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POSTER ABSTRACTS

Effective Hamiltonians for antiferromagnetic frustrated systems in a magnetic field

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We use a real space renormalization technique in order to derive effective models for antiferromagnetic frustrated systems in a magnetic field.

More precisely, we work with the *Contractor Renormalization (CORE)* method which is a non-perturbative approach. It is capable of reproducing the low-energy physics and reducing the complexity of the system at the same time. For the spin-1/2 Heisenberg model we consider the two-leg ladder, the bilayer, and the Shastry-Sutherland geometry and discuss the existence of magnetization plateau.

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Ultrashort Lifetime Expansion for Indirect Resonant Inelastic X-ray Scattering

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In indirect resonant inelastic X-ray scattering (RIXS) an intermediate state is created with a core-hole that has an ultrashort lifetime. The core-hole potential therefore acts as a femtosecond pulse on the valence electrons [1]. We will show that this fact can be exploited to integrate out the intermediate states from the expression for the scattering cross section. By doing so we obtain an effective scattering cross section that only contains the initial and final scattering states. This effective cross section turns out to be a linear combination of the charge response function $S(\mathbf{q}, \omega)$ and the dynamic longitudinal spin density correlation function, each with a resonant pre-factor [2]. This result is asymptotically exact for both strong and weak local core-hole potentials and ultrashort lifetimes. The resonant scattering pre-factors are shown to be weakly temperature dependent. Also a sum-rule for the total scattering intensity is derived and the results are generalized to multi-band systems. One of the remarkable outcomes is that one can change the relative charge and spin contribution to the inelastic spectral weight by varying the incident photon energy.

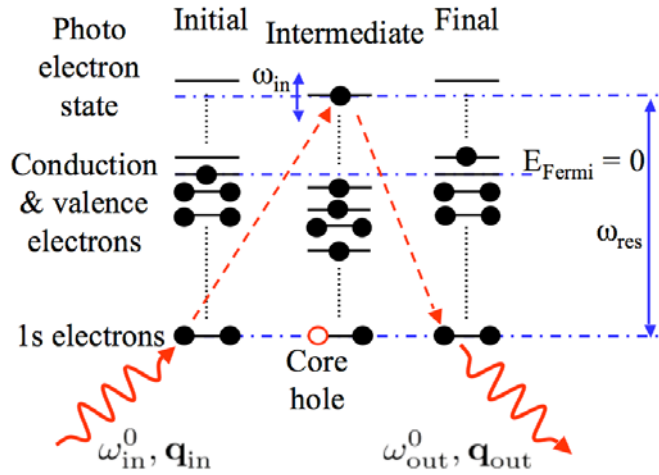


Figure 1: Schematic representation of the indirect resonant inelastic X-ray scattering (RIXS) process. The energy and momentum of the incoming photon are ω_{in}^0 and \mathbf{q}_{in} , respectively, and of the outgoing photon ω_{out}^0 and \mathbf{q}_{out} . The potential of the core-hole in the intermediate state scatters the valence and conduction electrons.

[1] J. van den Brink and M. Veenendaal, Europhys. Lett. **73**, 121 (2006).

[2] L.J.P. Ament, F. Forte and J. van den Brink, Phys. Rev. B **75**, 115118 (2007).

Unusual properties of the electromagnetic response in quantum-dot nanorings

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In the present work, we investigate nanorings consisting of N quantum dots (QDs) described by the extended Hubbard model with parameters for Ag-QDs taken from literature. By changing the interdot spacing, the parameters (t , U and V) can be smoothly tuned in wide ranges ($0.05 < U/4t < 15$, $0.035 < V/4t < 3.6$, $0.25 < V/U < 0.7$). In this way, the nanoring can be smoothly driven from the weak correlation regime to the strong correlation regime, and to visualize this we present results e.g. on the populations of the molecular orbitals (MOs). They demonstrate that the MO-picture completely breaks down, as we showed earlier by studying the so-called HOMO-ionization [1]. In view of the strong correlations, one might expect rich optical absorption and ionization spectra, with many transitions to the numerous excited states allowed by symmetry (point group D_{Nh}). The results we present here, obtained by exact numerical diagonalization, reveal that this is not the case. Both optical and photoionization spectra are very sparse, and can still be qualitatively understood within the MO-picture. An extreme case is that of closed shells, where the optical absorption spectrum is practically monochromatic, as reported recently [2]. These findings generalize the interpretation we proposed in [2] in terms of hidden quasisymmetries of the extended Hubbard model.

References:

- [1] I. Baldea and L. S. Cederbaum, Phys. Rev. Lett. **89**, 133003 (2002).
- [2] I. Baldea and L. S. Cederbaum, Phys. Rev. B **75**, 125323 (2007).

SPIN CORRELATIONS AND INTERACTIONS IN FRUSTRATED SPINEL
COMPOUNDS $\text{Cu}_y\text{Cr}_y\text{Zr}_{2-y}\text{Se}_4$

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Magnetic compounds with frustrated exchange due to geometric constraints became the subject of current theoretical and experimental interest. No systematic investigations of the magnetic properties of $\text{Cu}_y\text{Cr}_y\text{Zr}_{2-y}\text{Se}_4$ for $y = 1.05, 1.15$ to 1.30 have been reported in the literature. To get information on local and macroscopic magnetic properties we used completely techniques of DC magnetization, AC susceptibility and electron-spin resonance (ESR). The Curie temperature, the effective magnetic moment and the temperature range, for which magnetic susceptibility can be regarded as linear, were given for $y = 1.00, 1.05, 1.15, 1.20, 1.25$ and 1.30 . The examination of the $\text{Cu}_y\text{Cr}_y\text{Zr}_{2-y}\text{Se}_4$ formulation, shows that it derives from CuCr_2Se_4 , it's obtained by substituting half of Cr by Zr [1, 2], where the rate occupancy function of the composition ($y = 1.00, 1.05, 1.15, 1.20, 1.25$ et 1.30). The breakdown of ferromagnetism and the re-entrant transition to the spin-glass phase in CuCrZrSe_4 takes place in the dilute ferromagnetic system based on the ferromagnet CuCr_2Se_4 . The re-entrant spin glass phase in CuCrZrSe_4 originates from the random weak links of disordered clusters resulting from dilution and geometrical frustration [3].

[1] Y. Iijima, Y. Kamei, N. Kobayashi, J. Awaka, T. Awasa, S. Ebisu, S. Chikazawa, and S. Nagata, *Philosophical Magazine*, Vol. **83**, N°21, 2521-2530, 2003.

[2] T. Furubayashi, H. Suzuki, N. Kobayashi and S. Nagata, *Solid State Commun.* Vol.**131**, pp. 505–508, 2004.

[3] S. Abiko, S. Niidera, and F. Matsubara, *arXiv:cond-mat 0504615* Vol.**1**, 25, 2005.

Magnetothermoelectric Response at a Superfluid–Mott Insulator Transition

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We investigate the finite temperature magnetothermoelectric response in the vicinity of a superfluid–Mott insulator quantum phase transition. We focus on the particle-hole symmetric transitions of the Bose–Hubbard model, and combine Lorentz invariance arguments with quantum Boltzmann calculations. By means of an epsilon expansion, we find that a non-vanishing thermoelectric tensor and a finite thermal conductivity are supported in this quantum critical regime. We comment on the singular Nernst effect in this problem.

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- [1] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, *Nature* **415**, 39 (2002).
 - [2] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, 1999).
 - [3] Z. A. Xu, N. P. Ong, Y. Wang, T. Kakeshita, and S. Uchida, *Nature* **406**, 486 (2000).
 - [4] Y. Wang, L. Li, M. J. Naughton, G. D. Gu, S. Uchida, and N. P. Ong, *Phys. Rev. Lett.* **95**, 247002 (2005).
 - [5] I. Ussishkin, S. L. Sondhi, and D. A. Huse, *Phys. Rev. Lett.* **89**, 287001 (2002).
 - [6] A. S. Sørensen, E. Demler, and M. D. Lukin, *Phys. Rev. Lett.* **94**, 086803 (2005).
 - [7] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, *Phys. Rev. B* **40**, 546 (1989).
 - [8] M. P. A. Fisher, G. Grinstein, and S. M. Girvin, *Phys. Rev. Lett.* **64**, 587 (1990).
 - [9] M.-C. Cha, M. P. A. Fisher, S. M. Girvin, M. Wallin, and A. P. Young, *Phys. Rev. B* **44**, 6883 (1991).
 - [10] K. Damle and S. Sachdev, *Phys. Rev. B* **56**, 8714 (1997).
 - [11] A. G. Green and S. L. Sondhi, *Phys. Rev. Lett.* **95**, 267001 (2005).
 - [12] A. G. Green, J. E. Moore, S. L. Sondhi, and A. Vishwanath, [cond-mat/0605615](#).
 - [13] N. R. Cooper, B. I. Halperin, and I. M. Ruzin, *Phys. Rev. B* **55**, 2344 (1997).
 - [14] M. J. Bhaseen, A. G. Green, and S. L. Sondhi, in preparation.
 - [15] M. Vojta, Y. Zhang, and S. Sachdev, *Int. J. Mod. Phys. B* **14**, 3719 (2000); T. Senthil, unpublished.
 - [16] E. Shimshoni, N. Andrei, and A. Rosch, *Phys. Rev. B* **68**, 104401 (2003).
 - [17] J. D. Jackson, *Classical Electrodynamics* (John Wiley & Sons, Inc., 1998), 3rd ed.
 - [18] J. M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, 1964).

Possible Deconfined Quantum Phase Transition between Non-Collinear Magnet and VBS in Spin ($S=1/2$) Systems.

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Abstract

Recent developments in the field of Quantum Phase Transitions has brought into light the need for a broader framework of study than perceived in the Landau-Ginzburg-Wilson (LGW) paradigm. One such class of transitions that are not captured by the LGW picture are the Deconfined Quantum Phase Transitions [1]. In this work we present the possibility of existence of a generic second order quantum phase transition between the non-collinear magnet to the Valence Bond Solid (VBS) in two different spin($S=1/2$) systems (on frustrated anisotropic rectangular and triangular lattices). This transition belongs to the deconfined class. We have constructed an effective field theory for describing such a transition that correctly incorporates the effect of quantum “Berry phases” that play an important role in these transitions. The results of the anisotropic triangular lattice may be of experimental significance for the compound Cs_2CuCl_4 [2].

References:

[1] Deconfined Quantum Critical Points, T. Senthil, Ashvin Vishwanath, Leon Balents, Subir Sachdev, Matthew P. A. Fisher, *Science*, Vol. 303, 1490(2004).

[2] Extended scattering continua characteristic of spin fractionalization in the two-dimensional frustrated quantum magnet Cs_2CuCl_4 observed by neutron scattering, R. Coldea, D. A. Tennant, and Z. Tylczynski, *Phys. Rev. B* 68, 134424 (2003).

Evidence for long range in-plane and out of plane ordering in the frustrated system $\text{Ca}_3\text{Co}_2\text{O}_6$

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The topics of low-dimensional magnetism and topological magnetic frustration have attracted a lot of attention in recent years. In this respect, the family of compounds of the type $(\text{Sr},\text{Ca})_3\text{ABO}_6$ containing magnetic ions A and B is notable, as the crystal structure provides an opportunity to study both the phenomena in a single family of compounds. Preliminary results of a resonant x-ray investigation performed on a single crystal of the most famous member of this family ($\text{Ca}_3\text{Co}_2\text{O}_6$) at the Co K edge are presented.

The evolution of the in plane and out of plane magnetic correlation lengths as function of the temperature confirms the strong Ising character of the system but also points out that below the antiferromagnetic transition both the intra and inter-chains magnetic correlations involve a large number of sites.

What seems to indicate that the models [2,3] proposed to explain the behavior of this system might not entirely describe the complex nature of the system.

The better reciprocal space resolution of the x-ray also allowed the measure of a slight deviation of the magnetic reflections from the commensurate position determined with neutrons.

[1] Aasland S., Fjellvag H., Hauback B., Solid State Communications, Volume 101, Number 3, January 1997, pp. 187-192(6)

[2] Kudasov Y.B., Phys. Rev. Lett. 96, 027212 (2006)

[3] Maignan A, J. Mater. Chem., 2004, 14, 1231 - 1234,

**Magnetic properties of a novel S=1/2 Heisenberg antiferromagnetic two-leg
ladder BiCu₂PO₆**

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The polycrystalline samples of a new Heisenberg antiferromagnetic two-leg spin ladder compound BiCu₂PO₆ were synthesized by conventional solid-state reaction techniques. Magnetic susceptibility $\chi(T)$ and specific heat $C_p(T)$ were measured as function of temperature in the range 2 K to 300 K. The magnetic susceptibility exhibits a broad maximum at about 56 K and decreases exponentially at lower temperatures, revealing the spin-gap behavior. We have fitted the susceptibility data with the isolated spin-ladder expression given by Ref.[1] and exchange interactions along the leg and rung coupling were found to be $J_1/k_B = 80$ K and $J_2/k_B = 70$ K respectively. The spin-gap (Δ/k_B) was found to be 34 K. Significant inter ladder interactions and next nearest neighboring exchange interaction along the leg are suggested from susceptibility and band structure analysis. We have also synthesized various types of doped samples BiCu_{2(1-x)}Zn_{2x}PO₆ ($0 \leq x \leq 1$), and BiCu_{2(1-y)}Ni_{2y}PO₆ ($0 \leq y \leq 0.3$). In the case Zn (S=0) doping at Cu site, we found that low temperature $\chi(T)$ deviates from curie below 5 K. Magnetic specific heat $C_m(T)$ also shows cusp like anomaly at about 5K, possibly indicating spin-glass/disordered magnetism of the Zn-induced local moments. $\chi(T)$ and $C_p(T)$ measurements in Ni-doped (S = 1) samples indicate a spin-glass like behavior at about 6K.

Reference [1]: D. C. Johnston, M. Troyer, et al., cond-mat/0001147

Electronic structure and Fermi surface topology of Na_xCoO_2

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The Na_xCoO_2 compounds, already interesting because of their huge thermoelectric power, became even more popular after the discovery of their unexpected superconductivity, with controlled doping and hydration. In fact, their rich and complicated phase diagram [1] raises many questions on the nature of pairing and its connection to high-temperature superconducting cuprates. Detailed knowledge of their electronic structure is necessary to understand their puzzling electronic and magnetic properties. First principle band calculations [2, 3] have predicted that Na_xCoO_2 has a large Fermi surface associated with the a_{1g} band centered around the Γ point and six small hole pockets of mostly e'_g character near the K points, for a wide range of x . This Fermi surface topology is the starting point for several proposed models on non-phonon mediated superconductivity, and the existence of small hole pockets is essential for these theories. However, recent ARPES experiments [4–7] seem to show only the central feature, while the pockets 'sink' below the Fermi energy.

Here we construct an effective Hamiltonian for the motion of T_{2g} highly correlated states in Na_xCoO_2 . We solve exactly a multiband model in a CoO_6 cluster with electronic occupation corresponding to a nominal Co valence of either +3 or +4 [8]. Using the ensuing ground states, we calculate the effective O mediated hopping $t = 0.10$ eV between many-body T_{2g} states, and estimate the direct hopping $t' \sim 0.04$ eV. The trigonal splitting $3D = 0.315$ eV is taken from recent quantum chemistry calculations [9]. The resulting effective Hamiltonian is solved using a generalized slave-boson mean-field approximation. The results show a significant band renormalization and a Fermi surface topology that agrees with experiment, in contrast to predictions using the local-density approximation.

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- [1] M. L. Foo *et al.*, Phys. Rev. Lett. **92**, 247001 (2004).
 - [2] D. J. Singh, Phys. Rev. B **61**, 13397 (2000).
 - [3] M. D. Johannes *et al.*, Phys. Rev. Lett. **93**, 097005 (2004).
 - [4] M. Z. Hassan *et al.*, Phys. Rev. Lett. **92**, 246402 (2004).
 - [5] H. B. Yang *et al.*, Phys. Rev. Lett. **92**, 246403 (2004).
 - [6] H. B. Yang *et al.*, Phys. Rev. Lett. **95**, 146401 (2005).
 - [7] M. Z. Hasan *et al.*, condmat/0501530.
 - [8] T. Kroll *et al.*, Phys. Rev. B **74**, 115124 (2006).
 - [9] T. Landron *et al.*, Phys. Rev. B **74**, 184507 (2006).

Ground-state phase diagram of geometrically frustrated Ising-Heisenberg model on the diamond-like decorated planar lattices

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Ground-state phase diagram of the mixed spin-1/2 and spin-1 Ising-Heisenberg model on the diamond-like decorated planar lattices is examined using the generalized decoration-iteration mapping transformation. A particular attention is paid to the investigation of the effect of uniaxial single-ion anisotropy and exchange anisotropy on a character of the magnetic ordering of the spin system under investigation. It is shown that the mutual competition between the Ising interaction, the Heisenberg interaction and the uniaxial single-ion anisotropy gives rise to several interesting ground-state phases. In addition to the spontaneously ordered classical ferrimagnetic phase, the unusual ordered quantum ferrimagnetic phase and the disordered geometrically frustrated phase are detected within the ground-state phase diagram. It is worthy to notice that the ordered quantum ferrimagnetic phase does not have any classical analogue and its peculiar spin ordering can be understood only within the valence-bond-solid picture [1]. The ground-state boundaries between different phases are evaluated analytically and the macroscopic degeneracy of the geometrically frustrated phases is found in dependence on the exchange and single-ion anisotropies.

[1] I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki, *Commun. Math. Phys.* 115 (1988) 477.

Competing stripe-phases in the doped t - J model

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Considering the t - J model at $x=1/8$ doping, we investigate a possible instability of the uniform d-wave RVB phase, a well-known candidate for the high- T_c cuprate superconducting phase, towards a modulated superconducting stripe phase. It is found that (half-filled) charge domains separated by $2/x=4$ lattice spacings can spontaneously form along one of the crystal axis leading to modulated superconducting order.

The key feature of our proposal is the out-of-phase nature of the d-wave order parameters in two neighboring domains (they change signs), hence doubling the actual periodicity in the direction perpendicular to the stripes. Interestingly, a closely related instability is found in the Staggered Flux state (or d-density wave), a candidate for the normal pseudo-gap phase. Modulated and uniform phases are found to be very close in energy both at the mean-field level and in many-body Variational Monte Carlo calculations. We argue that the modulated RVB state bears strong similarities to the recently observed pattern of unidirectional domains found in STM studies of the two different families Na-CCOC and Dy-BSCCO of high- T_c superconductors [1].

[1] Y. Kohsaka et al. *Science* **315**, 1380 (2007).

Classical and quantum topological order: the birth of a coherent picture

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We calculate exactly the von Neumann and topological entropies of the toric code as a function of system size and temperature. We do so for systems with infinite energy scale separation between magnetic and electric excitations, so that the magnetic closed loop structure is fully preserved while the electric loop structure is tampered with by thermally excited electric charges. We find that the topological entropy drops to half its zero-temperature value for any infinitesimal temperature in the thermodynamic limit, and remains constant as the temperature is further increased. Such discontinuous behavior is replaced by a smooth decreasing function in finite-size systems. If the separation of energy scales in the system is large but finite, we argue that our results hold at small enough temperature and finite system size, and a second drop in the topological entropy occurs as the temperature is raised so as to disrupt the magnetic loop structure by allowing the appearance of free magnetic charges. We interpret our results as an indication that the underlying magnetic and electric closed loop structures contribute equally to the topological entropy (and therefore to the topological order) in the system. Since each loop structure *\emph{per se}* is a classical object, we interpret the quantum topological order in our system as arising from the ability of the two structures to be superimposed and appear simultaneously.

[1] C.Castelnovo and C.Chamon, arXiv:0704.3616.

Spin dynamics in magnetically frustrated $\text{Tb}_2\text{Sn}_2\text{O}_7$

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Magnetic frustration of geometric origin arises when the spatial arrangement of the spins is such that it prevents the simultaneous minimization of all the interaction energies. A large degeneracy of the ground state is expected [1]. This behavior is present in several crystal lattices where spins are arranged on triangles or tetrahedra with antiferromagnetic interaction between nearest neighbors.

The $\text{Tb}_2\text{Sn}_2\text{O}_7$ compound is such a system: it crystallizes in the pyrochlore structure (*i.e.* a three dimensional arrangement of corner-sharing tetrahedra), with space group $Fd-3m$ and lattice parameter $a = 10.426 \text{ \AA}$. Its specific heat shows a well-defined magnetic transition peak at 0.88 K, at a temperature much lower than expected from the magnetic interaction magnitude.

We investigated this system at low temperature and we carried out neutron powder diffraction measurements at the Paul Scherrer Institute (Villigen, Switzerland). We observed a broadening of the magnetic reflections beyond the instrument resolution in agreement with the literature [2]. The small magnetic domain picture being not adapted, we analyze this result with a quasielastic picture which is more appropriate. It gives the order of magnitude for the neutron energy transfer in the scattering process: $\Delta E \sim 80 \text{ \mu eV}$. Using the energy-time Heisenberg inequality, a bound for the spin fluctuation time is estimated: $\tau_{sc} \geq 10^{-11} \text{ s}$ [3, 4]

The muon spin relaxation spectra obtained at the Rutherford Appleton Laboratory (Chilton, United Kingdom) and at the Paul Scherrer Institute do not show spontaneous precession in the ordered phase and are well fitted to an exponential function. It is concluded that the Tb^{3+} magnetic moments are dynamical and their fluctuation time is estimated: $\tau_c \sim 10^{-10} \text{ s}$ [3].

The analysis of the dynamical magnetic structure factor measured by neutron spin echo (NSE) measurements performed at the Institut Laue Langevin (Grenoble, France) on the same system enable to estimate a spin fluctuation time $\tau_{\text{NSE}} \sim 10^{-10} \text{ s}$ [4].

In conclusion, the different experimental investigations at the microscopic level of the $\text{Tb}_2\text{Sn}_2\text{O}_7$ system lead to a consistent picture: although magnetic reflections are observed in neutron scattering, the ground state at low temperature is dynamical with a fluctuation time is of order 10^{-10} s .

[1] J. Villain, Z. Phys. B **33** 31 (1979).

[2] I. Mirebeau, A. Apetrei, J. Rodriguez-Carvajal, P. Bonville, A. Forget, D. Colson, V. Glaskov, J. P. Sanchez, O. Isnard and E. Suard, Phys. Rev. Lett. **94**, 246402 (2005).

[3] P. Dalmas de Réotier, A. Yaouanc, L. Keller, A. Cervellino, B. Roessli, C. Baines, A. Forget, C. Vaju, P.C.M Gubbens, A. Amato and P.J.C King, Phys. Rev. Lett. **96**, 127202 (2006).

[4] Y. Chapuis, A. Yaouanc, P. Dalmas de Réotier, S. Pouget, P. Fouquet, A. Cervellino and A. Forget, submitted for publication.

Correlated Systems on Geometrically Frustrated Lattices. Localized Eigenstates

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In this paper we present recent studies on localized eigenstates of strongly correlated systems on some one- and two-dimensional frustrated lattices and discuss their influence on the low-temperature physics. We focus on frustrated quantum Heisenberg antiferromagnets where these localized magnon eigenstates become ground states in strong magnetic fields. We also discuss localized electron states for the sawtooth-chain Hubbard model. Some further details can be found in Refs. 1 and 2.

[1] J. Richter, O. Derzhko and T. Krokhmalskii, Phys. Rev. B **74**, 144430 (2006).

[2] O. Derzhko, A. Honecker and J. Richter, arXiv:cond-mat/0703295.

**Title: On the slow dynamics of systems with FLUCTUATION INDUCED FIRST ORDER
PHASE TRANSITIONS**

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Content of Abstract

Using the Hartree approximation we consider an effective Landau-Ginsburg Hamiltonian with an isotropic long range interaction term. The Langevin dynamic in the long times limit is solved for both ferromagnetic and disordered initial conditions. The result is compared with extensive numerical simulations.

Comparative *ab initio* calculations of Cs_2CuCl_4 and Cs_2CuBr_4 electronic properties

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We present first-principle density functional calculations of the electronic properties of the layered spin-1/2 frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 and discuss the origin of their different magnetic behaviour.

Entropy analysis for the XY spin chain

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The Abdus Salam I.C.T.P.

Abstract

We study the bi-partite entanglement in the ground state of the one-dimensional XY spin $1/2$ model, by calculating the Von Neumann and the Renyi Entropy of a block of neighboring spins. We consider the double-scaling limit in which the block size is much bigger than unity, but still much smaller than the length of the whole chain. In this limit we achieve the first completely analytical description of these entanglement estimators, which allows us to study their behavior in the phase diagram and their analytical properties. One striking feature that emerges is the existence of a point, which we call Essential Critical Point, where the entropy is highly singular. Close to this point, the entropy can assume any positive real value between zero and infinity and small variation of the parameters of the model can change the entropy macroscopically.

Understanding the Bose Ferromagnets

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Although ferromagnetism has been intensively studied in the context of condensed matter physics, the description of ferromagnetism is not yet complete. The conventional ferromagnets are usually comprised of either classical particles (insulating ferromagnets) or fermions (itinerant ferromagnets) while Bose systems are seldom touched.

The achievement in cooling alkali atomic gases, such as ^{87}Rb , ^{23}Na and ^7Li , to quantum degeneracy opens up a way to study magnetism in spinor bosons, because these constituent atoms usually carry a hyperfine spin degree of freedom. Recently, the ferromagnetically coupled spinor Bose gas, such as ^{87}Rb has attracted numerous research interest [1].

The ferromagnetic coupling induces a ferromagnetic transition at the critical temperature called the Curie point. Moreover, the Bose gas undergoes an intrinsic phase transition, i.e., the Bose-Einstein condensation. Within mean-field theory, we suggested that the ferromagnetic Bose gas displays a quite surprising phase diagram. Its Curie point can be larger by magnitudes than the energy scale of the ferromagnetic interaction between bosons, and never below the Bose-Einstein condensation temperature [2]. It means that once the Bose gas condenses, it is already spontaneously magnetized. The phase diagram was also investigated by other groups later [3].

Moreover, we calculated thermodynamic quantities of the system [4]. The magnetic susceptibility obtained fits the Curie-Weiss law very well at all temperatures above the Curie point. The specific heat exhibits quite different behaviors at the two transition points.

[1] Q. Gu, Progress in Ferromagnetism Research, Ed. by V.N. Murray, (Nova Science, NewYork, 2006) Chap. 6.

[2] Q. Gu, K. Bongs, and K. Sengstock, Phys. Rev. A **70**, 063609 (2004); Q. Gu and R.A. Klemm, Phys. Rev. A **68**, 031604(R) (2003).

[3] K. Kis-Szabo, P. Szepfalusy, and G. Szirmai, Phys. Rev. A **72**, 023617 (2005).

[4] C. Tao, P. Wang, J. Qin, and Q. Gu, unpublished.

Hole dynamics in the J_1 - J_2 model.

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The dynamics of a hole injected in an antiferromagnet matrix has been extensively studied as a possible starting point to understand the physics of doped Mott insulators. However, the effect of magnetic frustration on the hole dynamics has been little explored in the literature. In this work, we have analyzed the single hole dynamics in the different magnetic phases of the J_1 - J_2 model. For this purpose, we have used a generalized t - J model, solved with the well-known self-consistent Born approximation and Lanczos exact diagonalization methods. We were able to track microscopically the origin of the different features of the hole spectral function. As a general characteristic, we have found that the hole propagates coherently as a spin polaron excitation for all values of frustration within magnetically ordered phases. However, the quasiparticle spectral weight is largely reduced as quantum fluctuations are increased due to frustration. We also investigate the hole motion in the disordered intermediate phase using exact diagonalization. Finally, we discuss the possible implications of our results for photoemission experiments in $\text{Li}_2\text{VOSiO}_4$.

A three dimensional Kasteleyn transition ; spin ice in a [100] field

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Applying a field in the [100] direction of a nearest neighbour spin ice model, the magnetization saturates discontinuously at finite field in a three dimensional Kasteleyn transition. A non-local loop algorithm [1] is used to simulate the system at low temperature, showing that the magnetic discontinuity previously described [2] as a first order transition is in fact a non-equilibrium effect ubiquitously present for local dynamics. A similar transition occurs for a Bethe lattice of corner sharing tetrahedra and this system is solved analytically. Our results are compared with data from neutron scattering on Holmium Titanate [3].

[1] S.V. Isakov, K. Gregor, R. Moessner and S.L. Sondhi, Phys. Rev. Lett. **93** 167204 (2004)

[2] M.J. Harris, S.T. Bramwell, P.C.W. Holdsworth and J.D.M.Champion, Phys. Rev. Lett. **81** 4496 (1998)

[3] T. Fennell, S.T. Bramwell, D.F. McMorrow, P. Manuel and A. Wildes, private communication (2007)

Spin Gap Behaviour in the Frustrated Heisenberg Layered Cuprate (CuCl)LaNb₂O₇

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A novel layered magnetic material (CuCl)LaNb₂O₇, has been prepared by ion-exchange between non-magnetic perovskite derivative RbLaNb₂O₇ and CuCl₂. The lattice is of tetragonal symmetry (P4/mmm) with room temperature cell constants $a = 3.8839 \text{ \AA}$ and $c = 11.7516 \text{ \AA}$ confirmed by Rietveld analysis of polycrystalline sample. Here, Cu²⁺ ions form a two-dimensional square-lattice, separated by magnetically inert perovskite slabs. Since each chlorine ion is located at the centre of a square made by the neighboring four magnetic ions, the nearest and next-nearest interactions are expected to be comparable and the magnetic properties are mapped onto the J₁-J₂ model. Magnetic susceptibility data show a broad maximum at around 16 K which is a characteristic property of low dimensional antiferromagnets and the susceptibility decreases below 16 K revealing that the spin-singlet ground state is separated from the excited state with a finite energy gap. We have fitted the susceptibility data with a S=1/2 isolated AFM dimer model and a spin gap (Δ/k_B) of 27 K is obtained which is equal to the intra-dimer interaction. It has been suggested that geometrical frustration most likely arises from antiferromagnetic next-nearest bonds makes the triplet excitation extremely localised as in the case of the Shastry-Sutherland model based SrCu₂(BO₃)₂. High-field (0-9T) magnetisation data show that magnetisation increases linearly with field and the slope discontinuity observed at low temperature is attributed to the spin gap behaviour of the compound. Also the linear rise of magnetisation can be due to the suppression of zero point fluctuation by applied magnetic field. We are also currently looking at doping and impurity effects in this layered cuprate.

Origin of the magnetic anisotropy in tetranuclear Ni(II) cluster of S4 symmetry

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We present the model for description of magnetic properties in tetranuclear Ni(II) clusters of S4 symmetry. The group theoretical analysis of the cluster energy spectrum points unambiguously to the pronounced role of Dzyloshinski-Moriya interaction. Therefore the model includes the antisymmetric exchange term besides of the isotropic exchange and the local anisotropies that are non - collinear with the cluster coordinate system. Being combined with the irreducible tensor operator method (ITO) the model reproduces the experimental data like magnetic susceptibility and magnetization and reconstructs the high-frequency tail of INS spectrum.

NMR and magnetic susceptibility measurements on novel cuprates $\text{Na}_5\text{RbCu}_4(\text{AsO}_4)\text{Cl}_2$ and $\text{Cu}_4\text{Te}_5\text{O}_{12}\text{Cl}_4$

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Two novel cuprates $\text{Na}_5\text{RbCu}_4(\text{AsO}_4)\text{Cl}_2$ and $\text{Cu}_4\text{Te}_5\text{O}_{12}\text{Cl}_4$ have been studied using NMR, magnetic susceptibility and specific heat measurements. $\text{Na}_5\text{RbCu}_4(\text{AsO}_4)\text{Cl}_2$, which contains layers of coupled Cu_4O_4 tetramers, orders in zero magnetic field antiferromagnetically via a second-order low-entropy phase transition at $T_N = 15(1)$ K [1]. Measurements in $\text{Cu}_4\text{Te}_5\text{O}_{12}\text{Cl}_4$ (Cu-45124), composed of weakly coupled tetrahedral Cu clusters, evidence antiferromagnetic, frustrated correlations of the Cu spin moments and long range ordering with $T_C = 13.6$ K [2]. The magnetic behaviour of both cuprates will be discussed.

[1] R. Stern et al., Phys. Rev. B, 378 - 380 (2006) 1124 - 1125

[2] R. Takagi et al., Phys. Rev. B, 74 (2006) 014413

Diagrammatic Determinantal methods: projective schemes and applications to the Hubbard-Holstein model

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We extend the weak-coupling diagrammatic determinantal algorithm to projective schemes as well as to the inclusion of phonon degrees of freedom. The projective approach provides a very efficient algorithm to access zero temperature properties. To implement phonons, we integrate them out in favor of a retarded density-density interaction and simulate the resulting purely electronic action with the weak-coupling diagrammatic determinantal algorithm. Both extensions are tested within the dynamical mean field approximation for the Hubbard and Hubbard-Holstein models.

Magneto-elastic effects and magnetization plateaus in two dimensional systems

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We show the importance of both strong frustration and spin-lattice coupling for the stabilization of magnetization plateaus in translationally invariant two-dimensional systems. We consider a frustrated spin-1/2 Heisenberg model coupled to adiabatic phonons under an external magnetic field. At zero magnetization, simple structures with two or at most four spins per unit cell are stabilized, forming dimers or 2×2 plaquettes, respectively. A much richer scenario is found in the case of magnetization $m = 1/2$, where larger unit cells are formed with non-trivial spin textures and an analogy with the corresponding classical Ising model is detectable. Specific predictions on lattice distortions and local spin values can be directly measured by X-rays and Nuclear Magnetic Resonance experiments.

Spatial noise correlations of a chain of ultracold fermions - Fingerprint of the FFLO state

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We analyze the spatial noise correlations (density-density correlations in momentum space) of the one-dimensional attractive Hubbard model in the presence of spin polarization. Based on the results of our density-matrix renormalization group calculation, we discuss the distinct features of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state imprinted in the noise correlations. Our results directly apply to experiments with polarized gases of ultracold fermions in optical lattices, in which the noise correlations can be extracted from time-of-flight images of the expanding cloud. The fact that Cooper pairs with non zero momentum are unambiguously detectable in such a setup opens up an interesting possibility for experimental studies of FFLO states.

Novel Spin Correlations and Jordan-Wigner Transformation in the Kitaev Model

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We study a Frustrated Quantum Spin model on a Hexagonal lattice. which was originally proposed and analysed by A.Kitaev. He showed that the model has an infinite number of conserved quantities and computed the energy eigenvalues of the ground state energy and a set of low lying excited states exactly. Extending the Kitaev's fermionisation we have introduced the concept of bond fermion which greatly clarifies the dynamics of the spin and facilitates the computation of spin-spin correlation function. We have found, at all energy scale, fractionalization of a spin-flip into two infinitely massive pi-fluxes and a dynamical majorana fermion. In particular two spin dynamical correlation function is zero beyond nearest neighbour separation. This is true for any eigen state. Further we have applied Jordan-Wigner transformation on a torus for this model which yields a fermionic model with local interactions. We reproduce the earlier results on the spectrum of the model in the fermionic representation. We show that in the thermodynamic limit ground state is four fold degenerate.

Ref: G. Baskaran, Saptarshi Mandal, R Shankar, Phys Rev Lett, **98**, 247201(2007)

Uniform and Staggered Magnetizations induced by Dzyaloshinskii-Moriya Interactions in Frustrated Heisenberg Spin-1/2 Ladders in a Magnetic Field

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We investigate the interplay of Dzyaloshinskii-Moriya interactions and an external field in spin-1/2 dimers. For isolated dimers and at low field, we derive simple expressions for the staggered and uniform magnetizations which show that the orientation of the uniform magnetization can deviate significantly from that of the external field. In fact, in the limit where the D vector of the Dzyaloshinskii-Moriya interaction is parallel to the external field, the uniform magnetization actually becomes perpendicular to the field. For larger fields, we show that the staggered magnetization of an isolated dimer has a maximum close to one-half the polarization, with a large maximal value of $0.35g\mu_B$ in the limit of very small Dzyaloshinskii-Moriya interaction. We investigate the effect of interdimer coupling in the context of ladders with density-matrix renormalization-group (DMRG) calculations and show that, as long as the values of the Dzyaloshinskii-Moriya interaction and of the exchange interaction are compatible with respect to the development of a staggered magnetization, the simple picture that emerges for isolated dimers is also valid for weakly coupled dimers with minor modifications. The results are compared with torque measurements on $\text{Cu}_2(\text{C}_5\text{H}_{12}\text{N}_2)_2\text{Cl}_4$ (also called "Cu(Hp)Cl"). Recent results for the torque and the magnetizations in the presence of frustrating interactions on the ladder are discussed.

Soliton interaction in coupled spin-Peierls chains

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(Dated: July 12, 2007)

We reconsider the elementary excitations of quasi-one-dimensional spin-phonon systems taking into account the interchain coupling. It is expected that the effect of the interchain coupling will be to confine the spin one-half solitons corresponding to each isolated chain. We show that this is the case when the interchain coupling is not frustrated. In the frustrated case we show that free solitons could be the elementary excitations of the coupled two-dimensional model. The case of an elastic interchain coupling is analyzed on a general energetic consideration. For the simplified two-chain problem we use DMRG calculations. In this case we take into account the magnetic interchain coupling. We show that the deconfinement mechanism is effective even when the antiferromagnetic interchain coupling is present. Our results could be relevant for a further experimental determination of the magnetic spectra in the recently studied spin-Peierls system TiOCl.

Electric field gradients in $\text{PrBa}_2\text{Cu}_3\text{O}_7$: LSDA+U and comparison with experiment

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Abstract

Electric-field gradient (EFG) and asymmetry parameter (η) at all oxygen and copper sites of nonsuperconducting $\text{PrBa}_2\text{Cu}_3\text{O}_7$ (Pr123) compound were calculated using the full-potential (linearized)-augmented-plane-wave plus local orbitals method in the ferromagnetic ordering. Exchange and correlation effects were treated by LSDA+U for Cu(3d) and Pr(4f) electrons. The effects of changing screened Coulomb parameters U_{Pr} , U_{Cu1} , and U_{Cu2} on the results were individually studied. The calculated EFG of O2 site is close to the EFG of O3 site at variance with the experimental result. It was shown that by increasing superconducting holes in O2 and O3 sites the EFG at these sites increase and vice versa. The most famous theories which have been proposed to explain the suppression of superconductivity in perfect (without any mis-substitution or other defects) Pr123 compound are not consistent with the experimental EFG at O2 and O3 sites. By replacing one Pr atom at the Ba site on unit cell of Pr123 (Pr_{Ba}), it was shown that Pr_{Ba} mis-substitution reduces the superconducting holes in both O2 and O3 sites and could be responsible for the suppression of superconductivity in Pr123 samples. It is very probable that the unusual behaviors of experimental EFG at O2 and O3 sites of Pr123 are related to oxygen defects which are produced with Pr_{Ba} mis-substitution.

Classical Shastry-Sutherland lattice coupled to lattice distortions

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We investigate the classical Shastry-Sutherland lattice coupled to adiabatic phonons and under an external magnetic field.

In the absence of phonons the classical Shastry-Sutherland lattice does not present any magnetization plateau. The question we address is whether adiabatic phonons could stabilize a plateau for a given range of spin-lattice coupling.

This work is motivated by recent experiments on the TbB₄ compound which presents plateaux in its magnetization curve. In this classical compound the Tb atoms are located on the sites of a lattice that is topologically equivalent to the Shastry-Sutherland lattice.

Disordered superconductors: role of interaction strength

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We study the interplay between impurities and superconductivity, in the sense that one is interested in determining how much dirt can a superconductor take before it becomes a normal metal. This question is even more interesting in two dimensions, since the superconducting transition at finite temperatures is marginal (Kosterlitz-Thouless). In order to provide insight into this issue, the attractive Hubbard model is very convenient since the impurities are modelled allowing a fraction f of the sites on a square lattice to have a vanishing on-site attraction, while pairing is favoured in the remaining fraction of sites by an on-site coupling $U < 0$. For given U , disorder configuration, band filling n , and linear lattice size L , we use Quantum Monte Carlo simulations to calculate the uniform pairing structure factor, $P_s(L, n, f, \beta, U)$ (i.e., the $\mathbf{q} = 0$ Fourier transform of the site-dependent pairing correlation function), for different values of the inverse temperature, β . We then use different finite-size scaling *ansatze* to estimate the zero-temperature gap, Δ , as well as the superconducting critical temperature, T_c , as functions of impurity concentration, f , for fixed values of the remaining parameters. Here we report on results for the case of a half filled band, and focus on the behaviour with the magnitude of the attractive interaction. Contrary to mean-field predictions, we have found that: for weak couplings, superconductivity is wiped out of the ground state for any finite disorder; as U increases beyond a certain threshold, U_m , superconductivity is present below a critical f_c , which increases with U . We also discuss the behaviour of the zero-temperature gap, Δ , as a function of f for different values of U : while for strong couplings Δ initially rises, for weak couplings Δ monotonically decreases with f . And, finally, we compare the behaviour of T_c with f , for different values of U .

^{31}P NMR on frustrated ferromagnetic square lattice compounds $\text{Pb}_2(\text{VO})(\text{PO}_4)_2$ and $\text{SrZn}(\text{VO})(\text{PO}_4)_2$

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The magnetic properties of the frustrated ferromagnetic square lattice compounds $\text{Pb}_2(\text{VO})(\text{PO}_4)_2$ [1] and $\text{SrZn}(\text{VO})(\text{PO}_4)_2$ were investigated by means of ^{31}P Nuclear Magnetic Resonance (NMR) measurements. We report here detailed investigation of NMR shift, spin-lattice relaxation rate ($1/T_1$) and spin-spin relaxation rate ($1/T_2$) for $\text{SrZn}(\text{VO})(\text{PO}_4)_2$ and some preliminary results of $\text{Pb}_2(\text{VO})(\text{PO}_4)_2$. Our attention is more focused on $\text{SrZn}(\text{VO})(\text{PO}_4)_2$ since it is suspected to be located more close to the quantum critical region with a spin-liquid state in the J_1 - J_2 phase diagram[2]. For both compounds, NMR spectra give a superposition of two in-equivalent ^{31}P sites present in the crystal structure. The hyperfine coupling constants associated with the in-plane and off-plane ^{31}P sites were calculated to be (637 Oe/ μ_B and -186 Oe/ μ_B) and (-2025 Oe/ μ_B and -154 Oe/ μ_B) for $\text{Pb}_2(\text{VO})(\text{PO}_4)_2$ and $\text{SrZn}(\text{VO})(\text{PO}_4)_2$ respectively. For $\text{SrZn}(\text{VO})(\text{PO}_4)_2$, ^{31}P $1/T_1$ at high temperatures remains temperature independent as is expected theoretically in the paramagnetic region ($T \gg J$). For, $T \leq 10$ K, $1/T_1$ drops sharply instead of an increase towards the transition temperature (T_N). Similarly ^{31}P $1/T_2$ at high temperatures remains temperature independent and below 10K it drops sharply towards T_N . This unusual behaviour in $1/T_1$ and $1/T_2$ likely reflect the frustrated nature of the system. Sudden change in line width below T_N ($\approx 3.5\text{K}$ and 2.7K for $\text{Pb}_2(\text{VO})(\text{PO}_4)_2$ and $\text{SrZn}(\text{VO})(\text{PO}_4)_2$ respectively) confirms the presence of an internal field in the ordered state.

[1] E. E. Kaul, H. Rosner, N. Shannon, R. V. Shpanchenko, and C. Geibel, J. Magn. Magn. Mater. **272**, 922 (2004).

[2] B. Schmidt, N. Shannon, and P. Thalmeier, J. Phys.: Condens. Matter **51**, 207 (2006).

Observation of magnetoelastic coupling in the pyrochlore $\text{Y}_2\text{Mo}_2\text{O}_7$

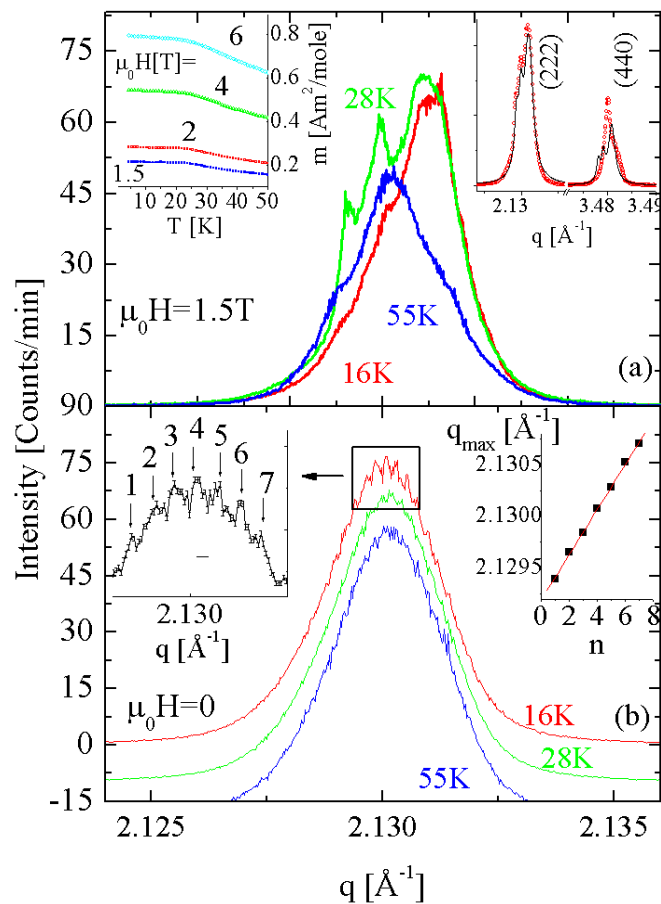
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We investigated the nature of the spin glass-like phase transition in the geometrically frustrated $\text{Y}_2\text{Mo}_2\text{O}_7$ using magnetic field-dependent x-ray and neutron scattering, and nuclear magnetic resonance (NMR). Our main finding is a dramatic change to Bragg scattering with the application of a magnetic field in high resolution X-ray diffraction. Especially, the (222) peak splits into three main peaks due to lattice deformation. The effect of the field is strongest near the spin-glass temperature T_g , but can be seen as high as 55K. The neutron experiment also shows field-induced lattice effects with similar temperature dependence. The NMR suggests that the deformation does not preserve the cubic symmetry. This finding clearly indicates that the low temperature properties of $\text{Y}_2\text{Mo}_2\text{O}_7$ are controlled by magneto-elastic coupling.



NMR STUDIES IN DOPED INTEGER SPIN CHAIN COMPOUND $\text{SrNi}_{1.93}\text{Mg}_{0.07}\text{V}_2\text{O}_8$

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Impurity effects in quantum spin chains with a singlet ground state have attracted recent interest, since even a nonmagnetic defect may disturb the correlated ground state of the bulk in a subtle manner and restore magnetic behavior. A good example is the extra spin- degree of freedom localized near an open end of an integer-spin Heisenberg chain, which has an excitation gap in the bulk. Earlier, from bulk susceptibility and heat capacity results it was shown that in $\text{SrNi}_2\text{V}_2\text{O}_8$, which is a integer spin chain system having a gap $\Delta \sim 25$ K, substitution of Ni^{2+} ions by nonmagnetic Mg^{2+} ions destroy the nonmagnetic ground state and restore AF ordered phase [1]. Furthermore, this impurity induced AF phase disappears above 4 T. Thus we have performed NMR studies in $\text{SrNi}_{2-x}\text{Mg}_x\text{V}_2\text{O}_8$ for $x=0.07$ in the temperature range 4 -300 K and in presence of external magnetic field 1.2 and 7 T to probe the system above and below 4 T microscopically. The ^{51}V NMR spectra in $\text{SrNi}_{1.93}\text{Mg}_{0.07}\text{V}_2\text{O}_8$ show large asymmetric broadening below 20 K [Fig.1(a),1(b)]. Whereas, the NMR line width in the pure compound was almost unaltered till 4 K [2]. This broadening of the ^{51}V

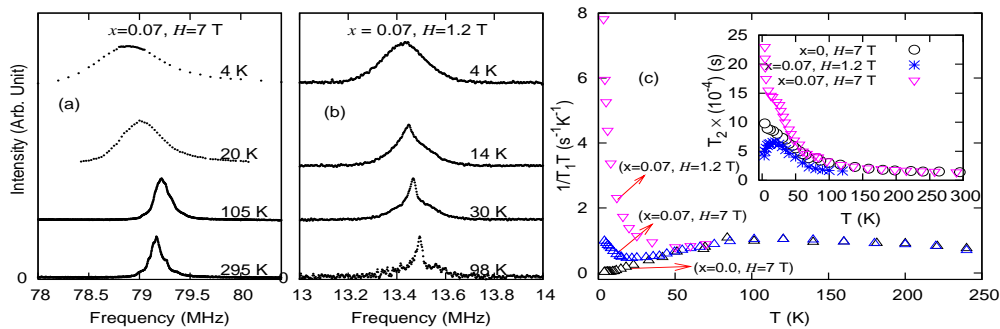


Figure 1: (a), (b) ^{51}V NMR spectra and (c) Variation of $1/T_1T$ and T_2 against T

NMR spectra for the Mg-doped compound is attributed to the presence of the localized $S \neq 0$ spins near the chain ends. The temperature dependence of spin-lattice relaxation rate ($1/T_1T$) [Fig.1(c)] of the doped compound shows a sharp enhancement below 20 K, wherein the pure system showed a continuous decrement. This suggests the predominance of another relaxation mechanism. Such feature may be attributed to the spins at the ends of the chains. Moreover, the enhancement of $1/T_1T$, measured at 1.2 T, is large compare to that of measured at 7 T. The temperature variation of spin-spin relaxation time (T_2) [Inset of Fig. 1(c)], measured at 1.2 T, indicates the formation of spin-spin correlation below 20 K. Whereas, the T_2 , measured at 7 T, does not show any indication of ordering. Thus the results of relaxations confirm that the impurity induced AF order disappears at 7 T.

REFERENCE

- [1] B. Pahari et al. *Physica B* **395** (2007) 138
- [2] B. Pahari et al. *Phys. Rev. B* **73** (2006) 012407

VALENCE BOND STATES AND LINKS MODELS

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An antiferromagnet spin-1 model is characterized on a 2D lattice with the following requirements:

- 1) The Hamiltonian is made out of nearest neighbor interactions.
- 2) It is homogeneous, translational and rotational invariant.
- 3) The ground state is a real singlet state of SU(2) (non-chiral).
- 4) It has a local spin-1 representation.

[1] Work in progress.

Magnetic properties and electronic Structure of $S = 1/2$ dimer system: $\text{BaCu}_2\text{V}_2\text{O}_8$

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(Dated: July 11, 2007)

We have investigated in details the electronic structure and magnetism of the proposed alternating spin chain compound $\text{BaCu}_2\text{V}_2\text{O}_8$ using both theory and experiment. Our magnetic susceptibility measurements on powder samples reveal that the magnetic behavior of this compound is best described by the isolated dimer model. We have also employed first principles calculations to study the electronic structure and magnetic properties of this low dimensional vanadate. We have calculated the Cu-Cu hopping parameters for various distances and found that the Cu-Cu hopping between the NNN(next nearest neighbor) is most dominant suggesting that the previously proposed alternating model is not valid thus confirming our experimental conclusion of the isolated dimer model. Our estimate of the alternation parameter $\alpha \approx 0$ from experiment compares very well with the ratio of the NN(nearest neighbor) exchange interaction to the NNN exchange interaction obtained from first principles calculation.

Dynamical correlation functions in the Ising model with a boundary

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Using scanning tunneling microscopy one can measure the local density of states in the presence of impurities. In one-dimensional systems, like stripes in high-temperature superconductors, an impurity is equivalent to a boundary. This motivates the study of correlation functions in models with boundaries. In particular, the low-energy properties of strongly correlated systems are typically described by boundary field theories. We have calculated the dynamical correlation functions in the semi-infinite quantum Ising chain in the presence of a boundary magnetic field. The used form-factor expansion is found to be fastly convergent for $R > 0.1\xi$, where R is the distance from the boundary and ξ denotes the correlation length. In particular, we find a light-cone effect and oscillations which influence the system far away from the boundary. The effect of a possible boundary bound state is analysed.

**Novel phases and magnetic refrigeration :
fine tuning entropy in a classical frustrated magnet**

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In this work we study the interplay between entropy and magnetic field in a frustrated magnet, using the classical J_1 - J_2 Heisenberg model on the square lattice as a paradigmatic example of a system which can be tuned from order to disorder. Special attention is paid to the change in temperature of the system with applied magnetic field h - the so-called Magnetocaloric Effect.

Both numerical (Monte Carlo simulation) and analytical (low temperature spin wave expansion) methods are employed. The results obtained explicitly relate the MCE to canted spin configurations at finite (h,T) , provide new insight into the magnetization plateau observed for $J_2 = J_1/2 > 0$, and demonstrate that a substantially enhanced MCE is accessible at low magnetic fields in the "frustrated ferromagnetic" region of the J_1 - J_2 phase diagram. Frustrated ferromagnets are proposed as possible materials for magnetic refrigeration.

Magnetization plateaus and sublattice ordering in easy axis Kagome lattice antiferromagnets

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We study the effects of easy axis single-ion anisotropy (D) in $S \geq 3/2$ kagome lattice antiferromagnets when the anisotropy dominates over the Heisenberg exchange J . For a broad range of magnetic fields $J^3/D^2 \lesssim B \lesssim JS$ along the easy axis, we establish the presence of a one-third magnetization ($m = 1/3$ in units of saturation magnetization) plateau with unusual low temperature order that breaks sublattice symmetry but not translation symmetry. In addition, we obtain a simple characterization of the collinear states selected by the exchange dynamics near $B = 0$ before the onset of the plateau.

[1] A. Sen, K. Damle, and A. Vishwanath, arXiv:0706.2362v1

Gap tuning in Cu²⁺ chain compounds Na₂Cu₂Si₄O₁₁·xH₂O (0 < x < 2)

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The copper silicate Na₂Cu₂Si₄O₁₁·2H₂O can be reversibly transformed to the dehydrated form Na₂Cu₂Si₄O₁₁ by heating without destruction of its framework [1]. The water molecules are included in first Cu²⁺ coordination sphere. The magnetic network of Na₂Cu₂Si₄O₁₁·2H₂O is constituted of edge-sharing chains of CuO₆ octahedra while that of Na₂Cu₂Si₄O₁₁ is made of chains of edge-sharing pyramids CuO₅. In both cases the strong alternation of exchange interaction within the chains stems from the topology of the chains.

In present work, we investigated magnetic and thermal properties of Na₂Cu₂Si₄O₁₁·2H₂O and Na₂Cu₂Si₄O₁₁ in the range 5 – 300 K. The temperature dependences of susceptibility $\chi(T)$ demonstrate broad maxima at 61 K in Na₂Cu₂Si₄O₁₁·2H₂O and 49 K in Na₂Cu₂Si₄O₁₄ and gradual decrease below these temperatures. At high temperatures the molar specific heat of Na₂Cu₂Si₄O₁₁·2H₂O is larger than that of Na₂Cu₂Si₄O₁₁ since the number of atoms per molecule in the first case is N = 25 and in the second case is N = 19. The specific heat of hydrated silicate exceeds that of the dehydrated compound below 20 K.

The experimental data were analyzed in the model for non – interacting dimers. The positions of $\chi(T)$ maxima were used to determine the exchange interaction parameters within the chains J_{\max} which amount 96 K in Na₂Cu₂Si₄O₁₁·2H₂O and 85 K in Na₂Cu₂Si₄O₁₁. The temperature dependences of susceptibility were fitted with the sum of temperature independent term χ_0 , Curie – Weiss term

$$\chi_{CW} = nN_A g^2 \mu_B^2 / 3k_B(t - \theta),$$

where $\theta = \Theta/J_{\max}$ is the reduced Weiss temperature, and dimer susceptibility term

$$\chi = (1-n)\exp(-1/t)/(t(1+3\exp(-1/t)))$$

for n segments of spin chains. The parameters obtained from magnetic properties were used to calculate magnetic specific heat for both compounds as

$$C_{\text{mag}} = \exp(-t)/(t(1+3\exp(-t))^2)$$

Theoretical value of C_{mag} for Na₂Cu₂Si₄O₁₁·2H₂O exceeds that of Na₂Cu₂Si₄O₁₁ at low temperatures which is indeed observed experimentally. The absence of well defined anomaly in C(T) dependences at low temperatures can be attributed to the predominant lattice contribution.

In conclusion, two new low dimensional compounds Na₂Cu₂Si₄O₁₁·2H₂O and Na₂Cu₂Si₄O₁₁ were found. The spin gap behavior is attributed to a strong alternation of exchange interaction within the Cu²⁺ chains. The unique possibility of gap tuning by water content in these compounds was established.

This work is supported by ISTC grant N 3501, RFBR grants N 07-02-00350, 06-02-16088 and DFG grant N 1824/3-1.

[1] P. Brandao, F.A. Paz, J. Rocha, Chem. Comm. **14**, 171 (2004).

Extended liquid phase in the Quantum Dimer Model on a Diamond Lattice

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Quantum dimer models (QDM's) provide the established paradigm for spin liquid states in frustrated quantum magnets. On bipartite lattices they can be mapped onto a $U(1)$ gauge theory, which can in principle support a liquid-like ground state with fractional excitations. However in two dimensions, these excitations are confined, except at the "Rokhsar-Kivelson (RK) point", a quantum critical point occurring for one specific ratio of parameters. Recently, it has been suggested that a $U(1)$ liquid might be stable for an extended set of parameters bordering on the RK point in the QDM on a 3D diamond lattice.

Here we present preliminary results for Green's Function Monte Carlo simulations which support this conjecture. In particular, we contrast the scaling of the gap between ground states in the relevant topological sectors for the QDM on a diamond lattice with that found in the QDM on a square lattice.

The phase diagram of the asymmetric Hubbard model: a DMRG analysis

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Using the density matrix renormalization group technique, we study the ground state quantum phase diagram of the one-dimensional asymmetric Hubbard model. A quantitative phase diagram of the model, at partial filling, is calculated for the first time. The phases obtained are charge density wave and phase separation, which are separated by a non-universal critical hopping. The critical hopping is an increasing function of the local on-site repulsion, for any fixed density, in agreement with previous results obtained for some limits of the model. We show the evolution of the system from the Falicov-Kimball to the Hubbard limit.

High pressure transport study of $\text{Co}_{1/3}\text{NbS}_2$

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$\text{Co}_{1/3}\text{NbS}_2$ belongs to the family of the transition-metal intercalated transition metal dichalcogenides. Co occupies octahedral positions between the trigonal prismatic layers of the host compound 2H NbS_2 , resulting in a $\sqrt{3} \times \sqrt{3}$ superlattice [1]. Two electrons per Co atom are transferred to the initially half-filled d_{z^2} -band of the host NbS_2 which thereby broadens and becomes 5/6 filled. The remaining seven electrons on the Co ion are localized and form magnetic moments with a quenched orbital contribution (3/2 spin-only moment). These moments order antiferromagnetically (known as the hexagonal ordering of the first kind) at the Néel temperature of 26 K. This transition is driven by two competing interactions: the RKKY and the superexchange via neighboring S ions [2]. A way to vary the relative strength of these interactions is by applying pressure. We have measured the electrical resistivity and thermopower at room pressure from 1.6 to 300 K and under pressures (up to 1.8 GPa in the temperature range of 1.6 to 300 K). In addition, thermal conductivity was measured at room pressure from 2 to 300 K. Resistivity is metallic-like with a change in slope at the Néel temperature. This is interpreted as diminution of the spin-disorder upon entrance into the antiferromagnetic state. Transition temperature is shifted to lower values with increasing hydrostatic pressure accompanied by development of a resistivity minimum. Thermopower on the other hand exhibits non-metallic behavior above 100 K and a small maximum at 10 K which diminishes and appears at lower temperatures upon applying pressure. Thermal conductivity is also unusual and bears very little change at the Néel temperature. This work was supported by the MoSES project No. 035-0352826-2848 and the SNF SCOPES project No. IB7320-111044.

[1] S. S. P. Parkin *et al.*, J. Phys. C: Solid State Phys. **16** (1983), 2765

[2] S. S. P. Parkin and R. H. Friend, Phil. Mag. B **41** (1980), 65

Heat conduction in spin-gap antiferromagnets

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The spin-gap antiferromagnets have a discrete spin-energy spectrum due to the existence of only short-range spin correlations. The thermal conductivity is a tool that probes the spin excitations and spin-phonon interaction. A variety of phenomena are observed: for example, in various strontium-cuprates thermal conductivity is strongly enhanced due to the opening of the heat channel carried by either magnons or spinons; in spin-Peierls compounds the heat transport exhibits rather unusual double peak at low temperatures, explained as a fingerprint of the spin-phonon resonance scattering. The thermal conductivity of strongly frustrated systems also shows the existence of spin-phonon resonance at low temperatures. We present the study of the thermal transport of several spin-gap antiferromagnets: (i) copper-tellurides, quasi-1D geometrically frustrated compounds with $S = 1/2$, (b) a "zigzag" frustrated spin ladder system LiCu_2O_2 ($S = 1/2$), and (c) quasi-2D $S = 1$ system nickel-telluride. We find that the thermal conductivity of these systems exhibits behavior typical for spin-phonon resonance coupling, and it gradually decreases as the dimensionality of the systems increases. This work was supported by the MoSES projects No. 035-0352826-2848 & 177-0352826-0478 and the SNF SCOPES project No. IB7320-111044.

Ordered Phases of the Anisotropic Kagome Lattice Antiferromagnet in a Magnetic Field

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The antiferromagnetic Heisenberg model on an anisotropic kagome lattice may be a good minimal model for real magnetic systems as well as a limit from which the isotropic case can be better understood. We study the nearest-neighbor Heisenberg antiferromagnet on an anisotropic kagome lattice in a magnetic field. Such a system should be well described by weakly interacting spin chains, and we motivate a general form for the interaction by perturbatively projecting out the inter-chain spins. In the spin $1/2$ case, we find that the system exhibits a quantum phase transition from a ferrimagnetic ordered state to an XY ordered state as the field is increased. Finally, we discuss the appearance of magnetization plateaus in the ferrimagnetic phase.

- [1] Z. Hiroi, M. Hanawa, N. Kobayashi, M. Nohara, H. Takagi, Y. Kato, and M. Takagawa. Spin- $1/2$ kagome-like lattice in volborthite $\text{Cu}_3\text{V}_2\text{O}_7(\text{OH})_2 \cdot 2\text{H}_2\text{O}$. *J. Phys. Soc. Jpn.*, 70:3377, 2001.
- [2] G. Fath. Luttinger liquid behavior in spin chains with a magnetic field. *Phys. Rev. B*, 68:134445, 2003.
- [3] T. Hikihara and A. Furusaki. Spin correlations in the two-leg antiferromagnetic ladder in a magnetic field. *Phys. Rev. B*, 63:134438, 2001.

Reentrant phase transitions of Ising-Heisenberg ferromagnet on a triangular lattice with diamond-like decorations

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The method based on the generalized decoration-iteration transformation is used to obtain the exact solution for the ferromagnetic Ising-Heisenberg model on a triangular lattice with diamond-like decorations. Our previous studies on this interesting quantum spin system have revealed an extraordinary rich ground-state phase diagram, which is composed of the classical ferromagnetic phase, the quantum ferromagnetic phase and the remarkable kind of disordered phase [1]. In spite of the pure ferromagnetic character of the model under investigation, we have found strong indications that the disordered phase arises as a result of a peculiar geometric spin frustration, which is closely connected to an interplay between the easy-plane Heisenberg- and the easy-axis Ising-like interactions.

It has been pointed out previously [2] that simple geometries composed solely of interconnecting diamonds often give rise to the interesting competition between the long-range magnetic order and quantum fluctuations. The purpose of present work is to clarify this issue in more detail by providing the global phase diagram of the model under investigation. It turns out that the competition between the long-range magnetic order and quantum fluctuations is responsible for an appearance of the complex finite-temperature phase diagram including closed loops of phase transition lines separating the long-range ordered phase(s) from the disordered one. This kind of global phase diagram implies that the competition causes multiply reentrant phase transitions between the long-range ordered and the disordered phases. The influence of single-ion anisotropy upon the occurrence of reentrant phase transitions is studied in particular. Our results are convincingly evidenced by detailed analysis of spontaneous magnetization, which represents the order parameter for the ferromagnetic system.

[1] J. Strečka and M. Jaščur, Phys. Stat. Sol. (b) 233 (2002) R12.

[2] M.W. Long and S. Siak, J. Phys.: Condens. Matter 2 (1990) 10321.

Heisenberg AF on Penrose tiling

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The Penrose tiling is a perfectly ordered two dimensional structure with fivefold symmetry and scale invariance under site decimation. Quantum spin models on such a system can be expected to differ significantly from more conventional structures as a result of its special symmetries. In one dimension, for example, aperiodicity can result in distinctive quantum entanglement properties. In this work, we study ground state properties of the spin-1/2 Heisenberg antiferromagnet on the Penrose tiling, a model that could also be pertinent for certain three dimensional antiferromagnetic quasicrystals.

We show, using spin wave theory and quantum Monte Carlo simulation, that the local staggered magnetizations strongly depend on the local coordination number z and are minimized on some sites of five-fold symmetry. We present a simple explanation for this behavior in terms of Heisenberg stars.

References:

- [1] R. Penrose, *The Math. Intelligencer* **2**, 32 (1979)
- [2] R. M. White, M. Sparks and I. Ortenburger, *Phys. Rev.* **139**, A450 (1965)
- [3] E. Manousakis, *Rev. Mod. Phys.* **63**,1 (1991)
- [4] S. Wessel and I. Milat, *Phys. Rev. B* **71**, 104427 (2005)
- [5] A. Jagannathan, A. Szallas, Stefan Wessel, and Michel Duneau, *Phys. Rev. B* **75**, 212407 (2007)

An Effective Low Energy Random Field Ising Model Description of the $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ Quantum Ising Magnet in a Transverse Magnetic Field

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Magnetic $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ in a transverse field has attracted a lot of attention over the past twenty years or so because it is an ideal system to study controlled quantum mechanical fluctuation effects in disordered systems. When a magnetic field is applied transversely to the Ho Ising magnetic moments in $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$, the field-induced transition behaves quite differently from theoretical expectations, as found in the case with $x = 0.167$ where the paramagnet to spin glass transition has been studied experimentally in some detail. In particular, experiments find that the cusp in the nonlinear susceptibility signaling the glass state decreases in size as the temperature is lowered and the critical transverse field increases. We show that in the presence of a transverse magnetic field B_x , the effective low-energy Hamiltonian of a general anisotropic dipolar interaction with non zero off-diagonal dipolar couplings is well described by a random field transverse Ising model. We show that how the random fields explain the smearing of the nonlinear susceptibility at the spin glass transition with increasing B_x in $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$.

[1] References if any

One-dimensional electronic systems by Jastrow correlated wavefunctions

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We apply the well known Jastrow variational wavefunction to a widely used and accepted model for describing the low-energy properties of interacting electrons in one dimension, namely the Luttinger model. The consequences are far-reaching. We demonstrate that the ground state of the Luttinger model is just a Jastrow-Slater variational wavefunction. Moreover, we show that not only the ground state, but also single-particle excitations of the Luttinger Liquid can be described within the variational scheme. Finally, we evaluate the single-particle spectral weight and the result obtained is consistent with the Luttinger Liquid theory.

Frustrated dimer models: interpolating between the square and triangular lattices

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Classical and quantum dimer models have close connections to frustrated magnetic systems: in particular, a 2D quantum dimer model was developed by Rokhsar and Kivelson[1] (“RK model”) 20 years ago to understand the properties of the Resonating-Valence-Bond phase of cuprate materials and its connection to superconductivity.

The properties of the RK model depend strongly on the lattice topology: a liquid phase was found on the triangular lattice[2], while on the square lattice[3] dimers order everywhere except at a critical point.

To understand these differences, we studied a classical dimer model, on a lattice interpolating between the square and triangular lattices[4]. With a

transfer matrix approach, we compute correlations on finite tori as well as the central charge and exponents of correlations, using conformal field theory arguments[5,6], and determine the domain of existence of the critical phase existing in the square lattice limit.

The main result of that study is that a critical phase is found in a finite temperature range on the triangular lattice (but with anisotropic, “non-frustrating” dimer interactions); in contrast, the critical phase is disfavored by the addition of frustrating interactions, going progressively towards the isotropic model . On the isotropic triangular lattice, no critical phase is found, but our results indicate that a dimer ordering occurs at low temperature, favored by an “order-by-disorder” mechanism.

[1] D.Rokhsar, S.Kivelson, PRL **61**, 2376 (1988)

[2] R.Moessner, S.L.Sondhi, PRL **86**, 1881 (2001)

[3] D.Poilblanc et al, PR B **74** , 014437 (2006)

[4] F.Trousselet, P.Pujol, F.Alet, D.Poilblanc, arXiv: 0705.4550

[5] F.Alet et al., PR E **74**, 041124 (2006)

[6] C.Castelnovo, C.Chamon, C.Mudry, P.Pujol, Ann.Phys. 322 (2007) pp.903-934

Evidence for a magnetic phase transition in the frustrated spin-1/2 Heisenberg chain compound near the quantum critical point

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We report thermodynamic properties of the novel low dimensional strongly frustrated spin – $\frac{1}{2}$ Heisenberg chain cuprate $\text{Li}_2\text{ZrCuO}_4$. The compound is close to the quantum critical point between ferromagnetic and spiral ordering [1].

The anomaly of unusual shape in the specific heat and the maximum in the derivative of the magnetic susceptibility $d\chi/dT$ at around 6 K as well as magnetization behavior of the low dimensional $\text{Li}_2\text{ZrCuO}_4$ allude to onset of a long range order in this compound. This suggestion is also supported by results of muon spin relaxation performed on a powder sample of $\text{Li}_2\text{ZrCuO}_4$, which show a spontaneous muon spin precession below 5.75 K. A peculiar rectangular shape of the static field distribution in the ordered state is consistent with an incommensurate helical spin structure predicted theoretically.

The ultra low specific heat exhibits an unusual linear contribution with a large Sommerfeld coefficient. Measurements of specific heat in high magnetic fields are also presented and discussed.

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[1] S.L. Drechsler et al. Phys. Rev. B **98**, 077202 (2007)

Short and long range order in silicates with Cu²⁺ chains

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The silicates can be used as proving ground for construction of new low dimensional compounds. These materials include isolated chains from edge or corner shared polyhedra of copper coordinated by oxygen. In the present work we report investigations of several members of this family of compounds Na₂Cu₂Si₄O₁₁·xH₂O (0 < x < 2) and Na₂Cu₅Si₄O₁₄. Their physical properties differ drastically.

The copper silicate Na₂Cu₂Si₄O₁₁·2H₂O and its dehydrated form Na₂Cu₂Si₄O₁₁ include the isolated edge – sharing CuO₆ (or CuO₅) chains [1]. They can be reversibly transformed to each other by heating. The water molecules are included in the first Cu²⁺ coordination sphere. So, the water content influences the parameters of the magnetic subsystems in these compounds. The structure of the chains presumes strong alternation of exchange parameters within the chains. The temperature dependences of specific heat and magnetic susceptibility confirm the spin gaps $\Delta = 96$ K in hydrated and $\Delta = 85$ K in dehydrated compounds.

The Na₂Cu₅Si₄O₁₄ compound includes chains which consist of dimers and trimers shared in turn through the corners. Every dimer (or trimer) is based on edge shared CuO₄ squares [2]. The temperature and field dependences of the magnetization indicate the formation of long range antiferromagnetic order below T_N ~ 7 K. This was confirmed by specific heat measurements.

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[1] P. Brandao, F.A. Paz, J. Rocha, Chem. Comm. **2**, 171 (2005).

[2] A. Moreira Dos Santos et al., Phys. Rev. B **72**, 092403 (2005).

Local-probe investigation of the kagomé-like compound $\text{Nd}_3\text{Ga}_5\text{SiO}_{14}$

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We report on the experimental investigation of a single crystal of the novel rare-earth based compound $\text{Nd}_3\text{Ga}_5\text{SiO}_{14}$. The Nd ($J = 9/2$) magnetic moments form a 2D lattice, which for dominant isotropic nearest-neighbor exchange coupling, is topologically equivalent to a kagomé lattice [1]. Due to significant spin-orbit coupling with respect to the crystal field, a pronounced magnetic anisotropy is observed in susceptibility measurements. This may significantly affect the ground-state properties of the investigated compound. In the limit of classical spins with Ising anisotropy, a collective paramagnetic state is expected.

In an attempt to throw a light on the interplay between magnetic anisotropy and fluctuations, governed by the frustrated topology of the magnetic lattice, we've initiated a comprehensive study of complementary local-probe techniques, including NMR, ESR and μSR . This approach allows us to follow the temperature evolution of the static magnetic properties on the local scale as well as the evolution of magnetic fluctuations in different frequency windows. Our μSR results demonstrate the persistence of a dominantly fluctuating regime down to at least 50mK with.

[1] P. Bordet et al., J. Phys.: Condens. Matter **18**, 5147 (2006).