



**The Abdus Salam  
International Centre for Theoretical Physics**



## **Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter**

**24-29 July 2011  
ICTP - Trieste, Italy**

**Venue: ICTP Leonardo Building - Main Lecture Hall -**

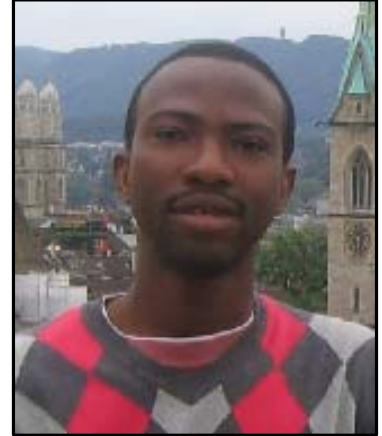
Co-Sponsored by:  
ICAM-I2CAM Institute for Complex Adaptive Matter; NSF Grant DMR-0844115  
and  
Boston University

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**Investigation on the applicability of lattice density functional theory for describing 1D correlated electronic systems in an electric field**

We describe theoretical investigation into the electrical properties of strongly correlated one-dimensional metals. Our studies are based on Bethe Ansatz local density approximation (BALDA) to the exchange correlation (XC) energy functional of ground state density functional theory on a lattice (LDFT) [1, 2]. The BALDA calculated values are compared with those obtained by numerically accurate methods, such as exact diagonalization and density matrix renormalization group, over a broad range of parameters. We validate the capability of LDFT with BALDA to compute static linear polarizabilities for finite 1D chains [3]. The response of the exact XC potential is found to point in the same direction as an external electric field. This is well reproduced by the BALDA approach, although fine details depend on the specific parameterization for the local approximation [3].

1. Lima, Silva, Oliviera and Capelle PRL \*90,\* 146402 (2003)
2. Xianlong \*et al\* PRB \*73,\* 165120 (2006)
3. Akande and Sanvito PRB \*82\*, 245114 (2010)

**E. ANDRADE**

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**Impurity driven order in gapped magnets**

We study magnetic order induced by non-magnetic impurities in quantum paramagnets with incommensurate host spin correlations. In contrast to the well-studied commensurate case where the defect-induced magnetism is spatially disordered but non-frustrated, the present problem combines strong disorder with frustration and, consequently, leads to spin-glass order. We numerically compute both thermodynamic quantities and neutron-scattering structure factors and find the spin-glass to display robust short-range order at the wavevector imprinted by the host correlations. We relate our findings to magnetic order in both  $\text{BiCu}_2\text{PO}_6$  and  $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$  induced by Zn doping.

**Sh. A. AYUPOV**

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## **OPERATOR ALGEBRAS AND QUANTUM DYNAMICS**

### ***Derivations and Automorphisms on Algebras of Measurable Operators***

Given an algebra  $A$ , a linear mapping  $\alpha : A \rightarrow A$  (respectively  $d : A \rightarrow A$ ) is called *an automorphism* (respectively, *a derivation*) if it satisfies the condition  $\alpha(xy) = \alpha(x)\alpha(y)$  (respectively,  $d(xy) = d(x)y + xd(y)$ ) for all  $x, y$  in  $A$ .

In this talk we study derivations and automorphisms on algebras of bounded and unbounded operators on a Hilbert space, emphasizing their properties such as innerness and spatialness. These notions are very important in the structure theory and cohomology of abstract ring and algebras and at the same time they have deep applications in quantum dynamics. Therefore we also discuss a physical background for derivations and automorphism of operator algebras.

Namely, in the quantum field theory the dynamical evolution is given by a group of automorphisms of an operator algebra  $A$  (of observables) and the infinitesimal motion is described by some form of Hamiltonian formalism incorporating the interpartical interaction. The *basic problem* which occurs in this approach – is the integration of this infinitesimal motion in order to obtain the dynamical flow. In terms of *operator algebras* this means: to prove that the given *derivation* on the algebra of observables is the infinitesimal generator of a one-parameter automorphisms group, moreover it is *spatial* (i.e. defined by some Hamiltonian operator) or even *inner* (i.e. the Hamiltonian operator itself is an observables in the considered physical system).

After exposition of some well-known result on bounded derivations on  $C^*$ -algebras and von Neumann algebras we consider open problems concerning derivations and automorphisms of unbounded operator algebras, namely algebra of measurable operators affiliated with von Neumann algebras and faithful normal semi-finite traces. Finally we give solutions of the mentioned problems for algebras of measurable operators affiliated with type I von Neumann algebras.

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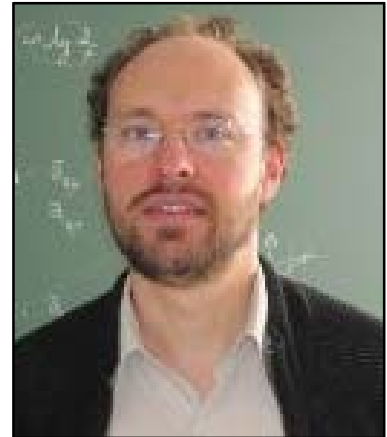


**Maximal entanglement of bipartite spin states  
in the context of quantum algebra**

In the framework of the  $U_q(\mathfrak{su}(2))$  quantum algebra, we investigate the entanglement properties of two-spin systems, of arbitrary spins  $j_1$  and  $j_2$ , defined in an entanglement of deformed spin coherent states of each of the spins. We derive the amount of entanglement and we give conditions under which bipartite entangled states become maximally entangled. Using these conditions, we construct a large class of Bell states for any choices of the parameters that specify the spin coherent states.

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### **Resonant color state and emergent chromodynamics in the kagome antiferromagnet**

With the recent discovery of a magnetic compound that does not order down to the lowest temperatures, the question of the existence of a "spin-liquid" phase has resurfaced. The herberthsmithite  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_3$  is a model compound of strongly interacting spins that has the geometry of the kagome lattice. While no long-range order is found, the dynamics is characterized by a broad power-law response, somehow similar to that of a "critical" state.

The large-S approach breaks down in this context and the resulting ground state is unknown. I will argue that the low-energy modes responsible for this breakdown can be described by non-linear oscillators which, when quantized, lead to a quantum loop model with a gauge symmetry analogous to that of chromodynamics. It turns out that the model has long-range Néel order together with topological order at zero temperature. In addition, there are unconventional excitations that can be described by an effective gauge theory, the parameters of which will be extracted from quantum Monte Carlo. We predict that these excitations trigger a very low-temperature phase transition to a "critical" state resembling the one observed experimentally (although it is a large-S approach).

[1] O. Cépas, A. Ralko, *cond-mat/ 1104.3033* (to appear in *Phys. Rev. B*).

**C.-C. CHEN**

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**Probing the degrees of magnetic frustration in iron pnictides**

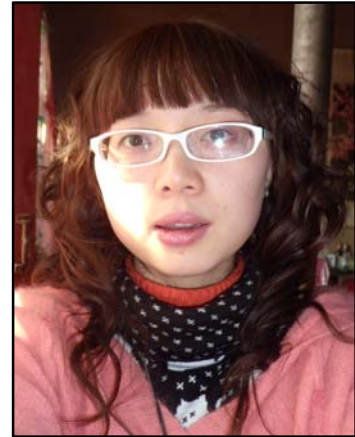
Being a central theme in condensed matter physics, magnetic frustration has now been widely discussed in iron-based superconductors. Theories for their collinear antiferromagnetism vary greatly in the amount of frustration and proximity to a quantum critical point. To distinguish these scenarios, the question is how frustration can be experimentally quantified.

We theoretically explore two possibilities to achieve the above goal. One way is to study the response of host antiferromagnets to non-magnetic impurities. We find that in a frustrated  $J_1$ - $J_2$  model, a non-magnetic impurity induces strong quantum fluctuations to its neighboring sites and results in reduced magnetic moments. In contrast, a spatially anisotropic but unfrustrated  $J_{1a}$ - $J_{1b}$ - $J_2$  model shows reduced fluctuations and enhanced local moments. The effects could be probed using  $^{75}\text{As}$  NMR and provide a benchmark to distinguish these models.

Another way is to study light scattering of two-magnon flips. We find that there exist low-energy two-magnon excitations in frustrated systems, while without frustration two-magnon flips would occur at a higher energy close to twice the single magnon bandwidth. Magnetic Raman scattering can thereby elucidate the role of frustration and help narrow models to understand magnetism in iron-based superconductors.

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**Academy of Sciences. My poster title is 'Study of Partial order of Anti-ferromagnetic Potts model by Tensor-based Numerical Method'.**

Phase transition is described by order parameter in Landau theory. At low temperature long range order exists, while at high temperature thermal fluctuation kill the long range order. Usually long range order means the system is ordered everywhere. However there could be partially ordered long range order, with only some of the lattice's sites ordered. Using the tensor-based method (TRG, SRG, iTEBD) developed recently we study this kind of order on AF Potts model. Compared to ferromagnetic Potts model the physics of anti-ferromagnetic is rich and complex, displaying many types of behavior as a function of  $q$  and of the lattice structure.

TRG is a real space coarse-graining method, while SRG is refined version of it. iTEBD is a power method by projecting transfer matrix on random vectors to derive the largest eigen value.. All these method could handle infinite size two dimensional classical statistical model by obtain the partition function. By noticing the work of  $q=3$  anti-ferromagnetic Potts model, which has partial order. We start to think whether this kind of order could appear on any other lattice.

By conjecture the partial order exist on  $q-1$  sublattices  $q$  state AF Potts model, we find order of  $q=4$  Potts model on union-jack lattice belong to this type, and the phase transition is to our knowledge never predicted by other people. Then we generalize this to other irregular lattice.



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**A DMRG Study of the Heisenberg Anti-Ferromagnet on the Kagome Lattice**

We use the Density Matrix Renormalization group to calculate the ground state of the anti-ferromagnetic Heisenberg model on the Kagome lattice. We find our results to be compatible with earlier studies by White et al. on the lattice sizes studied there and corroborate the proposed spin liquid ground state on even larger lattice sizes.

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**Continuous matrix product states for ground states and  
excited states of one-dimensional quantum fields**

The variational class of continuous matrix product states, recently developed by Verstraete and Cirac (PRL 104, 190405 (2010)), is ideally suited to study one-dimensional non-relativistic quantum field theories. In this poster, we present some recent (unpublished) results for both the ground state as well as the spectrum of low-lying excited states, as studied with the continuous matrix product state ansatz. We use imaginary time evolution according to the time-dependent variational principle to locate the variational optimum and use the tangent plane of the variational manifold at the variational optimum as an ansatz for studying the low-lying excitations. Examples for two exactly solvable models are presented.

**F. HEIDRICH-MEISNER**

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**Metamagnetism in isotropic frustrated ferromagnetic spin chains in an external magnetic field**

We show that frustrated,  $SU(2)$ -symmetric spin- $S$  chains with ferromagnetic nearest-neighbor interactions exhibit metamagnetic behavior under the influence of an external magnetic field for small  $S$ , in the form of a first-order transition to the fully polarized state. The magnetization jump increases gradually starting from an  $S$ -dependent critical value of exchange couplings and takes a maximum in the vicinity of a Lifshitz point. The metamagnetism results from resonances in the dilute magnon gas caused by an interplay between quantum fluctuations and frustration. In addition, we compute the central charge for  $S=1$  on both the ferromagnetic and the antiferromagnetic side to identify one and two-component gapless phases. The former are candidates for long-range vector chiral order.

**Y.-D. HSIEH**

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### **1D Entanglement Renormalization Implementation on GPU**

We have developed a code for 1D Multi-scale Entanglement Renormalization Ansatz (MERA), which is highly extensible code for further application on 2D or fermionic systems. To achieve higher computational performance, we have also developed a GPU version of MERA code based on Nvidia CUDA.

For 1D MERA, we have implemented the translation-invariant and scale-invariant versions of MERA. We benchmark the 1D translation- and scale-invariant MERA code on the 1D transverse-field Ising model.

**Y. IQBAL**

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### **Competing phases of the kagome $S=1/2$ quantum Heisenberg antiferromagnet**

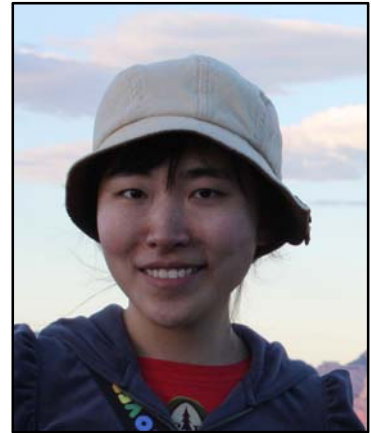
Within the class of full Gutzwiller-projected fermionic wave functions, using quantum variational Monte Carlo simulations we investigated the energetics of all possible Z2 spin liquids (gapped and gapless) on the kagome lattice which can potentially occur as ground states of the nearest-neighbor and next-nearest-neighbour  $S=1/2$  quantum Heisenberg antiferromagnet. We conclusively show that all gapped and gapless Z2 spin liquids are higher in energy compared to the U(1) gapless spin liquids in whose neighbourhoods they lie (Ref. [1]). These results contradict the recent proposal made using the density-matrix renormalization group (DMRG) method, that the ground state of the nearest neighbour  $S=1/2$  quantum Heisenberg antiferromagnet is a fully gapped Z2 spin liquid (Yan, et. al Science, 332, 1173 (2011)). In particular, the most promising gapped Z2 spin liquid (the  $Z_2[0,\pi]\backslash\beta$  state) conjectured to describe the ground state (Lu, et. al Phys. Rev. B. 83, 224413 (2011)) is always higher in energy compared to the U(1) Dirac spin liquid for both the nearest and next-nearest neighbour  $S=1/2$  quantum Heisenberg antiferromagnet. Thus, within the Schwinger fermion approach to the spin model the U(1) Dirac spin liquid has the best variational energy. We also report our earlier work (Ref. [2]) concerning the extension of the U(1) Dirac spin liquid and uniform RVB spin liquid to include 2nd nearest-neighbour hopping terms, and studied its local and global stability towards various valence bond crystal (VBC) patterns. In particular, we found that a non-trivial 36 site valence bond crystal phase is stabilized upon addition of a small ferromagnetic exchange coupling, whereas on the antiferromagnetic side we have a gapless U(1) Dirac state. It is worth mentioning that we use a sophisticated implementation of the stochastic reconfiguration optimization method within the variational Monte Carlo scheme, which enables us to obtain highly accurate values of the variational parameters.

[1]. Yasir Iqbal, Federico Becca, and Didier Poilblanc; *Phys. Rev. B* 00, 000400(R) (2011). (in press) - *arXiv: 1105.0341*

[2]. Yasir Iqbal, Federico Becca, and Didier Poilblanc; *Phys. Rev. B* 83, 100404(R) (2011). - *arXiv: 1011*.

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**Numerical studies of Resonant Inelastic  
X-ray Scattering (RIXS) in Cuprates**

We present our small cluster exact diagonalization study on momentum-resolved RIXS in cuprates, using both multi-orbital and single-band Hubbard models. We also compare RIXS and the dynamical structure factor  $S(q,w)$ , and present their qualitative distinction for insulating and electron-/hole-doped cuprates. The implementation of large-scale paralleled eigen-solver and bi-conjugate gradient stabilized method enables us to treat this complicated photon spectroscopy problem in an effective fashion.

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### **Coulomb interaction driven Pomeranchuk instability in half-integer filled Landau levels**

We investigate the Coulomb interaction driven Pomeranchuk instability mechanism of electronic nematic formation in half-integer filled higher Landau levels by calculating Fermi liquid parameters. It has been long known that  $\nu=1/2$  is a non-Fermi liquid,  $\nu=5/2$  is an incompressible quantum Hall state and  $\nu=9/2$  is an anisotropic fluid: an electronic nematic[1]. However, there has been little theoretical understanding regarding the competition between the electronic nematic phase and the quantum Hall state. Noting the former can be a consequence of Pomeranchuk instability with the Fermi liquid parameter  $F_2$  becoming less than -1, we calculate the Fermi liquid parameters for different half-filled Landau levels to test for the Pomeranchuk instability. We use composite fermion many-body wave functions on a toroidal geometry. For different Landau levels, Coulomb interaction amounts to different effective interactions for composite fermion wave function projected to lowest Landau level[2]. We calculate the excitation energy for eight independent particle-hole pair excitation configurations as well as the ground state energy using a quantum Monte Carlo algorithm through correlated sampling. For each Landau level, these nine energy values will allow us to determine the Fermi liquid parameters[3].

[1] M. P Lilly, K. B Cooper, J. P Eisenstein, L. N Pfeiffer, and K. W West, *Phys. Rev. Lett*, 83 824 (1999)

[2] F. D. M Haldane. *The Quantum Hall Effect*, edited by R.E. Prange and S.M. Girvin (Springer, New York, 1990), p.303

[3] Yongkyung Kwon, D. M Ceperley, and Richard M Martin. *Phys. Rev. B*, 50 1684, (1994)

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**Resonant inelastic x-ray scattering spectra of  
one-dimensional Mott insulators**

We present excitation spectra of resonant inelastic x-ray scattering (RIXS) processes in one-dimensional Mott insulators. The RIXS cross section of Hubbard and extended Hubbard models on finite half-filled rings is evaluated using exact diagonalization. The fundamental features of the obtained spectra reveal the different magnetic excitations occurring in indirect and direct RIXS processes, corresponding to copper K- and L-edge resonances in experiments on quasi-1D cuprates. It is shown that, whereas for indirect RIXS the prominent magnetic excitations are magnon pairs, in direct RIXS single-magnon excitations arise due to spin-orbit coupling, making it a complementary technique to inelastic neutron scattering. The analysis of the dependence of the spectral features on model parameters allows us to estimate physical parameters, such as the core-hole lifetime.



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**Triplon mean-field theory of an antiferromagnetic model with an exact fourfold degenerate Shastry-Sutherland ground state**

In a recent work [Phys. Rev. B **77**, 014419 (2008)], a quantum spin-1/2 model having an exact fourfold degenerate Shastry-Sutherland ground state was constructed, and studied using finite-size numerical exact diagonalization. There, a schematic quantum phase diagram suggesting many competing phases was also proposed. In the present work, this model is investigated using the dimer and plaquette triplon mean-field theories. The corresponding quantum phase diagram (in the thermodynamic limit) is found to have many interesting phases: commensurate and incommensurate magnetically ordered phases, and columnar dimer, Shastry-Sutherland and plaquette spin-gapped phases. Among themselves, these phases undergo a continuous or a level-crossing transition.

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### **Emergent gauge dynamics of highly frustrated magnets**

Condensed matter exhibit a wide variety of exotic emergent phenomena, such as the topological order in the fractional quantum Hall effect and the ``cooperative paramagnetic" response of geometrically frustrated magnets. I consider the constrained classical Hamiltonian dynamics of spins exploring the large configuration space associated with the latter using a method introduced by Dirac[1]. It suggests, at the semi-classical level, that all frustrated magnets have gauge dynamics. Remarkably, in the kagome lattice model I consider as an example, these dynamics are similar to the ``topological" (Chern-Simons) gauge dynamics of electrons in the fractional quantum Hall effect and have non-locally entangled edge modes as the only low energy degrees of freedom. This topological dynamics, which may be found in any nearest neighbor exchange dominated kagome-like antiferromagnet, provides a natural explanation for the apparent insensitivity of the ground state of Herbertsmithite to the out-of-plane impurity moments.

[1] Dirac, P. A. M. *{\it Generalized hamiltonian dynamics}*. *Can. J. of Math.* **{\bf 2}**, 129 (1950)

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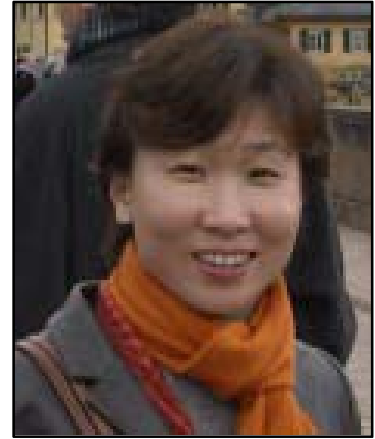
### **Spin ice in a $[100]$ field with 2nd nearest-neighbour interaction**

**Abstract:** We examine the statistical mechanics of spin-ice material with second nearest-neighbor interaction in an external magnetic field along  $[100]$ . The simulation is studied with a Monte Carlo cluster algorithm. The survival of the three dimensional Kasteleyn transition, which occurs in the nearest-neighbor spin ice model, is examined.

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### **Neel to valence-bond solid transitions in generalized amplitude-product states with correlated weights**

An amplitude-product state is a superposition of valence-bond states with the expansion coefficients being products of individual bond amplitudes that depend only on the bond shape. In two dimensions, these states have Neel order or are spin liquids, but they never have any valence-bond solid order. We construct generalized amplitude-product states on the square lattice which include correlated weights for short-range bonds. Using these states, we explore phase transitions between Neel phase, valence-bond solid phases, and spin liquid.

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**Variational cluster mean-field study of a frustrated two-orbital spin model  
on the square lattice**

We study the two-orbital frustrated spin model introduced by Si and Abrahams to describe magnetism in the iron pnictides. The "double-spin" model has an on-site Hund's coupling and inter-site interactions extending to the second-nearest neighbors on the square lattice. Dividing the lattice into small clusters, we fully optimize the cluster-product wave function for clusters with up to 8 sites (65536 cluster wave-function coefficients). We confirm the presence of two phases previously studied with spin-wave theory and exact diagonalization - a "hidden order" phase in which there is long-range magnetic order by not net on-site moment, as well as a canted phase, in which the standard ordered collinear state (when the second-nearest-neighbor interactions are strong) acquires a modulation with a canting angle that depends on the interaction parameters. The canted phase is smaller than in spin-wave theory, however with phase boundaries that are well converged as a function of the cluster size. A more general case of the double-spin model is also studied when more parameters in the Hamiltonian are subject to change. We discuss the ability of the double-spin model to describe the reduced magnetic moment of the iron-pnictides.

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### **Length- and temperature-dependent crossover of charge transport across molecular junctions**

We study the electronic transport in a molecular junction, in which each unit is coupled to a local phonon bath, using the non-equilibrium Green's function method. We observe conductance oscillates with the molecular chain length.

We observe the oscillation length period of the conductance in odd-numbered chains depends strongly on the applied bias, and the oscillatory behavior is smeared out for the bias voltage near the phonon energy. In addition, a crossover from tunneling to thermally activated transport as the length of the molecule increases is found for the phonon-free case. In the presence of electron-phonon interaction, transport is related to thermal and a transition from the thermally suppressed to assisted conduction is observed.

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**From entanglement entropy to entanglement spectrum: 1+1D CFT  
embedded in 2D valence bond solid**

We study the Affleck-Kennedy-Lieb-Tasaki (AKLT) model defined on two-dimensional symmetric graphs, whose ground state is known to be in valence bond solid (VBS) order. The entanglement entropy of 2D VBS states can be calculated from the reduced density matrix of the subsystem, defined on the boundary which separates two symmetric parts of the lattice. We investigate both square lattice and hexagonal lattice with various sizes and aspect-ratios. We show that the von Neumann entropies in our systems deviate (is less than)  $\ln 2$ — known result for 1D AKLT model.

We further study the entanglement spectrum of VBS states. We show that the reduced density matrix of the subsystem can be mapped into “entanglement Hamiltonian”, the spectrum of which resembles that of Heisenberg quantum spin chain. We observe that the low-energy entanglement spectrum of our 2D AKLT model reflects the underlying 1+1D conformal field theory with the central charge  $c = 1$ . We further investigate nested entanglement entropy (NEE) of the system to confirm our conjecture. Finite size scaling results of NEE can be well fit by CFT prediction.

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**Pairing of critical Fermi-surface states**

States of matter with a sharp Fermi-surface but no well-defined Landau quasiparticles are expected to arise in a number of physical systems. Examples include i) the spinon Fermi-surface ( $U(1)$  spin-liquid) state of a Mott insulator, ii) the Halperin-Lee-Read composite fermion liquid state of a half-filled Landau level and iii) the quantum critical point associated with the formation of nematic order in a metal. In this work, we use renormalization group techniques to investigate possible instabilities of such non-Fermi-liquids to pairing. We show that in the case of the nematic transition, the attractive interaction mediated by order parameter fluctuations always leads to a superconducting instability, which preempts the non-Fermi-liquid effects. On the other hand, the spinon Fermi-surface and the Halperin-Lee-Read states are stable against pairing for a sufficiently weak attractive short-range interaction. However, once the strength of attraction exceeds a critical value, pairing sets in. We describe the ensuing quantum phase transition between i) the  $U(1)$  and the  $Z_2$  spin-liquid states, and ii) the Halperin-Lee-Read and Moore-Read states.



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### **Competing Phases of Bosonic Atoms in 'Rotating' Optical Lattices**

For cold atomic gases on optical lattices, there is now a multitude of schemes for generating effective magnetic fields – equivalent to rotating the entire lattice, but more suitable to experimental realisations. Here we address some interesting questions about the many-body physics in such 'rotating lattices' where strong correlations are favoured by the simultaneous presence of a lattice and the effect of high magnetic fields. We review how the mapping bosons to composite fermions (CF) leads to the prediction of quantum Hall fluids that have no counterpart in the continuum [1]. Here, we focus particularly on the nature of states in the vicinity of flux density  $n\phi = 1/2$ . We show that precisely at this high symmetry point, no strongly correlated phases occur: the groundstates are Bose condensates at any density [2]. These can be thought of as vortex lattices breaking translational and time-reversal invariance. We discuss how to detect the broken symmetry by expansion images of the gas, and show that the expansion images are gauge dependent. Our general CF theory can be used to formulate trial wavefunctions for strongly correlated states at general values of the flux density. Near simple rational fractions  $n\phi = 1/k$ , it had also been proposed to treat the problem by expanding the interactions in a basis of states with periodicity  $k$  [3]. We take this expansion to the next level in the parameter  $\epsilon = 1/2 - n\phi$  for  $k = 2$ , and show that the effective interaction in the resulting two-subband state stabilises a form of pairing [4].

[1] G. Möller, N. R. Cooper, "Composite Fermion Theory for Bosonic Atoms in Optical Lattices", *Phys. Rev. Lett.* 103, 105303 (2009). [2] G. Möller, N. R. Cooper, "Condensed ground states of frustrated Bose-Hubbard models", *Phys. Rev. A* 82, 63625 (2010). [3] R. Palmer, D. Jaksch. "High-Field Fractional Quantum Hall Effect in Optical Lattices", *Phys. Rev. Lett.* 96, 180407 (2006). [4] L. Hormozi, G. Möller, S. H. Simon, to be published.

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**SU(2)-invariant Majorana spin liquid with stable parton Fermi surfaces  
in an exactly solvable model**

We construct an exactly solvable spin-orbital model on a decorated square lattice that realizes an SU(2)-invariant Majorana spin liquid with parton Fermi surfaces, of the kind discussed recently by Biswas et al., [arXiv:1102.3690]. We find power-law spin correlations as well as power-law spin-nematic correlations with the same dominant  $1/|\mathbf{r}|^3$  envelope. The model is solvable also in the presence of Zeeman magnetic field. One fermion species carries  $S^z=0$  quantum number and its Fermi surface is not altered in the field, while the Fermi surfaces of the other species evolve and can disappear. In particular, we find an interesting half-magnetization plateau phase in which spin excitations are gapful while there remain spinless gapless excitations that still produce metal-like thermal properties. In the fully-magnetized phase, the model reduces to the one proposed by Baskaran et al., [arXiv: 0908.1614v3] in terms of the orbital degrees of freedom.

*AND*

Author: Tiamhock Tay

**Variational study of J1-J2 Heisenberg model on Kagome lattice using  
projected Schwinger boson wave functions**

Motivated by the unabating interest in the spin-1/2 Heisenberg antiferromagnetic model on the Kagome lattice, we investigate the energetics of projected Schwinger boson (SB) wave functions in the  $J_1$ -- $J_2$  model with antiferromagnetic  $J_2$  coupling. Our variational Monte Carlo results show that Sachdev's  $Q_1=Q_2$  SB ansatz has a lower energy than the Dirac spin liquid for  $J_2 \gtrsim 0.08 J_1$  and the  $\mathbf{q}=0$  Jastrow type magnetically ordered state. This work demonstrates that the projected SB wave functions can be tested on the same footing as their fermionic counterparts.

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*Other authors: J. T. Chalker; P. Serna;  
M. Ortuno and A. M. Somoza.*

**Loop models, vortex lines, and sigma models in three dimensions**

Many statistical mechanics problems can be framed in terms of ensembles of random curves. In the first part of this poster we consider three dimensional classical loop models which are prototypes for such ensembles. We show that their continuum descriptions are (compact)  $CP^{n-1}$  sigma models or supersymmetric variants, where  $n$  is a loop fugacity. Using Monte Carlo simulations we identify continuous transitions for  $n=1,2,3$  and first order transitions for  $n \geq 5$ . Next we consider vortex lines in random (short-range correlated) complex fields, and show that the  $CP^{k|k}$  model describes the statistics of these defects.

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**N=4 Supersymmetric non linear sigma Models and  
Generalized Monodromy Matrix**

Two-Dimensional N=4 Supersymmetric non linear sigma Models with non Compact lie Groups  $O(d,d)/O(d) \times O(d)$  models are constructed. These large Symmetries lead to basis solutions with well defined transformations properties of T-duality. Under this latter, we construct the Generalized Monodromy Matrix  $M$  of two-Dimensional String Effective action by introducing the general Integrability conditions.

**V. OHANYAN**

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**Magneto-Thermal Properties Of The Ising-Heisenberg Orthogonal-Dimer Chain With Quantum Xxz-Triangles**

We consider an exactly solvable model of orthogonal-dimer chain with Ising and Heisenberg bond. Using the modified classical transfer-matrix technique we find exact expression for partition function and, thus, for all thermodynamic functions of the system. We investigate the issue of vast variety of its ground states, especially ones with spontaneous breaking of the translational symmetry. Analyzing ground states properties we obtain several  $T = 0$  ground states phase diagrams which correspond to different sets of the parameters. Depending of the values of parameters the system exhibits the magnetization curves with the following transitions between various magnetization plateau  $M = 0 \rightarrow M = 1$ ,  $M = 0 \rightarrow M = 1/2 \rightarrow M = 1$ ,  $M = 0 \rightarrow M = 1/4 \rightarrow M = 1/2 \rightarrow M = 1$ ,  $M = 0 \rightarrow M = 1/4 \rightarrow M = 1$ ,  $M = 1/2 \rightarrow M = 1$  and  $M = 1/4 \rightarrow M = 1/2 \rightarrow M = 1$ . The general mechanism of unit cell doubling in the lattice models with block structure and left-right asymmetry is discussed. Finally, we present a comparison of the magneto-thermal properties of the underlying purely quantum model (orthogonal-dimer chain with four various couplings) and exactly solvable system with Ising and Heisenberg bonds.

**R. ORUS**

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Germany



**Studying the robustness of topological phases with  
infinite-PEPS and pCUT methods**

We investigate the stability of the topological phases of the  $Z_2$  and  $Z_3$  Toric Code models in the presence of uniform magnetic fields by means of infinite Projected Entangled Pair State algorithms (iPEPS) and perturbative Continuous Unitary Transformations (pCUT). We find that when the perturbation is strong enough, the system undergoes a topological phase transition whose first- or second-order nature depends on the field orientation and symmetry. The phase diagrams of these systems are explored, and we see that they offer a very rich behavior in terms of different universality classes and phase transitions breaking topological order.

**F. ROSHANI**

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### **Generalized model of rumor spreading on complex social networks**

We introduce the generalized model of rumor spreading on complex networks. We derive the mean-field equations characterizing the dynamics of a rumor process and solve these equations theoretically. Our results predict under what conditions will the maximum of spreading occur? Computational results on some complex networks (scale-free (SF), small-world (SW) and random graph (ER)) are well consistent with the theoretical predictions. Our results show when the spreader choose the nodes with small degree to spread the rumor, spreading can be maximized. The time that society reaches the steady state with respect the rumor is great importance for potential applications, so we investigate the conditions that leads to less or more time of spreading the rumor.

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### **Effective models for spin liquid phases in Hubbard models**

The Hubbard model is one of the most studied microscopic models in condensed matter physics. It describes on a very simple level the interplay between the kinetics and the Coulomb interaction of electrons in solid state systems. Generically, one expects at half filling a metallic phase for large kinetics while a Mott insulator is present for large interactions. In most cases the Mott phase shows additionally long-range spin order, since the Hubbard model can be mapped to a Heisenberg model in the strong-coupling limit. A direct transition between the metal and the long-range ordered Mott insulator was considered to be the standard case for a long time.

But in recent years there are more and more evidences that especially on frustrated lattices there is the possibility of exotic and insulating intermediate phases without long-range order. It is therefore an obviously relevant question what kind of effective low-energy theory describes such Mott phases and how to derive them. This is particular complicated when the spin liquid is located close to the metal-insulator transition as for the recently discovered spin liquid of the Hubbard model on the honeycomb lattice. In this talk we discuss these issues for the Mott phase of the Hubbard model on the triangular and on the honeycomb lattice.

*H.Y. Yang, A. Laeuchli, F. Mila, and K.P. Schmidt,  
Effective spin model of the spin-liquid phase of the Hubbard model on the triangular  
lattice  
Physical Review Letters 105 , 267204 (2010)*

*H.Y. Yang and K.P. Schmidt,  
Effective models for gapped phases of strongly correlated quantum lattice models  
European Physics Letters 94 , 17004 (2011)*

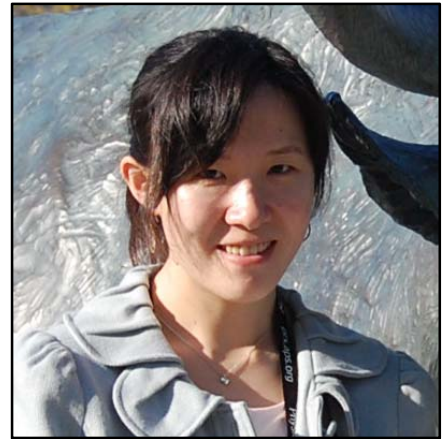


**Y. TANG**

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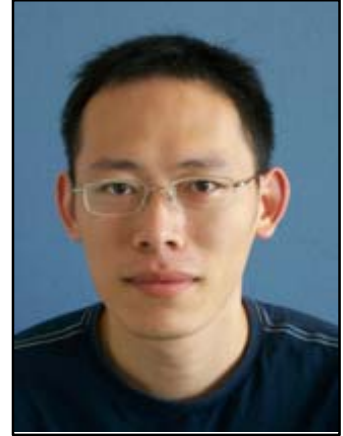
### **Method to characterize spinons as emergent elementary particles**

We develop a technique to directly study spinons (emergent spin  $S=1/2$  particles) in quantum spin models in any number of dimensions. The size of a spinon wave packet and of a bound pair (a triplon) are defined in terms of wave-function overlaps that can be evaluated by quantum Monte Carlo simulations. We show that the same information is contained in the spin-spin correlation function as well. We illustrate the method in one dimension. We confirm that spinons are well defined particles (have exponentially localized wave packet) in a valence-bond-solid state, are marginally defined (with power-law shaped wave packet) in the standard Heisenberg critical state, and are not well-defined in an ordered Néel state (achieved in one dimension using long-range interactions). We also show a method to determine whether two spinons in  $S=1$  excitation are deconfined or confined.

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### **Effective field theory for the $SO(n)$ bilinear-biquadratic spin chain**

We present a low-energy effective field theory to describe the  $SO(n)$  bilinear-biquadratic spin chain. We start with  $n=6$  and construct the effective theory by using six Majorana fermions. After determining various correlation functions we characterize the phases and establish the relation between the effective theories for  $SO(6)$  and  $SO(5)$ . Together with known results for  $n=3$  and 4, a reduction mechanism is proposed to understand the ground state for arbitrary  $SO(n)$ . Also, we provide a generalization of the Lieb-Schultz-Mattis theorem for  $SO(n)$ . The implications of our results for entanglement and correlation functions are discussed.

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**Bold Diagrammatic Monte Carlo: A new approach for  
strongly correlated fermions**

Expansion in Feynman diagrams is a standard tool of quantum many-body theory. Usually, one is restricted to a few low-order diagrams. Bold diagrammatic Monte Carlo (DiagMC) is a new technique to perform the summation of skeleton diagrams built on dressed propagators up to high order. With DiagMC, we simulate the balanced unitary gas in the normal phase. The method works directly in the thermodynamic limit and with zero-range interactions. The diagrammatic series is found to be strongly oscillating but resummable. The obtained equation of state is in good agreement with recent experiments. The contact and the critical temperature can also be extracted. The method is expected to work equally well for the imbalanced gas.

**G. WACHTEL**

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**Renormalization of the Superfluid Density in Composite Superconductors**

Underdoped cuprate superconductors exhibit high pairing energies, but low critical temperatures due to strong phase fluctuations in the pairing order parameter. It has been demonstrated experimentally, and studied theoretically within a mean-field framework, that it is possible to overcome these fluctuations by coupling the superconductor to a metallic layer. Beyond the mean-field level, we show using Monte Carlo simulations, that fluctuations considerably renormalize the superfluid density. An effective weak coupling theory is constructed in order to explain this within an analytical framework.

**L. WANG**

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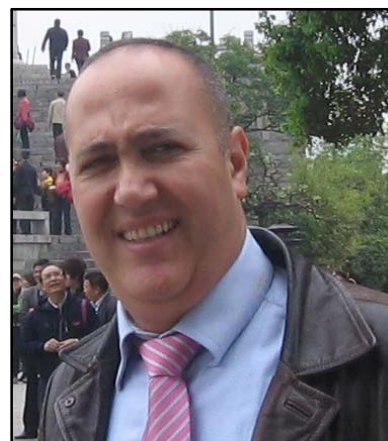
### **The J1-J2 Heisenberg Antiferromagnets on square lattice**

We studied the J1-J2 Heisenberg Antiferromagnets on square lattice via tensor network method. A grand state of fairly large bond dimension upto 10 was reached. Though finite size scaling, a vanishing of antiferromagnetic order was observed near the coupling ratio  $g=0.45$ . A small valence bond solid order emerges afterwards. Our result was compared to the exact diagonalization result upto  $N=40$ , energies differences are within 1% upto  $g=0.6$ .

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**Theoretical study of Uranyl Adsorption on Kaolinite surfaces**

In the present study, we performed various adsorption complexes depending on the degree of deprotonation of Al(o) surface hydroxyl group and the degree of deprotonation of silanol group in the defect site. We modeled 4 inner-sphere complexes where two neighboring O centers connected to the same Al atom and we also modeled 4 inner-sphere complexes with the same three different contribution surface OH center but the surface oxygen centers bound to the neighboring Al of kaolinite. Besides we have also optimized an outer-sphere complex. In this model, we did not consider SiOH defect in the Si(o) surface. A neutral system was constructed with the substitution of solvated uranyl by the corresponding neutral dihydroxide complex.