum, Ann. Phys. **327** (2012)]. Our high-quality real-frequency NRG results confirm the existence of a Fermi-liquid regime at low temperatures and a crossover to an incoherent normal state. Further, we analyse the interplay of spin and orbital degrees of freedom to gain insights into the relevant energy scales of the coherence-incoherence crossover and the corresponding renormalization group flow. In addition the lattice model is investigated within DMFT employing fdmNRG as impurity solver.

P23 **Combining Projector Quantum Monte Carlo with Tensor Network methods**
Brecht Verstichel (Ghent University)

We discuss a combination of tensor network state (TNS) techniques and projector quantum Monte Carlo (QMC) to overcome both the high computational scaling of TNS and the sign problem in QMC. As a first example, we describe the performance of phaseless auxiliary field quantum Monte Carlo with matrix product states (MPS-AFQMC). MPS-AFQMC improves significantly on the variational MPS ground-state energy, at a computational cost which scales only quadratically in the MPS bond dimension. We show results of our technique on the J_1-J_2 Heisenberg model, observing for all couplings an order of magnitude reduction of the error compared to the variational MPS energy. A second application focusses on the combination of Green's Function Monte-Carlo (GFMC) with projected entangled pair states (PEPS). We prove the feasibility of the approach by obtaining exact results for the sign-problem free 2D Heisenberg model for lattice sizes up to 20×20, using a variationally optimized PEPS as a trial wave function.

P24 **Berezinskii-Kosterlitz-Thouless phase transition of spin-orbit coupled Fermi gas in optical lattice**

Tang Ho Kin (National University of Singapore)

We extend the use of determinant quantum Monte Carlo simulation to study the Rashba spin-orbit coupled Fermi gases in square optical lattice. Notably, we show that the Berezinskii-Kosterlitz-Thouless phase transition temperature can be enhanced by the spin-orbit coupling. Using DQMC, we also study the pairing mechanism by obtaining pairing susceptibility and spin susceptibility.

P25 **Composite boson mean field for strongly correlated systems**

Daniel Huerga (Universitï Stuttgart)

We present a method applicable to spin and bosonic model Hamiltonians of strongly correlated systems. The method is based on the identification of clusters of the original spin and/or bosonic degrees of freedom as the building blocks which capture the essential quantum correlations to describe the phases emerging in the model. We present a canonical mapping which relates the original spin and bosonic operators to a new set of composite boson operators that describe the quantum states of the cluster. As the mapping is canonical, we can rewrite the original Hamiltonian in terms of the new set of composite boson operators and approach it by standard many-body techniques, with the advantage that short-range correlations are computed exactly from the onset. A simple Gutzwiller wave function of CBs allows us to uncover the phase diagram of two-dimensional frustrated models such as a model of spins with ring-exchange interaction or a system of bosons in the presence of artificial magnetic fields. A Bogoliubov approach to the CB quantum fluctuations allows us to accurately describe the recently measured Higgs and Goldstone excitation modes of a system of cold atoms loaded in a two-dimensional optical lattice. The algebraic framework set by the mapping may allow for further extensions of the method.

P26 **SYMETTS - Symmetric Minimally Entangled Typical Thermal States**

Benedikt Bruognolo (LMU Munich)

The Density Matrix Renormalization Group is the most powerful exact numerical method for describing 1-dimensional (1D) quantum many-body systems regarding their static ground-state, dynamic, as well as thermodynamic properties. However, its efficiency is compromised when used to study low but finite temperature properties. A recently proposed method based on sampling small ensembles of so-called Minimally Entangled Typical Thermal States (METTS) promises to overcome this restriction. However, this approach suffers from a severe constraint: the ensemble states cannot be efficiently chosen such that they conserve inherent symmetries of the system. With SYMETTS, we propose an intuitive extension that allows using a symmetry-conserving METTS sample and provide proof-of-principle calculations for a Heisenberg spin-chain. We expect that this work will allow the finite temperature treatment of significantly more complex 1D systems than hitherto possible, with possible extensions to 2D lattice simulations for fermions or frustrated spin systems.

P27 **Calculating Conserved Currents and Fermionic Force for the Lanczos Approximation to the Overlap Dirac Operator**

Matthias Puhr (Universität Regensburg)

The overlap Dirac operator obeys the Ginsparg-Wilson equation and offers a possibility to introduce chiral symmetry on the lattice. Evaluating the overlap operator is numerically very expensive and one has to rely on approximation methods. At finite chemical potential the overlap operator can be efficiently computed with the two-sided Lanczos algorithm. To calculate conserved currents on the lattice, or to evaluate the fermionic force in HMC calculations, one needs to compute derivatives of the Dirac operator. We present a method to simultaneously compute the action of the overlap operator and its derivative on a source vector.

P28 **Towards a Matrix Product State based description of steady-state non-equilibrium physics in 1D correlated quantum systems using Lindblad driving**

Frauke Schwarz (Ludwig-Maximilians-Universität München)

The Kondo effect in quantum impurity models in equilibrium is well-understood by means of the Numerical Renormalization Group (NRG). To extend the description of Kondo physics to situations of steady state non-equilibrium, we want to combine the ideas of NRG with the Lindblad approach to open quantum systems. For this purpose, we introduce additional reservoirs described by Lindblad terms in the Liouville equation which restore the continuum properties of the discretized leads that are coupled to the impurity. This enables us to define the temperature and the chemical potential for each lead independently. To reduce the dimensionality of the problem we employ the stochastic quantum trajectory approach to solve the underlying Lindblad equation. Several ideas on how to define adequate Lindblad operators will be

presented together with their implications for the calculation of the quantum trajectories based on Matrix Product States.

P29 **Measurement-driven dynamics of large quantum spin systems**
Hebenstreit Florian (Bern)

We study the real-time evolution of large quantum spin systems in two spatial dimensions, whose dynamics is entirely driven by a dissipative coupling to the environment. We consider different measurement processes of spin pairs and investigate the dynamics from an ordered phase at initial times towards a disordered phase at late times. The corresponding Kossakowski-Lindblad equation is solved via an efficient cluster algorithm for different spin models (Heisenberg model, XY-model). We find that the symmetry of the measurement process determines the time scales which govern the approach towards a new equilibrium phase at late times. Most notably, we find an exponentially slow equilibration if the dissipative coupling conserves any of the magnetization Fourier modes. In these cases, the dynamics can be interpreted as a diffusion process of the quantum spins.

P30 **An integrability-based class of non-orthogonal geminal wavefunctions for the description of strongly-correlated systems**
Pieter Claeys (Ghent University)

Integrable systems take a special place within the theory of quantum many-body systems, having been used to describe a wide variety of physical phenomena. Due to the underlying algebraic structure, all correlations can be captured exactly within a Bethe Ansatz wavefunction at a fraction of the usual computational cost. Unfortunately, the demands for integrability are quite stringent, allowing only for an exact description of a limited number of Hamiltonians. However, the structure of the eigenstates of these systems can also be used as a starting point for the description of nonintegrable systems, either from a variational or a projected point of view. This method has been proposed in quantum chemistry starting from a so-called XXX RG model, leading to a novel family of non-orthogonal geminal wavefunctions capable of describing strongly-correlated atoms and molecules at a cost that scales polynomially (instead of exponentially) with system size. Here we propose an extension of this method starting from the class of more general XXZ Richardson-Gaudin systems.

P31 **Effective spin models for edge magnetism in graphene zigzag ribbons**
Cornelie Koop (RWTH Aachen)

We consider the effective magnetic interactions among edge states in zigzag graphene-based nanoribbons. To leading order, there has previously been shown to emerge a direct ferromagnetic intra-edge coupling and an antiferromagnetic coupling between opposite edges. We study the electronic system by an effective model, yielding a separation between edge and bulk states, and systematically investigate bulk-state corrections within a Schrieffer-Wolff transformation. Using both numerical and analytical methods, fermionic and spin correlation functions are calculated. We show that the reduction to pure edge-state models is well justified for a wide range of general ribbon geometries. Our framework enables a systematic exploration of electronic correlation physics in graphene-based nano-structures beyond the often-employed mean-field approximation on realistically large system sizes.

P32 **Spin and charge dynamics of a quasi-one-dimensional antiferromagnetic metal**
Marcin Raczkowski (LMU Munich)

We use quantum Monte Carlo simulations to study a finite-temperature dimensional-crossover-driven evolution of spin and charge dynamics in weakly coupled Hubbard chains with a half-filled band. The low-temperature behaviour of the charge gap indicates a crossover between two distinct energy scales: high-energy one-dimensional (1D) Mott gap due to umklapp process and a low-energy gap which stems from long-range antiferromagnetic (AF) spin fluctuations. Away from the 1D regime and at temperature scales above the charge gap, the emergence of zero-frequency Drude-like feature in the interchain optical conductivity implies the onset of a higher-dimensional metal. In this metallic phase, enhanced quasiparticle scattering off finite-range AF spin fluctuations results in incoherent single-particle dynamics. The coupling between spin and charge fluctuations is also seen in the spin dynamical structure factor displaying damped spin excitations (paramagnons) close to the AF wave-vector and particle-hole continua near 1D momentum transfers spanning quasiparticles at the Fermi surface. We furthermore compare the results for the single-particle spectral function with the ones obtained within a cluster extension of the dynamical mean-field theory. Finally, we discuss the relationship of our results to the charge deconfinement in quasi-1D organic Bechgaard-Fabre salts.

P33 **Linear to zigzag transition in dipolar chains**
Florian Cartarius (Universität des Saarlandes)

In very anisotropic confinement cold dipolar particles can arrange in linear chains. By relaxing the transverse confinement these chains split into a zigzag structure. We consider a chain of dipolar bosons superimposed by an optical lattice, where the particles can tunnel from one site to the next. In deep optical lattices the coupling to the axial phonons can be neglected and it is possible to describe the behaviour of the system by two coupled extended Bose-Hubbard Hamiltonians close to the transition [1]. We present the solution of this model using a path integral Monte Carlo method.

[1] P. Silvi, T. Calarco, G. Morigi, and S. Montangero, Phys. Rev. B **89**, 094103 (2014).

P34 **Quantum Monte Carlo Study of Long-Range Transverse-Field Ising Models on the Triangular Lattice**

Stephan Humeniuk (Universität Stuttgart)

Motivated by recent experiments with a Penning ion trap quantum simulator, we perform Stochastic Series Expansion quantum Monte Carlo simulations of long-range transverse-field Ising models on a triangular lattice for different decay powers α of the interactions. The phase boundary for the ferromagnet is obtained as a function of α. For antiferromagnetic interactions we find that the transverse field stabilizes a clock ordered phase with sublattice magnetization $(M, -\frac{M}{2}, -\frac{M}{2})$ with $M \approx 1$ in a process known as "order by disorder" similar to the nearest neighbour antiferromagnet on the triangular lattice. Connecting the known limiting cases of nearest neighbour and infinite-range interactions, we obtain a semiquantitative phase diagram. In the appendix we give magnetization curves for the ferromagnet for experimentally relevant system sizes and with open boundary conditions.

P35 **Localized excitations on top of a PEPS ground state**

Laurens Vanderstraeten (University of Ghent)

Starting from a PEPS ground state of a gapped two-dimensional quantum spin system, we present a variational ansatz for capturing the elementary excitations. Our variational method is applied to frustration-free Hamiltonians with a PEPS as an exact ground state. We have calculated both the magnon dispersion relation of the 2D AKLT model on a square lattice and the spectrum of the toric code with local filtering.

P36 **Extended density-density interactions in auxiliary field QMC**

Michael Golor (RWTH Aachen University)

In quantum Monte Carlo simulations, the fermionic sign problem poses a major obstacle and essentially restricts the class of accessible problems. We explain how Hubbard-like models with extended interactions can be simulated efficiently and sign-problem-free, allowing to study the interplay of competing interactions at least to a certain extent. We discuss applications to the honeycomb lattice and the square lattice bilayer.

P37 **Néel transition temperatures for the Hubbard model on layered honeycomb lattice**

Jakub Imriska (ETH Zurich)

We study the Hubbard model on a layered honeycomb lattice for different interlayer couplings and interaction strengths. We provide estimates of the Néel transition temperature based on the dynamical cluster approximation. The lattice susceptibility is obtained based on the approximation of the irreducible lattice vertex by the irreducible cluster impurity vertex. The approach leads to consistent results with the direct measurement of the order parameter when allowing for the symmetry breaking.

P38 **Strongly Correlated Phases and Ferromagnetic Phases of Fermions in an Optical Flux Lattice Model**

Simon Davenport (University of Cambridge)

We study a theoretical model of a 2-dimensional ultracold atomic gas subject to an "optical flux lattice": a particular laser configuration where Raman-dressed atoms experience a strong effective magnetic field, which can lead to a bandstructure of narrow energy bands with non-zero Chern numbers. In this optical flux lattice we place spin-$1/2$ fermions that interact via a Feshbach-resonance induced contact interaction, coupling spin-up and spin-down particles. Atoms restricted to the lowest band are described by an effective model of spinless fermions with a tunable interaction coupling states in a momentum-dependent manner across the Brillouin zone. This non-local interaction is due to the Raman coupling between spin-up and spin-down levels. We present a summary of results from a detailed exact diagonalization study of the effective lowest band model. In particular we offer evidence indicating the presence of strongly correlated phases and ferromagnetic phases.

Wednesday Sessions at a Glance

Wednesday 1 — Chair: A. Honecker

09:00–09:40 **O3**	**BCS regime of the two-dimensional fermionic Hubbard model: ground-state phase diagram** *Nikolai Prokof'ev (University of Massachusetts)*
09:40–10:10 **F3**	**Tensor network algorithms for 2D strongly correlated lattice systems** *Juan Osorio (ETH Zurich)*
10:10–10:30 **C9**	**Diagrammatic methods for lattice gauge theories with staggered fermions** *Hélvio Vairinhos (ETH Zurich)*

Wednesday 2 — Chair: M. Hohenadler

11:00–11:30 **I13**	**Exact diagonalization for topological phases driven by interaction** *Maria Daghofer (University of Stuttgart)*
11:30–12:00 **I14**	**Matrix product state formulation of frequency-space dynamics at finite temperatures** *Salvatore Manmana (University of Göttingen)*
12:00–12:20 **C10**	**Phase diagram of repulsive spinless fermions on the honeycomb lattice** *Sylvain Capponi (Université Paul Sabatier Toulouse)*

Wednesday 3 — Chair: Z. Meng

14:00–14:30 **F4**	**MPS based quantum impurity solvers** *F. Alexander Wolf (LMU Munich)*
14:30-15:00 **F5**	**Entanglement Structure of the Hubbard Model in Momentum Space** *Georg Ehlers (University of Marburg)*
15:00–15:20 **C11**	**Geometric stability of topological lattice phases** *Gunnar Möller (University of Cambridge)*

Wednesday 4 — Chair: Z. Meng

16:00–16:20 **C12**	**A generalized perspective on non-perturbative linked cluster expansions** *Kai P. Schmidt (TU Dortmund)*
16:20–16:40 **C13**	**Entanglement Entropy for Many-Fermion Systems** *Peter Bröcker (University of Cologne)*

Social program

17:30	**Meet at the Frankoniabrunnen for a guided tour of the Residenz.**
19:00	**Conference dinner in the Fürstensaal of the Residenz.**

09:00–09:40 **BCS regime of the two-dimensional fermionic Hubbard model: ground-state phase diagram**
O3 *Nikolai Prokof'ev (University of Massachusetts)*

09:40–10:10 **Tensor network algorithms for 2D strongly correlated lattice systems**
F3 *Juan Osorio (ETH Zurich)*

I will introduce the main ideas behind a tensor network algorithm, providing a quick overview on the main aspects of an infinite projected entangled-pair states (iPEPS) implementation. A recent application of the iPEPS algorithm to the so-called Kitaev-Heisenberg model, proposed as a candidate model describing the low energy physics in Iridate compounds of the form A_2IrO_3 (A=Na,Li) will be presented. Finally, in a more technically oriented part of the talk, I will discuss recent efforts aimed at coping with the (relatively) large computational costs of an iPEPS implementation both from a hardware as well as an algorithmic perspective

10:10–10:30 **Diagrammatic methods for lattice gauge theories with staggered fermions**
C9 *Hélvio Vairinhos (ETH Zurich)*

The sign problem is a major obstacle to our understanding of the phase diagram of QCD at finite baryon density. Several methods have been proposed to tackle this problem in the framework of lattice gauge theory, but a full solution to the sign problem is still elusive. Motivated by this problem and by recent advances in diagrammatic Monte Carlo methods, we find a new exact representation of the partition function of pure lattice gauge theory that contains no link variables. This approach can be easily extended to include staggered fermion fields, and results in a diagrammatic representation of gauge theory states, which consists of monomers, dimers, and fermionic loops saturating the spacetime lattice. Our models are exact for any value of the lattice coupling, and extend previous models that are only valid in the strong coupling limit $\beta = 0$ and at order β. As a concrete example, we construct a monomer-dimer-polymer representation of compact lattice QED.

11:00–11:30 **Exact diagonalization for topological phases driven by interaction**
I13 *Maria Daghofer (University of Stuttgart)*

Topologically nontrivial kinetic energy due to spin-orbit coupling and strong magnetic fields are two established ways to topologically nontrivial phases. We study alternative mechanisms, where electron-electron interaction, together with exotic magnetic states, might stabilize topologically nontrivial features [1]. Tools are either exact diagonalization or the variational cluster approach based on this method. We apply exact diagonalization to interacting Chern bands to detect signatures of "fractional Chern insulators", analogs of fractional quantum-Hall states, as well as of a more exotic pinball liquid that combines topological and conventional "Landau" order [2]. We also employ the variational cluster approach to investigate symmetry breaking of interacting fermions, possibly into topologically nontrivial phases [3].

[1] J. W. Venderbos, S. Kourtis, J. van den Brink, and M. Daghofer, Phys. Rev. Lett. **108**, 126405 (2012).

[2] S. Kourtis and M. Daghofer, Phys. Rev. Lett. **113**, 216404 (2014).

[3] M. Daghofer and M. Hohenadler, Phys. Rev. B. **89**, 035103 (2014).

11:30–12:00 **Matrix product state formulation of frequency-space dynamics at finite temperatures**
I14 *Salvatore Manmana (University of Göttingen)*

Based on a Liouvillian formulation of the problem, we present a flexible matrix product state approach to calculate finite-temperature spectral functions of one-dimensional strongly correlated quantum systems directly in frequency space. Using this approach, we study finite-temperature properties of dynamical spectral functions of spin-$1/2$ XXZ chains with Dzyaloshinskii- Moriya interactions in magnetic fields and analyze the effect of these symmetry breaking interactions on the nature of the finite-temperature dynamic spin structure factor.

12:00–12:20 **Phase diagram of repulsive spinless fermions on the honeycomb lattice**
C10 *Sylvain Capponi (Université Paul Sabatier Toulouse)*

We investigate the phase diagram of spinless fermions with competing interactions on the honeycomb lattice at half-filling. Using Exact Diagonalization technique and a careful choice of finite-size clusters, we determine the different charge orderings that occur for large interactions, in particular confirming the existence of Kekule pattern that has been proposed in the literature, but also proposing new types of charge ordering for very large interaction strengths. We also investigate in details the stability of the quantum Hall phase that was found in mean-field studies. While there is definitely some short-range correlations in the (charge) current correlations, our data indicate the absence of this topological phase in the thermodynamic limit.

14:00–14:30 **MPS based quantum impurity solvers**
F4 *F. Alexander Wolf (LMU Munich)*

We present recent advancements in the solution of MPS represented quantum impurity problems. These are benchmarked within equilibrium DMFT and its extensions (DCA) and nonequilibrium DMFT.

14:30-15:00 **Entanglement Structure of the Hubbard Model in Momentum Space**
F5 *Georg Ehlers (University of Marburg)*

We study the properties of the ground states of the one- and two-dimensional Hubbard models using entanglement-based measures, which we calculate quasi-exactly numerically using the momentum-space DMRG. In particular, we investigate quantities such as the single-site entropy and two-site mutual information of single-particle momentum states as well as the behaviour of the bipartite subsystem entropy for partitions in momentum space. The distribution of these quantities in momentum space gives insight into the fundamental nature of the ground state, insight that can be used to make contact with weak-coupling-based analytic approaches and to optimize numerical methods, the momentum-space DMRG in particular. We study the site and subsystem entropy as a function of interaction strength U and system size. In both the one- and two-dimensional cases, we find that the subsystem entropy scales proportionally to U^2 for weak U and proportionally to volume. Nevertheless, the optimized momentum-space DMRG can obtain variationally competitive results for the two-dimensional Hubbard model at weak coupling for moderate system sizes.

15:00–15:20 **Geometric stability of topological lattice phases**
C11 *Gunnar Möller (University of Cambridge)*

The possibility of realizing fractional quantum Hall (FQH)-like phases in lattice models has attracted intense interest recently, both as a more experimentally accessible venue for FQH phenomena and to provide possible generalizations of FQH physics which have been largely unexplored theoretically. For both of these purposes, we investigate quantitatively the physical relevance of band geometric criteria such as the flatness of the Berry connection and the Fubini study metric in determining the stability of such phases, both criteria quantifying deviations from the Landau level physics of the FQHE. We conduct extensive numerical many-body simulations on a variety of lattice models and find remarkable correlation between these criteria and the many-body gap for the Laughlin state, and (to a lesser extent) for the Moore-Read state. This leads us to propose a *geometric stability hypothesis*, namely that these single-particle criteria usefully quantify destabilizing effects on many-body FQH-like phases.

16:00–16:20 **A generalized perspective on non-perturbative linked cluster expansions**
C12 *Kai P. Schmidt (TU Dortmund)*

We identify a fundamental challenge for non-perturbative linked cluster expansions (NLCEs) resulting from the reduced symmetry on graphs, most importantly the breaking of translational symmetry, when targeting the properties of excited states. A generalized notion of cluster additivity is introduced, which is used to formulate an optimized scheme of graph-based continuous unitary transformations (gCUTs) allowing to solve and to physically understand this fundamental challenge. Most importantly, it demands to go beyond the paradigm of using the exact eigenvectors on graphs.

16:20–16:40 **Entanglement Entropy for Many-Fermion Systems**
C13 *Peter Bröcker (University of Cologne)*

The precise determination of the entanglement of an interacting quantum many-body systems is now appreciated as an indispensable tool to identify the fundamental character of the ground state of such systems. This is particularly true for unconventional ground states harbouring non-local topological order or so-called quantum spin liquids that evade a standard description in terms of correlation functions. With the entanglement entropy emerging as one of the central measures of entanglement, recent progress has focused on a precise characterization of its scaling behaviour, in particular in the determination of (subleading) corrections to the prevalent boundary-law. While much progress has been made for spin and bosonic quantum many-body systems, fermion systems have proved to be more difficult. For a large class of interacting fermionic systems, the numerical method of choice for unbiased, large-scale simulations is Determinantal Quantum Monte Carlo (DQMC) for which a generalization of the replica techniques developed to calculate entanglement entropies for spin and bosonic systems has remained an open question. Here we show one possibility how to construct the corresponding algorithm in DQMC and demonstrate its strength by studying the ground state and finite temperature properties of the entanglement entropy in one-dimensional Hubbard systems. We also compare our results to another recent approach based on free fermion Green's functions. Recent work is focused on the numerical stabilization of the presented algorithm.

Thursday Sessions at a Glance

Thursday 1

Chair: A. Filinov

09:00–09:40	**TBA**
O4	*Frank Verstraete (University of Vienna)*
09:40–10:10	**Continuous-time quantum Monte Carlo for electron-phonon models**
F6	*Manuel Weber (University of Würzburg)*
10:10–10:30	**Breakdown of antiferromagnetism and the Coulomb phase for RVB states on anisotropic three-dimensional lattices**
C14	*Kevin Beach (University of Mississippi)*

Thursday 2

Chair: M. Raczkowski

11:00–11:30	**Cluster Quantum-Monte-Carlo Methods for Frustrated Spin Systems**
F7	*René J. Kerkdyk (University of Göttingen)*
11:30–11:50	**Self-consistent screening in graphene**
C15	*Shaffique Adam (Yale-NUS College)*
11:50–12:20	**Spin Dynamics in Two-dimensional Quantum Spin Systems**
F8	*Stefan Wessel (RWTH Aachen University)*

09:00–09:40 **TBA**
O4 *Frank Verstraete (University of Vienna)*

09:40–10:10 **Continuous-time quantum Monte Carlo for electron-phonon models**
F6 *Manuel Weber (University of Würzburg)*

The continuous-time quantum Monte Carlo (CTQMC) method relies on the imaginary-time path-integral formulation of the partition function and samples the weak-coupling perturbation expansion of a fermionic action. This action-based formulation makes the CTQMC method applicable to a variety of models. In this talk, we will focus on electron-phonon models, where the phonons can be integrated out exactly to arrive at an effective fermionic action with retarded interactions. We will show selected applications to metal-insulator transitions driven by the Peierls instability. In particular, we will present results for the phonon spectral function, which can be recovered from fermionic correlation functions using generating functionals.

10:10–10:30 **Breakdown of antiferromagnetism and the Coulomb phase for RVB states on anisotropic three-dimensional lattices**
C14 *Kevin Beach (University of Mississippi)*

Nearest-neighbour (NN) resonating-valence-bond (RVB) wave functions are often invoked as prototype ground states for various frustrated models in two dimensions because of their lack of long-range magnetic correlations. In three dimensions, though, such states are generally not featureless, and their tendency is toward robust antiferromagnetic order. For the NN RVB states on the cubic and diamond lattices, for example, antiferromagnetism coexists with power law dimer correlations characteristic of the "Coulomb phase" (in analogy with classical hardcore dimer models). The introduction of increasingly strong spatial anisotropy, however, leads to the destruction of these long-range and algebraic correlations, leaving behind an apparent short-range spin liquid state. Using quantum Monte Carlo, we characterize the critical exponents at the phase boundaries for wave functions built from products of SU(2) singlets as well as their SU(N) generalizations; we discuss attempts to construct a field theory that describes the transitions.

11:00–11:30 **Cluster Quantum-Monte-Carlo Methods for Frustrated Spin Systems**
F7 *René J. Kerkdyk (University of Göttingen)*

Quantum-Monte-Carlo (QMC) methods face severe difficulties when applied to frustrated spin models due to the infamous sign problem. We suggest that this problem can be alleviated or even eliminated for certain highly frustrated magnets using a cluster basis. This idea is illustrated by Stochastic Series Expansion (SSE) QMC simulations for a highly frustrated spin-$1/2$ ladder. While here the sign problem can indeed be eliminated, one still needs to deal with large autocorrelation times at low temperatures in standard SSE simulations. The highly frustrated spin-$1/2$ ladder is known to exhibit a first-order quantum phase transition between a rung singlet and a Haldane phase. Close to this transition, we observe that the maximum of the specific heat shifts to lower temperatures as compared to the broad maximum of the magnetic susceptibility.

11:30–11:50 **Self-consistent screening in graphene**
C15 *Shaffique Adam (Yale-NUS College)*

About seven years ago, a new electronic material appeared – notable not only for its ease of preparation and theoretical simplicity, but also by its promise for future electronic devices [1]. Single monotonic sheets of carbon, known as graphene, have an electronic dispersion that is reminiscent of light, in that they can be described as a massless Dirac particle. More recently, such Dirac fermions have also been observed on the surfaces of some bulk insulators with strong spin-orbit coupling (called topological insulators) [2]. In many ways, these Dirac fermion systems are a textbook system to test physical models – and part of the success in understanding these materials is because the effects of electron-electron interactions are quite weak. In this talk, I will first discuss how the electronic properties of the Dirac point provide an intriguing example of how the competing effects of disorder, electron-electron interactions, and quantum interference conspire together to give a surprisingly robust state whose properties can be described using semi-classical methods. Then, I will examine some very recent experiments that claim to observe the effects of strong electron-electron interaction in graphene and will report on our theoretical progress towards understanding correlation effects in graphene and other Dirac materials.

[1] S. Das Sarma, S. Adam, E. H. Hwang, and E. Rossi, Rev. Mod. Phys. **83**, 407 (2011).

[2] D. Kim, S. Cho, N. P. Butch, P. Syers, K. Kirshenbaum, S. Adam, J. Paglione, M. S. Fuhrer, Nature Physics **8**, 460 (2012).

11:50–12:20 **Spin Dynamics in Two-dimensional Quantum Spin Systems**
F8 *Stefan Wessel (RWTH Aachen University)*

List of Participants

Abdelwahab	Anas	University of Hanover
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Barman	Himadri	Tata Institute of Fundamental Research
Beach	Kevin	University of Mississippi
Becker	Jonas	RWTH Aachen University
Bercx	Martin	University of Würzburg
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Mariën	Michael	Ghent University
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