We study the quantum critical phase of an SU(2) symmetric spin-2 chain obtained from spin-2 bosons in a one-dimensional lattice. We obtain the scaling of the finite-size energies and entanglement entropy by exact diagonalization and density-matrix renormalization group methods. From the numerical results of the energy spectra, central charge, and scaling dimension we identify the conformal field theory describing the whole critical phase to be the SU(3)1 Wess-Zumino-Witten model. We find that, while the Hamiltonian is only SU(2) invariant, in this critical phase there is an emergent SU(3) symmetry in the thermodynamic limit.

B06-04 Invited
Quantum Monte Carlo study of Disordered Spin Systems
Dao-Xin Yao1, 2, *, Nvsen Ma1, Anders W Sandvik2
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We use quantum Monte Carlo method to study the disordered S=1/2 quantum spins on the square lattice with three different nearest neighbor interactions J1, J2 and J3. Here J1 represents weak bonds, and J2 and J3 correspond to stronger bonds which are randomly distributed on columnar rungs forming coupled 2-leg ladders. By tuning the average value of J2 and J3, the system undergoes Neel-glass-paramagnetic quantum phase transition. A wide range of Mott glass phase has been found. We notice that its uniform susceptibility in the glass phase follows $\chi \sim \exp(-b/T^\alpha)$, where 0<$\alpha$<1. This dimerized disordered quantum spin system shows the violation of Harris criterion. Furthermore, we study a disordered quantum spin chain, which shows a new power law decay for the dimer-dimer correlation function.


B06-05 Keynote
Quest for Deconfined Criticality in Two-Dimensional Heisenberg Model
Naoki Kawashima
Institute for Solid State Physics, University of Tokyo, Japan
The deconfined critical phenomena (DCP) is characterized by unbinding of spinon pairs. Thus created free spinons condense to form magnetically ordered state. In this sense, the deconfined criticality is a form of magnetic phase transition. What makes this phase transition unique is that in lattice systems, before unbinding, the spinon pairs align with each other breaking the lattice rotational symmetry. Therefore, the symmetry is broken on both sides of the transition with different types of the broken symmetry; spin-rotational symmetry broken on the condensed side and lattice-rotational symmetry on the confined side. Since these theoretical predictions [1], there have been a number of attempts at detecting this transition in two-dimensional quantum systems. Now it is widely accepted that the DCP in two dimensions is quite elusive if it exists at all. After summarizing previous attempts, I present our latest results on this issue based on quantum Monte Carlo simulation. [2] We studied SU(N) Heisenberg model with 3- or 4- body interaction terms to control the quantum fluctuation up to the system size of L=384. We observed quantum phase transitions in SU(N) (N=2,3,4) models on square and honeycomb lattices. Finite-size scaling plot seems to work reasonably well, indicating very long correlation lengths even if the transition is of the first order. However, the estimated values of critical exponents systematically drifts toward the values expected for the first order transition as we change the set of system sizes to be used in the analysis.

B06-06 Invited
Neel to valence-bond-solid phase transitions in correlated valence-bond states
Yu-Cheng Lin
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We study generalizations of the singlet-sector amplitude-product (AP) states in the valence-bond basis of S = 1/2 quantum spin systems. In the standard AP states, the weight of a tiling of the system into valence bonds (singlets of two spins) is a product of amplitudes depending on the length of the bonds. We introduce generalized AP states which include correlated weights for short-range bonds. With these correlated amplitude product (CAP) wave functions, Neel to columnar/ plaquette valence-bond solid (VBS) phase transitions are realized as a function of some parameter describing the bond correlations. We study such phase transitions of CAP wave functions on the two-dimensional square lattice. We find examples of direct first-order Neel-VBS transitions, as well as cases where there is an extended U(1) spin liquid phase intervening between the Neel and VBS states. In the latter case the transitions are continuous and we extract critical exponents and address the issue of a possible emergent U(1) symmetry in the near-critical VBS.

B06-07 Invited
Quantum Monte Carlo Study of Quantum Criticality on SO(N) Bilinear-Biquadratic Chains
Kenji Harada1,*, Kouichi Okunishi2
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Using a generalized Jordan-Wigner transformation combined with the defining representation of the SO(N) spin, we map the SO(N) bilinear-biquadratic spin chain into the N-color bosonic particle model[1]. Since the Jordan-Wigner transformation disentangles the symmetry-protected topological entanglement, this bosonic model becomes negative-sign-free in the context of quantum Monte Carlo simulation. There are two quantum critical points at the both ends of the original symmetry-protected topological phase. One of them has an SO(N) symmetry, and the other has an SU(N) symmetry. We report their quantum criticality in the SO(N)=3,4,5,6) cases from quantum Monte Carlo simulations[2].

B06-08 Keynote
Superconducting mechanisms of iron-based and cuprate superconductors
Masatoshi Imada
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Two families of high temperature superconductors whose critical temperatures are higher than 50K are known. One is the copper oxides and the other is the iron-based superconductors. Here we first present an overview of the ab initio numerical method developed for strongly correlated electron systems. This multi-scale ab initio scheme for the correlated electrons is applied to an electron-doped iron-based superconductor LaFeAsO. The superconductivity is reproduced in the variational Monte Carlo calculations in accordance with the experiments. The mechanism of the superconductivity is identified as enhanced uniform density fluctuations by one-to-one correspondence with the instability toward inhomogeneity driven by first-order antiferromagnetic (AF) and nematic transitions. The mechanism is analyzed in terms of the underlying orbital selective Mottness. Despite many differences, certain common features with the copper oxides are found. The emergence of the superconductivity in the copper oxides is further analyzed by the dynamical mean-field calculations. From one-to-one correspondence of the gap function and the Green’s function between the model for the cuprates and a simple two-component fermion model, we show evidence for the existence of hidden fermions that give birth to the strongly bound Cooper pairs. The hidden fermions survive even above Tc and generate the strange-metal pseudogap phase.

B06-09 Invited
New scheme to calculate superconductivity instabilities in correlated electronic systems beyond single-site DMFT
Zi Yang Meng
Institute of Physics, Chinese Academy of Sciences, Beijing, China
In this talk, I will present a new numerical scheme to calculate the non-local, two-particle vertex functions beyond the dynamical mean field theory (DMFT) simulations, in which one first measures the local vertex functions in DMFT, then introduces the momentum-dependence into the two-particle vertex and correlation functions with the help of two-particle diagrammatic techniques-Bethe-Salpeter equation and Parquet equations. After that, I will present the application of such scheme to the measurement of superconductivity instabilities in several strongly correlated systems: in Hubbard model on square lattice with type-II van Hove singularity, a topological p+ip triplet pairing instability is found; in the t2g multi-orbital correlated system with strong spin-orbit coupling, a two-fold degenerate, odd-parity, p-wave triplet pairing instability is observed when Hund’s coupling is comparable with spin-orbit coupling, and a d-wave singlet pairing state is found in when Hund's coupling is small.
2. arXiv:1408.1407

B06-10 Invited
Quantum criticality, fractal nodal surface and the scaling behavior of the entanglement entropy in an interacting Fermion system
Tao Li
Renmin University of China, Beijing, China
Entanglement entropy has emerged as an important way to characterize the intricate quantum structure of many body systems in recent years. At a quantum critical point, entanglement entropy will exhibit exotic scaling behaviors. Early on, it has been proposed that the transition from the Fermi liquid to the non-Fermi liquid phase in an interacting Fermion system is accompanied by the appearance of fractal nodal surface in the many body wave function and can be driven by changing the strength of the back-flow correction. In this talk, we will first introduce our efforts to improve the efficiency of the Monte Carlo algorithm to simulate the entanglement entropy of gapless Fermion systems. We will then discuss the application of the new algorithm to the back-flow wave function. The phase structure of the many body wave function is found to play an crucial role in the entanglement property of the system.

B06-11 Keynote
Tensor-network algorithms and frustrated quantum magnetism
Frederic Mila
École polytechnique fédérale de Lausanne
Frustrated quantum magnetism remains a very lively field of research after more than two decades of intensive activity for two reasons: the impressive progress in the synthesis and characterization of frustrated magnets (e.g. the spin-1/2 kaogme herbertsmithite), and the lack of reliable theoretical approaches (paradigmatic models such as the spin-1/2 kaogme antiferromagnet or the J1-J2 model on the square lattice are still heavily debated). In this talk, I will review the results recently obtained on various problems using the newly developed tensor-network algorithms, with emphasis on the iPEPS algorithm (infinite Product of Entangled Pair States) that has allowed to solve the 15-year old puzzle of the magnetization plateau of SrCu2(BO3)2.
Spin Liquids on the Kagome Lattice

Andreas Lauchli

Institut für Theoretische Physik, Universität Innsbruck, Austria

In this talk I will present recent results for S=1/2 and S=1 spin models on the Kagome lattice and provide new insights into proposed spin liquid phases.

Tensor Renormalisation using Projected Entangled Simplex States: New Insight into the Kagome Conundrum

Bruce Normand

Renmin University of China, Beijing, China

We propose a new class of tensor-network states, the projected entangled simplex states (PESS), for studying the ground-state properties of quantum lattice models. These states extend the pair-correlation basis of projected entangled pair states (PEPS) to a simplex. PESS are an exact representation of the simplex-solid states and provide an efficient trial wavefunction that satisfies the area law of entanglement entropy. We implement a simple-update scheme for evaluating PESS wavefunctions based on imaginary-time evolution and the higher-order singular-value decomposition of tensors. By applying this method to the spin-1/2 antiferromagnetic Heisenberg model on the Kagome lattice, we obtain accurate and systematic results for the ground-state energy, which approach the lowest upper bounds yet estimated for this quantity.

Supersolid phases in the extended Shastry-Sutherland model

Keola Wierschem

National Taiwan University

The low temperature magnetic properties of several rare-earth tetraborides have been shown to be well-characterized by an extension of the Shastry-Sutherland model (SSM) to include additional next-nearest-neighbor bonds and anisotropic spin exchange interactions. In the case of ferromagnetic transverse exchange, this model is equivalent to a system of hard-core bosons with unfrustrated hopping and is free of the quantum Monte Carlo (QMC) sign problem. Using large-scale QMC simulations, we study the phase diagram of the extended SSM in a parameter regime that stabilizes a zero-temperature phase transition to a spin supersolid phase. By comparing the overall magnetization process to experimental observations of ErB4, a rare-earth tetraboride with ground-state columnar antiferromagnetic ordering, we speculate that a field-induced supersolid phase may be present in ErB4. Finally, we briefly consider supersolid phases in other parameter regimes of the SSM and discuss criteria for searches of the novel Bose condensation.

Correlated topological insulators

Fakher Assaad

Universität Würzburg, Germany

Topological insulators have become one of the most active research areas in condensed matter physics. They combine the interplay between spin-orbit coupling and correlations. In this talk I will review recent numerical results, pertinent to the understanding of correlations effects on edge states of topological insulators as well as correlation induced topological insulators possibly realized in the heavy fermion compound SmB6.

Chiral and Time-reversal Invariant Spin Liquids in Anisotropic Kagome Antiferromagnets

Yang Chen

Laboratory of Advanced Materials, Fudan University, China

Kalmeyer-Laughlin (KL) chiral spin liquid (CSL) is a type of quantum spin liquid without time-reversal symmetry, and it is considered as the parent state of exotic anyon superconductor. Such an exotic state has been sought for more than twenty years; however, it remains unclear whether it can exist in a realistic system where time-reversal symmetry is breaking spontaneously. Within the matrix renormalization group, we show that KL CSL exists in a frustrated anisotropic kagome antiferromagnets, which has time-reversal symmetry breaking. We find that our model has two topological degenerate ground states, which exhibit nonvanishing scalar chirality order and are protected by finite excitation gap. Furthermore, we identify this state as KL CSL by the characteristic edge conformal field theory from the entanglement spectrum and the quasiparticles braiding statistics extracted from the modular matrix. Next we study spin-liquid phases of spin-1/2 XXZ kagome antiferromagnets. We find that the emergence of the spin-liquid phase is independent of the anisotropy of the XXZ interaction. In particular, the two extreme limits—the Ising and the XY—host the same spin-liquid phases as the isotropic Heisenberg model. Both a time-reversal-invariant spin liquid and a chiral spin liquid are obtained. We show that they evolve continuously into each other by tuning the second and the third-neighbor interactions.

Violation of the spin statistics theorem and the Bose-Einstein condensation of particles with half integer spin.

Harley D. Scammell, Oleg P. Sushkov

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The usual wisdom is that only particles with integer spin obey Bose statistics and hence only those particles can form a Bose condensate. However, in some cases the spin-statistics relation can be violated and particles with half integer spin obey Bose statistics. Examples of such violation are under discussion in solids and in cosmology (dark matter).

In the work we bring the following messages.

(i) Topological excitations in spin systems, spinons and antispinons, have spin 1/2 and they are bosons.
(ii) Spinons Bose condense under some conditions.
(iii) The Bose condensate is very unusual, particularly unusual are Goldstone modes of the condensate which do not support Landau criterion of superfluidity.
(iv) We discuss criteria for searches of the novel Bose condensation in QMC simulations.

Half-magnetization plateau of a dipolar spin ice in a [100] field

Sheng-Ching Lin
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Ying-Jer Kao

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We report here numerical results of the low-temperature behavior of a dipolar spin ice in a magnetic field along the [100] direction. Tuning the magnetic field, the system exhibits a half-magnetization plateau at low temperature. This half-polarized phase should correspond to a quantum solid phase in an effective 2D quantum boson model, and the transition from the Coulomb phase with a power-law correlation to this state can be regarded as a superfluid to a quantum solid transition. We discuss possible experimental signatures of this half-polarized state.

Solving fermion sign problem in quantum Monte Carlo by Majorana representation

Zi-Xiang Li, Yi-Fan Jiang, and Hong Yao

B06-19 Invited

B06-18 Invited

B06-15 Keynote

B06-14 Invited

B06-13 Invited

B06-12 Invited
In this talk, we shall discuss a recently-discovered quantum Monte Carlo (QMC) method to solve the fermion sign problem in interacting fermion models by employing Majorana representation of complex fermions. We call it "Majorana QMC" (MQMC). Especially, MQMC is fermion sign free in simulating a class of spinless fermion models on bipartite lattices at half filling and with arbitrary range of (unfrustrated) interactions. To the best of our knowledge, MQMC is the first auxiliary field QMC method to solve fermion sign problem in spinless (more generally, odd number of species) fermion models. MQMC simulations can be performed efficiently both at finite and zero temperatures. We believe that MQMC could pave a new avenue to solve fermion sign problem in more generic fermionic models.

[1] Zi-Xiang Li, Yi-Fan Jiang, and Hong Yao, arXiv:1408.2269
[2] Zi-Xiang Li, Yi-Fan Jiang, and Hong Yao, arXiv:1411.7383

B06-20 Invited
Practical linear scaling simulation of Born-Oppenheimer dynamics
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Born-Oppenheimer molecular dynamics (MD) is increasingly being applied to a wide range of problems in physics, chemistry, and materials science. However, the large cost to calculate the electronic energy at each time step makes existing linear-scaling methods impractical. Here we present an extension of the stochastic kernel polynomial method that benefits from any type of density matrix decay. By carefully introducing correlations between the random vectors, we improve the rate of stochastic convergence. Our GPU-based implementation of this linear scaling algorithm enables practical MD simulation of tens of thousands of atoms, for tight-binding models of insulators and metals.