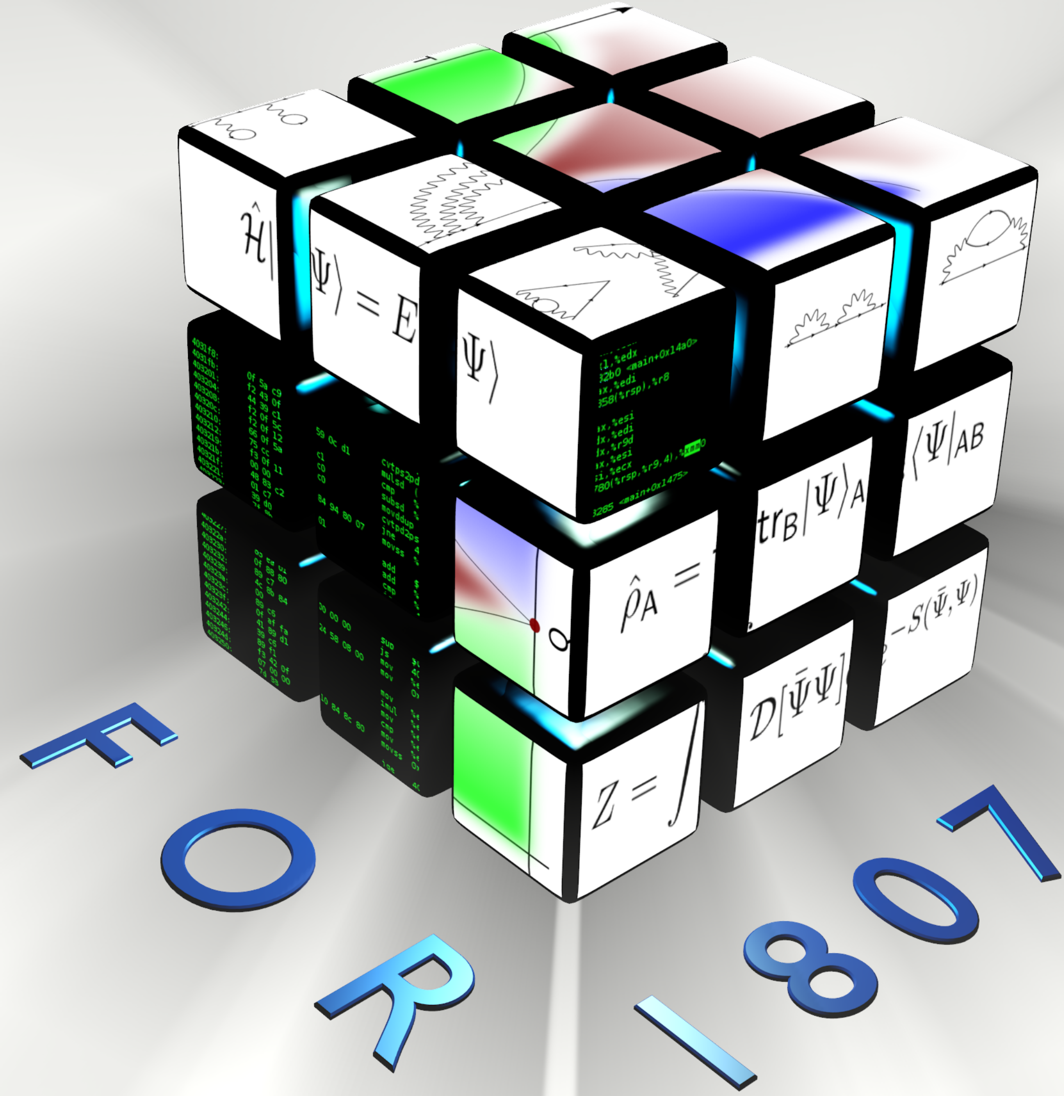
Advanced Numerical Algorithms for Strongly Correlated Quantum Systems



Würzburg, February 23 - 26 2015

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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.