

## TT 36: Focus Session: Advanced Algorithms for Strongly Correlated Quantum Matter

One of the aims of simulations of correlated electron systems is to understand the emergent collective phenomena inherent to this system class. The Focus Session will review recent highlights in this domain and address the following questions. What role can we expect quantum computing to play? Which models possess topologically ordered phases and how do we detect this exotic state of matter? How do we understand quantum phase transitions beyond the Landau paradigm, and can we find numerically solvable model systems which confirm exotic scenarios? Answers to the above questions are based on innovative algorithmic work in the domains of tensor networks, DMRG, and quantum Monte Carlo.

Organizer: Fakher Assaad (Uni Würzburg)

Time: Tuesday 9:30–12:15

Location: HSZ 03

**Invited Talk** TT 36.1 Tue 9:30 HSZ 03  
**Quantum Computing and Strongly Correlated Materials** —  
 ●MATTHIAS TROYER — ETH Zurich

Feynman's proposal of using quantum mechanics to solve hard quantum problems was the origin of the field of quantum computing. The same idea is at the heart of optical lattice quantum simulators, which can be viewed as special-purpose analog quantum computers. As successful as optical lattice quantum simulators are in emulating the Hubbard model and variants thereof, they suffer from several limitations: they can only simulate particular models that arise naturally from the underlying quantum system used to build the simulator, and reaching low effective temperatures is a challenge. Both of these problems can be overcome on (future) universal quantum computers. With small quantum computers becoming feasible in the next years it is time to think about how a quantum computer can help us solve strongly correlated electron problems. In this talk I will thus review quantum algorithms for the simulation of quantum systems and will estimate what size quantum computer could outperform a classical computer for these problems. I will also show that the exact ab-initio simulation of materials will be infeasible even on quantum hardware and that thus the model-based approach of first mapping materials to effective models will remain crucial.

**Invited Talk** TT 36.2 Tue 10:00 HSZ 03  
**Quantum Monte Carlo Simulations of Deconfined Quantum-Criticality** — ●ANDERS SANDVIK — Boston University, USA

I will discuss recent results, based on quantum Monte Carlo (QMC) simulations, for the quantum phase transition from the standard Neel state of a 2D antiferromagnet into a non-magnetic valence-bond solid state. The transition has been achieved in two different classes of models which are amenable to large-scale QMC simulations. These models can be defined with  $SU(N)$  spins for several different values of  $N$ , and results for these models can be compared with  $1/N$  expansions of the quantum field-theory proposed to describe the "deconfined" transition. I will also discuss results for thermodynamics, which indicate that deconfined spinons can describe the excitation spectrum at criticality.

**Invited Talk** TT 36.3 Tue 10:30 HSZ 03  
**Characterizing Entanglement Entropy with Quantum Monte Carlo** — ●ROGER MELKO — University of Waterloo 200 University Ave. W. Waterloo, ON N2L 3G1

An understanding of entanglement across a bipartition can give novel perspectives on correlations in condensed matter systems. Entanglement probes geometric and topological properties of the bipartition, and resultant paradigms such as the "area" law have led to important resources for characterizing quantum phases and phase transitions. The full power of these resources has only recently been exploited in two dimensions and higher, since the advent of algorithms to cal-

culate the Renyi entanglement entropies in quantum Monte Carlo (QMC). Estimators for the Renyi entropies, mostly based on replica-trick methods borrowed from quantum field theory, are now routinely exploited in almost all flavours of QMC, including Stochastic Series Expansion,  $T=0$  Projector, Auxiliary Field, and Path Integral Monte Carlo for particles in the continuum. In this talk, I will discuss the common underpinning of all replica-trick methods, as well as some advanced algorithmic tactics required to obtain statistical control of the Renyi entropy estimators. Finally, I will illustrate the use of Renyi entropies as a resource in condensed matter systems, e.g. measurement of topological entanglement entropy in spin liquid phases, identification of broken continuous symmetries, and calculation of universal quantities at quantum critical points.

15 min. break.

**Invited Talk** TT 36.4 Tue 11:15 HSZ 03  
**Field-Induced Superfluids and Bose Liquids in Projected Entangled Pair States** — ●DIDIER POILBLANC — CNRS & University of Toulouse, Toulouse, France

In two-dimensional incompressible quantum spin liquids, a large enough magnetic field generically induces "doping" of polarized  $S=1$  triplons or  $S=1/2$  spinons. We review a number of cases such as spin-3/2 AKLT or spin-1/2 Resonating Valence Bond (RVB) liquids where the Projected Entangled Pair States (PEPS) framework provides very simple and comprehensive pictures. On the bipartite honeycomb lattice, simple PEPS can describe Bose condensed triplons (AKLT) or spinons (RVB) superfluids with transverse staggered (Neel) magnetic order. On the Kagome lattice, doping the RVB state with deconfined spinons or triplons (i.e. spinon bound pairs) yields uncondensed Bose liquids preserving  $U(1)$  spin-rotation symmetry. We find that spinon (triplon) doping destroys (preserves) the topological  $Z_2$  symmetry of the underlying RVB state. We also find that spinon doping induces longer range interactions in the entanglement Hamiltonian, suggesting the emergence of (additive) log-corrections to the entanglement entropy.

[1] D. Poilblanc, N. Schuch, and J.I. Cirac, Phys. Rev. B 88, 144414 (2013) and references therein.

**Invited Talk** TT 36.5 Tue 11:45 HSZ 03  
**Nature of the Spin Liquid Ground State of the Kagome Model** — ●ULI SCHOLLWÖECK — Department of Physics, University of Munich

In this talk, I will discuss the identification of the spin liquid ground state of the Heisenberg antiferromagnet on a kagome lattice by ground state analysis, gap calculations and topological entanglement. All the numerical evidence obtained by the density-matrix renormalization group points to a  $Z_2$  quantum spin liquid.