# Posters

P–1 **Berry phase investigation of spin-S ladders**
**Chepiga Natalia, EPFL**
We investigate the properties of antiferromagnetic spin-S ladders with the help of local Berry phases defined by imposing a twist on one or a few local bonds. In gapped systems with time reversal symmetry, these Berry phases are quantized, hence able in principle to characterize different phases. In the case of a fully frustrated ladder where the total spin on a rung is a conserved quantity that changes abruptly upon increasing the rung coupling, we show that two Berry phases are relevant to detect such phase transitions: the rung Berry phase defined by imposing a twist on one rung coupling, and the twist Berry phase defined by imposing a twist on all couplings between two rungs, i.e. by twisting the boundary conditions along the legs. In the case of non-frustrated ladders, we have followed the fate of both Berry phases when interpolating between standard ladders and dimerized spin chains, with the surprising conclusion that, at least far enough from dimerized chains, they define different domains in parameter space. A careful investigation of the spin gap and of edge states shows that a change of twist Berry phase is associated to a quantum phase transition at which the bulk gap closes, and at which, with appropriate boundary conditions, edge states appear or disappear, while a change of rung Berry phase is not necessarily associated to a quantum phase transition. The difference is particularly acute for regular ladders, in which the twist Berry phase does not change at all upon increasing the rung coupling from zero to infinity while the rung Berry phase changes 2S times. By analogy with the fully frustrated ladder, these changes are interpreted as cross-overs between domains in which the rungs are in different states of total spin from 0 in the strong rung limit to 2S in the weak rung limit. This interpretation is further supported by the observation that these cross-overs turn into real phase transitions as a function of rung coupling if one rung is made arbitrarily strongly ferromagnetic, or equivalently if one rung is replaced by a spin 2S impurity.

P–2 **A variational cluster approach to strongly correlated quantum systems out of equilibrium**
**Martin Nuss, TU-Graz**
The theoretical understanding of the non-equilibrium behaviour of strongly correlated quantum many-body systems is a long standing challenge, which has become increasingly relevant with the progress made in the fields of molecular-and nano- electronics, spintronics, spectroscopy or quantum optics and simulation. We report on the development of non-equilibrium cluster perturbation theory, and its variational improvement, the non-equilibrium variational cluster approach for steady-state situations. The non-equilibrium extensions of the well established cluster perturbation theory and the variational cluster approach are based on the Keldysh Green's function method which allows, in this case, accessing single particle dynamic quantities. These flexible and versatile techniques can in principle be applied to any fermionic / bosonic lattice Hamiltonian, including multi-band and multi-impurity systems. Within this framework it is possible to work in the thermodynamic limit and therefore exchange particles with a bath and/or dissipate energy. We present results for the steady-state of molecular / nano devices under bias including the effects of electron-electron interactions.

P–3 **Non-linear electron-phonon coupling in the Holstein model,**
**Clemens Adolphs, UBC**
We point out an inconsistency in the most widely used theoretical models that describe systems with strong electron-phonon coupling. Both the Holstein and the Froehlich models assume that lattice distortions are sufficiently small to justify treating them to linear order. At strong coupling, however, it is well established that these models predict the formation of a small polaron, with potentially considerable local lattice distortions, invalidating the original assumption. Here we use the momentum average approximation to study the effect of higher-order coupling terms in the Holstein model. We show that they have drastic consequences on the properties of the polaron when compared to the linear model, and that these effects cannot be captured by a linear model with renormalized parameters.

P–4 **Quantum Phase Transition between Kondo Polarons**
**Julian Rincon, ORNL**
We study a mobile spin-1/2 impurity, coupled antiferromagnetically to a one-dimensional gas of fermions. Combining perturbative ideas and extensive density matrix renormalization group calculations, we study the interplay between the screening of the impurity by the electrons and the kinetic and magnetic properties of the impurity. We show that this problem displays a quantum phase transition between one- and two-channel Kondo physics. Using finite-size scaling, we construct a ground-state phase diagram and discuss various non-trivial regimes.

P–5 **Single magnetic impurities in the Kane-Mele model**
**Florian Goth, David J. Luitz, and Fakher F. Assaad, Würzburg**

The realization of the spin-Hall effect in quantum wells has led to a plethora of studies regarding the properties of the edge states of a two-dimensional topological insulator. These edge states constitute a class of one-dimensional liquids, called the helical liquid, where an electron's spin quantization axis is tied to its momentum. In contrast to one dimensional conductors, magnetic impurities — below the Kondo temperature — cannot block transport and one expects the current to circumvent the impurity. To study this phenomenon, we consider the single impurity Anderson model embedded into an edge of a Kane-Mele ribbon with up to 512 x 80 sites and use the numerically exact continuous time quantum Monte Carlo method (CTQMC) to study the Kondo effect. We present results on the temperature dependence of the spectral properties of the impurity and the bulk system that show the behaviour of the system in the various regimes of the Anderson model. A view complementary to the single particle spectral functions can be obtained using the spatial behaviour of the spin spin correlation functions. Here we show the characteristic, algebraic decay in the edge channel near the impurity.
Journal Reference: Phys. Rev. B 88, 075110 (2013)

P–6 **Coexistence of topological and Landau order from strong correlations in Chern bands**
**Stefanos Kourtis, IFW-Dresden**
Several lattice models featuring topologically non-trivial and flat bands have been recently studied as potential hosts of fractional quantum-Hall states in the absence of a magnetic field. Such states, dubbed fractional Chern insulators (FCI), were shown to arise in an effective model originally derived from a 3-orbital model describing layered transition-metal oxides, if short-range repulsion between particles is taken into account. To this end, the eigenpairs of the model Hamiltonian were obtained and studied as a function of filling, interaction strength and band dispersion using exact diagonalization of small clusters. Using symmetry arguments as well as appropriate observables, such as the Hall conductivity and the static charge-structure factor, FCI and charge-density wave (CDW) ground states are identified at various filling fractions. After discussing the competition between FCI and CDW phases, a class of states, in which the FCI topological order is induced by the presence of CDW order, will be introduced and established by interpreting numerical evidence for a few cases.

P–7 **Towards a Numerical Renormalization Group description of the steady-state nonequilibrium single-impurity Anderson model using Lindblad driving**
**Frauke Schwarz (1), Ireneusz Weymann (2), Andreas Weichselbaum (1), and Jan von Delft (1)**
**(1) Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich (2) Institute of Physics, Adam Mickiewicz University, Pozna**
Wilson's Numerical Renormalization Group (NRG) allows to describe the single-impurity Anderson model (SIAM) in equilibrium in a nonperturbative way. However, it remains a challenge for NRG to treat situations of steady-state nonequilibrium, such as transport through a quantum dot at finite source-drain bias, or to describe the dynamics of relaxation processes. To model such situations, we envisage considering additional baths, which are coupled to the leads. The effect of these baths on the leads can be described by using Lindblad operators [1] in the Liouville equation for the density matrix of the dot and the leads. The action of these operators can, in principle, be chosen such that the leads are effectively held in thermal equilibrium. An efficient way of solving this Liouville equation is to use the stochastic quantum trajectory method [1]. The intermediate time evolution needed to generate such trajectories can be done with time-dependent NRG (tNRG) based on complete basis sets. Here we present our preliminary results illustrating the above ideas.
[1] C.W. Gardiner, P. Zoller, Quantum Noise (Springer, Berlin, 2000

P–8 **Martin Zonda, Charles University, Prague**
Modern unconventional Josephson junctions (JJ), can have a current-phase relation $I(\phi) = I_1 \sin\phi + I_2 \sin 2\phi$ where the second harmonic $I_2$ plays an important role. Typical example of such systems are $\phi$ junctions, where the second harmonics is negative. We numerically study the influence of the negative second harmonic on the phase dynamics and voltage noise of JJs within the resistively and capacitively shunted junction (RCSJ) model. We evaluate the noise as well as the full counting statistics of the phase dynamics by the matrix continued fraction method. The analysis of the results enables us to identify the various components contributing to the overall noise such as the thermal noise close to equilibrium (small current-bias regime), switching noise for higher biases and the shot noise of (multiple) phase slips in the intermediate range of biases. We focus on the phase-slips regime, characterized by the plateau in the Fano factor (voltage noise normalized by the mean voltage) as a function of the current bias, in more detail. Depending on the relative importance of the first ($I_1$) and second ($I_2$) harmonic, we observe the crossover from the unitary Fano factor corresponding to elementary $2\pi$ phase slips to the Fano factor value of one half revealing the fractional phase slips just by $\pi$. These findings are further supported by the analysis of the full counting statistics also exhibiting the presence of fractional phase slips via the non-trivial analytical properties of the cumulant generating function.

P–9 **Entanglement Entropy in Many-Fermion Systems**
**Peter Bröcker , Köln**

The concept of entanglement first garnered widespread attention in the 1930s when Einstein, Podolsky and Rosen conducted a thought experiment to show that the prevailing formulation of quantum mechanics was incomplete. The experiment included two entangled particles that were created simultaneously and then separated by an arbitrarily long distance. However, they remained correlated and, most importantly, this correlation appeared to spread faster than the speed of light. This could either be explained by missing, hidden variables that had to be included in the theory or by accepting that quantum mechanics is a non-local theory. Today we know that quantum mechanics does indeed allow to interweave two quantum mechanical objects into a collective state with highly non-trivial entanglement.

Since then, two- and few-particle entangled states have been studied extensively, both theoretically and experimentally. Many-particle entanglement on the other hand has only recently moved into focus and much of its properties are still left unexplored. One natural way to quantify it is by calculating the so-called entanglement entropy. The entanglement entropy does not depend on the system volume but typically follows a boundary law. Various correction terms to this boundary law allow to uniquely identify the quantum state of a system. Most notably, this includes states like spin liquids that lie outside the Ginzburg-Landau paradigm for which a very precise diagnostic criterion can be defined by the entanglement entropy.

We will present a new approach to calculate the entanglement entropy of many-fermion states in quantum Monte Carlo simulations. In particular, our method is applicable to two-dimensional systems where a full characterization of the respective quantum states is still incomplete.

P–10 **Theory of the magnetic properties of the bilayer iridate Sr3Ir2O7**
**Vera I. Schnells, Frdric Mila, Henrik M. Ronnow (EPFL)**

We propose a bilayer pseudospin-1/2 anisotropic Heisenberg model to describe the magnetic properties of the iridate Sr3Ir2O7 at zero temperature using a combination of analytical and numerical methods to explore the excitation spectrum of the system. From x-ray scattering (RIXS) experiments, it is known that the compound's lowest magnetic excitation has a large spin gap of 92 meV and a bandwidth of 70 meV. Treating our model using bond-operator mean-field theory, it was possible to reproduce these features accurately. The anisotropy selects an easy c-axis collinear antiferromagnetic ground state that has also been observed experimentally. In comparison to other proposed models, we were able to describe both the first and second magnetic excitation branches as transverse and longitudinal triplet excitations. To obtain complementary results on the compound and to verify the parameter range of the bond-operator mean-field theory, we also treated the system within an exact diagonalization approach. The results obtained so far support the accuracy of our proposed model.

P–11 **Determinant quantum Monte Carlo studies of the three-orbital Hubbard model.**
**Yvonne Kung, Standford**

Studying temperature and doping trends in strongly correlated materials is integral to understanding how their properties emerge and develop, and possibly can be tuned. To this end, determinant quantum Monte Carlo (DQMC) simulations are used to investigate the three-orbital Hubbard model as applied to the cuprate superconductors. Spectral functions relevant to photoemission measurements are calculated and various spectral features, such as the indirect charge-transfer gap and Zhang-Rice singlet band, are shown to vary with doping. In addition, these orbitally resolved calculations help shed light on proposed pictures of the pseudogap regime, such as oxygen spin ordering and orbital current loops.

P–12 **Magnetic Correlations in Short and Narrow Graphene Armchair Ribbons**
**Michael Golor, Cornelie Koop, Thomas C. Lang, Stefan Wessel, Manuel J. Schmidt, RWTH, Aachen**

Electronic states at the ends of a narrow armchair nanoribbon give rise to a pair of non-locally entangled spins. We propose two experiments to probe these magnetic states, based on magnetometry and tunneling spectroscopy, in which correlation effects lead to a striking, nonlinear response to external magnetic fields. On the basis of low-energy theories that we derive here, it is remarkably simple to assess these nonlinear signatures for magnetic edge states. The effective theories are especially suitable in parameter regimes where other methods such as quantum Monte-Carlo simulations are exceedingly difficult due to exponentially small energy scales. The armchair ribbon setup discussed here provides a promisingly well-controlled (both experimentally and theoretically) environment for studying the principles behind edge magnetism in graphene-based nano-structures.

P–13 **Spin-orbit physics of j=1/2 Mott insulators on the triangular lattice**
**Michael Becker, Köln**

We investigate the Heisenberg-Kitaev model on the triangular lattice which is thought to capture the essential

physics of the spin-orbital entanglement in a broad class of effective j=1/2 Mott insulators such as certain Iridate compounds – one potential candidate material being the recently synthesized Ba3IrTi2O9. While first results have recently been reported for the classical limit of this model, our focus is on its quantum version. Using a combination of numerical techniques, such as exact diagonalization and the density matrix renormalization group, which we complement with various analytical approaches, we can identify its entire phase diagram. The most interesting features of this phase diagram resemble what has already been found in the classical limit – a Z2 vortex lattice phase in the vicinity of the Heisenberg limit and a "nematic" phase around the antiferromagnetic Kitaev point.

P–14 **Quasi continuous-time impurity solver for dynamical mean-field theory with linear scaling in the inverse temperature**

**- Daniel Rost (1) , Fakher Assaad (2) , and Nils Blümer (1) - (1) Institute of Physics, Johannes Gutenberg-University, Mainz (2) Institute of Theoretical Physics and Astrophysics, University of Würzburg**

Diagrammatic quantum Monte Carlo impurity solvers (CT-QMC) provide numerically exact solutions for dynamical mean-field theory (DMFT), at a computational cost that scales cubically with the inverse temperature $\beta$. In contrast, a recently proposed approach [1], based on a Hamiltonian representation of the bath Green function and the BSS quantum Monte Carlo algorithm [2], scales linearly with $\beta$, but introduces a bias due to Trotter discretization. We present an algorithm, based on multigrid extrapolations of Green functions, that combines the advantages of both methods: (i) it retains the superior linear scaling of BSS and (ii) is free of significant Trotter errors. The accuracy of this quasi continuous-time method is established for the metal-insulator transition in the 1-band Hubbard model, in comparison with CT-QMC and exact diagonalization. We also analyze the impact of the bath discretization and conclude that the new method appears most promising for cluster DMFT studies at low temperatures.

[1] E. Khatami et al., PRE 81, 056703 (2010);
QUantum Electron Simulation Toolbox, *http* : *//www.cs.ucdavis.edu/bai/QUEST_public/*.
[2] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24, 2278 (1981).

P–15 **ALPS/diagonalization: Parallel Implementation of Exact Diagonalization**

**Ryo Igarashi, ISSP University of Tokyo**

We present a new implementation of exact diagonalization for generic quantum lattice models, ALPS/diagonalization, based on the ALPS (Algorithms and Libraries for Physics Simulations) library. Current exact diagonalization code in ALPS does not scale on multi-node clusters and our implementation aims to fill the gap.

P–16 **Spin dynamics of a quantum spin model on the kagome lattice exhibiting a $Z_2$ spin liquid phase**

**Maximilian Lohfer, RWTH Aachen**

We discuss a stochastic series expansion (SSE) algorithm similar to the one presented in [1] to simulate a S=1/2 XY model with four-site ring exchange on a kagome lattice [2]. This model was shown recently to exhibit a $Z_2$ spin liquid phase [2]. Here, we want to study the spin dynamical properties in the spin liquid regime. For this purpose, we employ an efficient continuous-time representation to access the longitudinal and transverse imaginary-time displaced correlation functions. For the analytic continuation of the obtained data from imaginary time to real frequency space, we consider to employ the stochastic analytical continuation as well as the statistical optimization method [3-5]. The poster focuses on the methodological details of this investigation.

[1]R.G. Melko, A. W. Sandvik PRE 72 026702 2005
[2]L. Dang, S. Inglis, R.G. Melko PRB 84 132409 2011
[3]K. S. D. Beach arXiv:cond-mat/0403055
[4]A. S. Mishchenko, N. V. Prokof'ev, A. Sakamoto, B. V. Svistunov PRB 62 10 2000
[5]A. S. Mishchenko Correlated Electrons: From Models to Materials

P–17 **Dimensional transitions for short-range resonating valence bond states**

**Jin Xu, Alberta**

Given the difficulty of obtaining the ground states of even simple model Hamiltonians, it is common to consider an alternative route that begins with a family of trial wave functions. A plausible starting point for strongly frustrated models is a state with no explicit symmetry breaking, made up of short range singlets. With this in mind, we construct a resonating valence bond trial wave function in a layered cubic lattice, allowing for a general anisotropy in the weights of the nearest-neighbour valence bonds along one axis. Worm Monte Carlo simulations reveal that several interesting quantum phases are stabilized as a function of the anisotropy parameter, with continuous quantum transitions appearing at critical values of the effective dimension. We investigate the critical properties and the emergence of well-defined topological sectors.

P–18 **A nonequilibrium Dynamical Mean Field Theory approach based on the Lindblad equation**
**Antonius Dorda, TU Graz**

In order to apply the Dynamical Mean Field Theory to nonequilibrium steady state situations, an auxiliary impurity problem has to be devised which exhibits dissipative mechanisms and thus enables the time evolution to a stationary state. For this purpose, we have introduced an effective model whereby the impurity is coupled to bath sites which in turn are connected to a Markovian environment [1]. This provides a description of the impurity system within a quantum master equation. A superfermionic representation is used to rewrite the Lindblad equation in a non-hermitian Hamiltonian form. With some modifications, the well-established exact diagonalization methods for sparse hermitian matrices can be adapted to the non-hermitian case, enabling us to address the steady state and the dynamics of this problem. The Single Impurity Anderson model is presented as a test case [2], and results are compared with those from Density-Matrix-Renormalisation-Group-like and cluster-embedding approaches.
[1] E. Arrigoni et al., Phys. Rev. Lett. 110, 086403 (2013)
[2] A. Dorda et al., in preparation

P–19 $\pi$ **Fluxes near the Edge of a Topological Insulator: Kondo Screening of a Soliton**
**Manuel Weber, Martin Hohenadler and Fakher F. Assaad, Würzburg**
The insertion of a $\pi$ flux into a quantum spin Hall insulator creates four spin-charge separated states: the two chargeons with $Q = \pm 1$ and the two spinons with $S_z = \pm 1/2$. In the presence of repulsive Coulomb interactions the charged states are gapped out and a local moment is formed. For both free and interacting systems the fluxons lead to a characteristic Curie law in the magnetic susceptibility. We consider the Kane-Mele-Hubbard model on a ribbon with zigzag edges to show that the spinon can be screened by the edge states of a quantum spin Hall insulator. At $U = 0$ their hybridization is dominated by the extent of the edge states, which becomes larger with increasing spin-orbit coupling $\lambda$. As the fluxons are exponentially localized, it is sufficient to include Hubbard interactions only at lattice sites directly around the $\pi$ flux. We have expanded the CTQMC method by global susceptibility measurements that reproduce the Curie law of a free $\pi$ flux even for this reduced interacting system. When the spinon is screened by the edge states, we observe deviations from the Curie law for different $U$ and $\lambda$ that follow the universal behavior obtained from a data collapse. Moreover, at low temperatures a Kondo resonance arises in the spectral function between two low-lying Hubbard peaks.

P–20 **DMRG study of the optical conductivity of the 1D Hubbard model**
**Alexander C. Tiegel, Piet E. Dargel, Andreas Honecker, and Thomas Pruschke**
**Institut für Theoretische Physik, Georg-August-Universität Gttingen**
The zero-temperature optical conductivity of the Hubbard model in one dimension is studied for various values of the on-site repulsion U and the electronic filling n by means of frequency-resolved density-matrix renormalization group (DMRG) methods. The focus of this work is the determination of the optical gap and the investigation of the leading frequency dependence at the onset of the finite-frequency conductivity. At half-filling, our data is compatible with a square-root increase above the band threshold, which is in agreement with conformal field theory and DDMRG results in the literature. Away from half-filling, we find an increasing pseudogap with the amount of doping. These results as well as the extracted exponents at the onset are directly compared to existing field-theoretical values.

P–21 **Exploiting non-abelian symmetries in the Dynamical Mean-Field Theory using the Numerical Renormalization Group**
**Katharina Maria Stadler, Münich**
The realistic description of strongly correlated materials, such as transition metal oxides, rare earth or actinide elements, is a huge challenge in condensed-matter physics. As the strength of electron-electron interactions is comparable to or larger than the kinetic energy, intriguing quantum many-body phenomena like the transition from a metallic to an insulating phase arise, but cannot be investigated by perturbative methods. The Dynamical Mean-Field Theory (DMFT) [1] provides a non-perturbative many-body approach to describe the local dynamics of strongly correlated systems by mapping a lattice model self-consistently onto an effective (single-site) quantum impurity model. The quantum impurity model is then solved by a non-perturbative method, such as Quantum Monte Carlo simulations (QMC) or the Numerical Renormalization Group (NRG) approach. QMC codes are widely used and have been highly refined over the last few decades. However, the data is obtained on the imaginary (Matsubara) frequency axis and has to be analytically continued to the real axis, a procedure that is mathematically ill-conditioned. Furthermore, possible limitations are very low temperatures and also the so called sign problem for fermionic systems. In my work, I exploit one of the most evolved codes in the field of NRG as an alternative to QMC impurity solvers within DMFT. The NRG method allows to calculate physical

quantities directly on the real frequency axis. Using the full density matrix approach (fdm-NRG, [2]) within the framework of complete many-body basis sets [3], our NRG solver can handle arbitrary temperatures in a clean, systematic and thus optimal manner. Moreover, our code is, to date, the only NRG framework, that is able to exploit arbitrary abelian and non-abelian symmetries [4], which leads to a significant reduction of numerical effort and makes it highly suitable for the investigation of multi-band models in the presence of intrinsic symmetries.

[1] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg. Rev. Mod. Phys., 68:13125, 1996
[2] A. Weichselbaum and J. von Delft. Phys. Rev. Lett., 99:076402, 2007
[3] F. B. Anders and A. Schiller. Phys. Rev. Lett., 95:196801, 2005
[4] A. Weichselbaum. Annals of Physics, 327(12):2972 3047, 2012

P–22 **Using DMRG to probe the honeycomb antiferromagnet**

**R. Ganesh, IFW Dresden**

We study the J1-J2 model on the honeycomb lattice which has attracted immense interest recently. We study the S=1/2 model using a combination of DMRG calculations and semi-analytical methods. As J2 is tuned, we find a Neel phase, a plaquette-ordered state and a dimer solid. To obtain an effective description of the intermediate plaquette phase, we develop a plaquette-operator approach. Surprisingly, the phase transitions between these states appear to be continuous Landau-forbidden transitions. Our study is the first to see a possible deconfined transition in a realistic Heisenberg-like model.

P–23 **Investigation of Berry Curvature and Intrinsic Spin Hall Conductivity of Bismuth**

**Cuneyt Sahin (1), Giovanni Vignale (2), Michael E. Flatte' (1)**
**(1) Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa, 52242, USA (2)Department of Physics and Astronomy, University of Missouri, Columbia, Missouri, 65211, USA**

Spin Hall effect describes the phenomenon of emergence of spin current perpendicular to an external electric current. The spin Hall conductivity (SHC) is then defined as ratio of the resultant spin current to the applied electric field. Materials with large SHC driven under the effect of spin-orbit interaction provide generation and control of spin currents with no external magnetic field and therefore they are significant candidates for spintronics applications. Bismuth which is a semimetal with large spin-orbit coupling is expected to exhibit a large spin Hall conductivity. Furthermore bismuth based materials with small band gaps and strong spin-orbit interactions such as bismuth selenide and bismuth telluride are known to exhibit novel properties such as three dimensional topological insulator states [1] as well as quantum Hall and quantum spin Hall effects [2].

In this work we have used a low-energy effective spin-orbit Hamiltonian for Bismuth which is based on a Slater-Koster type tight-binding model. [3] This Hamiltonian includes up to third neighbor interactions which is sufficient to mimic the characteristics of the electronic band structure and effective masses around the Fermi energy. Beginning with this low-energy Hamiltonian and band structure we calculate the intrinsic spin Hall conductivity using a Berrys phase technique in the clean static limit. Although SHC is assumed to scale with the strength of the spin-orbit coupling, curvature of the band plays a great role in determining the spin Hall angle. Considering that we have also investigated the behavior of the Berry curvature at high symmetry points in the first Brillouin zone. Vertex corrections due to impurity scatterings have been also considered and shown to be insignificant. In conclusion we report that robust spin-orbit coupling and Berry curvature in bulk bismuth results in orders of magnitude larger intrinsic SHC than conventional metals and semiconductors like GaAs, Ge, AlAs [4, 5] and it is as large as platinum. [6] As a result large SHC suggests the potential for novel spintronic applications of Bismuth based systems.

This work was supported by C-SPIN, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

[1] Chen, et al. Science 325, 178 (2009).
[2] Bernevig et al., Science 314, 1757 (2006).
[3] Y.Liu and R. Allen, Phys. Rev. B, 52, 1566 (1995).
[4] G. Guo et al. Phys. Rev. Lett. 94, 226601 (2005).
[5] Y. Yao and Z. Fang, Phys. Rev. Lett. 95, 156601 (2005).
[6] G. Guo, et al., Phys. Rev. Lett. 100, 1 (2008).

P–24 **Quantum Monte Carlo for Berry connection and local quantized Berry phase**

**Yuichi Motoyama, University of Tokyo**

We present path-integral quantum Monte Carlo method for gauge-fixed Berry connection using projection method

and the meron cluster algorithm, and applied this to the local quantized Berry phase [Hatsugai, JPSJ 75 (2006) 123601]. The local quantized Berry phase is one of the topological order parameter which characterize the gapped short range entangled state such as VBS. We calculate the local $Z_2$ Berry phase of antiferromagnetic Heisenberg model on chain, ladder, and square lattice with dimerization coupling. We also propose that the gauge-fixed Berry connection itself can be another effective tool to catch the quantum phase transition.

P–25 **Measurement of vertices and improved estimators in quantum Monte Carlo for general interactions**

**Markus Wallerberger(1) Emanuel Gull(2) Nicolaus Parragh(3) Alessandro Toschi(1) Giogrio Sangiovanni(3) Karsten Held(1)**
**(1) TU Wien, Austria (2) Univ. of Michigan, USA (3) Universität Würzburg, Germany**

P–26 **Non-equilibrium dynamics in the 1D Bose-Hubbard model**

**Felix ANDRASCHKO, Kaiserslautern**

We study the spreading of local impurities inserted into Bose-Hubbard chains in a prepared thermal or product state. By considering different interaction strengths, we draw a connection between the weakly interacting regime, in which the dynamics are dominated by Luttinger liquid-like behaviour, and the large-U regime, in which the impurities can be well described by a model of free fermionic quasiparticles. Making use of the Lieb-Robinson bound, we are able to perform numerical simulations in the thermodynamic limit using a Light Cone Renormalization Group algorithm based on corner transfer matrices.

P–27 **Is there Andreev-reflection in 1D Fermi-Hubbard systems?**

**Mirco Marahrens, Göttingen**

We investigate for the possibility of *directly* observing Andreev-reflection in the time evolution of an initial wave packet at a metal/superconductor junction in interacting one-dimensional Fermi-Hubbard systems. We apply the adaptive time-dependent density matrix renormalization group (t-DMRG) method to obtain the behaviour when the wave packet initially prepared in the metallic region (modelled by non-interacting electrons) hits the interface to the superconducting region which we model by an attractive Fermi-Hubbard model. Somewhat surprisingly, and at first sight in contradiction to the findings in [1,2], we do not obtain a clear signal for hole-reflection over a wide range of parameters. This appears to be different for bosonic systems, in which we identify hole-like reflection, in line with the findings of [2]. We discuss ongoing work on this issue and the different aspects of the results obtained so far.

[1]A.E. Feiguin, S.R. White, and D.J. Scalapino, PRB 75, 024505 (2007).
[2] A.J. Daley, P. Zoller, and B. Trauzettel, PRL 100, 110404 (2008).

P–28 **Wien Effect on a Lattice,**

**Vojtech Kaiser, MPIPKS**

External fields can strongly enhace the conductivity of charged systems by increasing the dissociation of Coulombically bound pairs. We show how numerical simulations can explore regimes of the Wien effect beyond the original theory of Onsager, while exploring the microscopic processes underlying the effect. *http* : *//dx.doi.org/*10.1038/*nmat*3729

P–29 **Temperature dependence of the spectral function in topological Kondo insulators**

**Jan Werner, Würzburg**

Heavy-fermion materials naturally combine strong spin-orbit interactions and electronic correlations. When there is precisely one conduction electron per impurity spin, the state is insulating. Recently is has been argued that this Kondo insulating state is in fact a topological insulator. By means of DMFT, we investigate a model for Kondo insulators with spin-orbit coupling. At sufficiently large interaction strength, we find a topological heavy fermion state, which is adiabatically connected to a non-interacting state with a non-trivial band topology. Our method allows us to track the evolution of the spectral function with temperature, where we observe the emergence of edge states as the temperature crosses the Fermi liquid coherence scale. Our results directly relate to recent investigations of SmB6, where the spectral function obtained by spectroscopic methods is a central quantity for identifying the topological state.

P–30 **Topological transitions of interacting bosons in one-dimensional bichromatic lattices**

**Xiaolong Deng and Luis Santos, Hannover**

Ultra-cold atoms in 1D bi-chromatic lattices constitute a surprisingly simple system for the study of topological insulators. We show that topological phase transitions constitute a general feature of bosons in 1D bi-chromatic lattices, and that these transitions may occur both as a function of the superlattice strength and due to inter-site interactions. We discuss in addition the topological character of incommensurate density wave phases in quasi-periodic lattices.

P–31 **Dimensional-Crossover-Driven Mott Transition: Variational Cluster Approach**
**Benjamin Lenz, Göttingen**
The dimensional-crossover-driven Mott transition has been studied recently in a frustrated Hubbard model with next-nearest neighbor hopping at finite temperatures [Raczkowski, Assaad, PRL 109 (2012)]. By means of variational cluster approximation (VCA) we investigate this system at zero temperature in a thermodynamically consistent way at half filling. The transition from one to two dimensions is studied for fixed frustration at several interaction strengths. VCA results for various dynamic and static quantities are presented as a function of cluster size.

P–32 **Series Expansion Methods for Lattice Models**
**Andreas Hehn, (ETHZ)**
We present an application for high order series expansions which is publicly available for calculations on quantum magnets and Bose-Hubbard models. The application we developed as part of the Swiss Platform for High-Performance and High-Productivity Computing (HP2C) is capable of calculating high-temperature series as well as ground-state series for various lattices. We explain the principles of the methods and discuss their scope and limitations. We present showcase examples and illustrate how to extract thermodynamic and critical properties such as susceptibilities, correlation functions or excitation gaps from the series.

P–33 **Multigrid Algorithm for the Density Matrix Renormalization Group**
**Michele Dolfi[1], Bela Bauer[2], Matthias Troyer[1], Zoran Ristivojevic[3]**
[1] **Theoretische Physik, ETH Zurich, [2] Physics Department, University of California, Santa Barbara, [3] Laboratoire de Physique Thorique-CNRS, Ecole Normale Suprieure, Paris**

The density matrix renormalization group (DRMG) method often fails to converge in systems with multiple length scales, such as lattice discretization of continuum optical lattices. The local optimizations employed by DMRG to optimize the wave function are ineffective in updating large scale features. Here we present a multigrid algorithm[1] that solves these convergence problems by optimizing the wave function at different spatial resolutions.

We demonstrate its effectiveness by simulating bosons in continuous space with an external optical lattice potential. We study non-adiabaticities when ramping up the strength of the external potential, and we suggest new ramping profiles to be employed in cold atoms experiments.

The algorithm can be generalized to tensor network methods, and be combined with the contractor renormalization group (CORE) method to study dilute and weakly doped lattice models such as Hubbard ladders.
[1] M. Dolfi, B. Bauer, M. Troyer and Z. Ristivojevic, Phys. Rev. Lett. 109, 020604 (2012)

P–34 **Time Evolution Within A Comoving Window**
**Valentin Zauner, University of Vienna**
We present a modification of Matrix Product State time evolution to simulate the propagation of signal fronts on infinite one-dimensional lattice systems. We restrict the calculation to a window moving along with a signal, which by the Lieb-Robinson bound is contained within an effective light cone. Signal fronts can be studied unperturbed for much longer times than on finite systems. Entanglement inside the window is naturally small, greatly lowering computational effort. We calculate the time evolution of signals in the Transverse Field Ising (TFI) model and in the XXZ spin-half antiferromagnet after local quantum quenches. In both models, we observe distinct magnetization plateaus. In the TFI model, their dynamical scaling follows universal power laws and the plateaus can be interpreted as individual propagating particles. In the XXZ model the dynamic scaling also follows power laws with exponents dependent on the model parameters.

P–35 **Quantum Monte Carlo Simulations of inhomogeneous wires**
**Denis Morath, Kaiserslautern**
Inhomogeneities are of fundamental importance in real one dimensional wires, e.g. in the form of impurities or contacts (leads). Even in perfect one-dimensional optical lattices for ultracold atomic gases, inhomogeneous trapping potentials need to be considered. We now use the Stochastic Series Expansion (SSE) to investigate transport through junctions in spinless inhomogeneous wires, ie. with changing hopping parameters, chemical potential and/or interaction strength along the wire. We compare our results to field theoretical calculations from Luttinger liquid theory. We can show that there exists an unstable conducting fixed point in two wires at arbitrary filling connected at a junction when we tune the bulk parameters of the wire appropriately. We analyze the density as well as correlation functions $\langle S^+S^-(\tau)\rangle$ in imaginary time, which confirms new exponents of a non trivial universality class that are influenced from both sides of the junction.

P–36 **Quantum Monte Carlo Simulations of Trimerized Antiferromagnetic Systems**
**Dominik Straßel, Kaiserslautern**
We consider linear clusters of three strongly coupled spins S = 1/2 (trimers), which are connected more weakly in a two dimensional lattice using Stochastic Series Expansion Quantum Monte Carlo simulations of the Heisenberg model in a magnetic field. In general these systems show a magnetization plateau at 1/3 saturation, which is already known from strongly coupled three-leg ladders. Interestingly the origin of the plateau is very similar to the 1/3 plateau in frustrated lattices (e.g. the triangular lattice) so that the analogous phase transitions can be analyzed using non-frustrated systems, which do not suffer from the infamous minus sign problem. With increasing coupling between the trimers, the plateaux vanishes and a critical point can be identified. We also analyze the behavior in the limit of weak inter-trimer coupling.

P–37 **Universal behavior beyond multifractality in quantum many-body systems**
**David Luitz, Toulouse**
How many states of a configuration space contribute to a wave-function? Attempts to answer this ubiquitous question have a long history in physics and chemistry, and are keys to understand e.g. localization phenomena. Quantifying this aspect has often been overlooked for interacting many-body quantum systems, mainly due to the exponential growth of the configuration (Hilbert) space. Here, we introduce two Monte Carlo schemes to calculate Shannon-Renyi entropies for ground-states of large quantum many-body systems that are out of reach for any other exact method. Our simulations reveal that the very nature of quantum phases of matter and associated transitions is captured by universal subleading terms in these entropies, on top of a generic dominant multifractal behavior.

P–38 **Antiferromagnetism in Metals, Beating the Sign-Problem**
**Max H. Gerlach and Simon Trebst, Köln**
The possibility of itinerant electrons to undergo a transition into a magnetically ordered state has long been appreciated as one of the necessary precursors to the onset of superconductivity in materials such the electron-doped cuprates or more recently the iron pnictides. Understanding such a quantum-critical transition in full detail has remained a key challenge for both analytical and numerical approaches. On the computational side, a numerically exact simulation of such itinerant electron systems via Monte Carlo studies has been precluded by the infamous fermion sign-problem – a situation which typically leaves little hope for further progress. As such the recent realization by Erez Berg and collaborators that one can deform the originally sign-problem-inflicted model in a controlled way, such that the universal properties of this quantum-critical point are preserved, while completely removing the sign-problem in a determinantal quantum Monte Carlo approach, opens an ingenious inroad into this long-standing problem. This poster will give a pedagogical introduction to the problem, outline the seminal conceptual approach of Berg et al., as well as show various numerical results which we obtained by implementing this adapted determinantal quantum Monte Carlo technique. Our results extend the perspective of Berg et al., thereby further improving our understanding of the rich physics of a relatively simple single-band electron model appropriate for the cuprates.

P–39 **Topological entropies for the toric code in a magnetic field**
**Johannes Helmes, Köln**
Although the concept of topological order  long-range order beyond the conventional paradigm of symmetry broken order  has been introduced more than two decades ago, its unambiguous identification and quantita- tive characterization has remained a challenging task for both theory and experiment. Since long-range quantum mechanical entanglement is a key factor in forming this peculiar order, it is natural to look for fingerprints of topolog- ical order in various measures of entanglement. Much progress has recently been achieved by carefully investigating entanglement entropies like the von Neumann or the Renyi entropies, which expose the precious information on long-range entanglement in their scaling behavior. Particularly the Renyi entropies have received much attention from the numerical community due to their accessibility in quantum Monte Carlo simulations. On this poster, we present a quantum Monte Carlo method to calculate Renyi entropies for a prototypical lattice model harboring a non-trivial topological phase  the toric code model augmented by a magnetic field. Using stochastic series expansion techniques we calculate the topological corrections to the entanglement entropies for various field strengths, which allows us to unambiguously track the topological phase up to a quantum phase transition into a trivial phase.

P–40 **Diagrammatic Monte Carlo for the Hubbard model**
**Jan Gukelberger, ETHZ**
Diagrammatic Monte Carlo (DiagMC) is a new technique for correlated fermionic systems based on sampling Feynman diagrammatic series. In contrast to conventional QMC methods, which are generally limited to small system sizes by the fermionic sign problem, DiagMC is formulated directly in the thermodynamic limit, while

the sign problem is related to the diagram expansion order. The latter fact is crucial for rendering the sign problem manageable. Although so far DiagMC applications have been mostly focused on accurate determination of equations of state, the approach can be straightforwardly extended to calculating two-particle correlation functions to access phase diagrams. We describe the method for the Hubbard model as an instructive case and present results in two and three dimensions.