Correlated states and excitations in d- and f-electron systems and ultracold Fermi gases

Summary

In this project we have considered the low temperature properties of strongly correlated materials when quantum effects are strong. Typical examples include magnetic materials with spin and orbital degrees of freedom, ultracold atoms in optical lattices and f-electron systems. Most of these systems are Mott insulators, i.e. the effective degrees of freedom are localized to the sites (atoms), such as the magnetic moments of an ion. The model describing the dynamics in such system is the Heisenberg model, in the simplest case it just exchanges the local quantum states of two neighboring atoms.

We treated these systems with analytical and numerical methods. While we conducted theoretical research, in many cases we were motivated by the experiments done on existing materials. On a few occasions we worked in a close collaboration with experimental researchers, as in the case of the Cu_2OSeO_3, a materials showing skyrmions, and in the case of the multiferroic $Sr_2CoGe_2O_7$. Our input proved to be essential to understand the experimental neutron spectra of the Cu_2OSeO_3 or to recognize the spin-quadrupolar excitations in the high field ESR spectra in $Sr_2CoGe_2O_7$.

To guide and motivate experiments, we were researching extreme quantum behavior in systems yet to be realized. Such an example is the chiral spin liquid we found in the SU(6) honeycomb lattice and SU(N) triangular lattice models with multiple exchange terms. Our implementation of a variational Monte Carlo Method has played a key role in describing the chiral phase in these models of ultracold atoms.

One of the highlights of our results is the identification of the topological character of the triplon excitations in the $SrCu_2(BO_3)_2$ quantum magnet, which would lead to a thermal Hall effect. The topological property of the excitations is due the relativistic spin-orbit interaction and the structure of the material.

We will discuss a selection of interesting results in detail following the list of publications.

In the last year of the project we have organized a workshop ”Topological properties in quantum magnets”, from August 30 – September 1, 2017. The workshop took place in the Wigner Research Centre in Budapest and was open to researchers who wished to listen to the talks. The accommodation of the invited foreign participants was covered by the grant. The list of the invited speakers is appended to this final report.

During the project two PhD student were involved: Miklós Lajkó (he completed his doctoral studies successfully in 2013), and Péter Balla.

Publications

Our results have been published in 22 refereed journals: 2 Nature Communications, 3 Physical Review Letters, 1 Scientific Reports, 14 Physical Review B, and 2 Journal of the Physical Society of Japan. The total impact factor is above 100.

The starred items in the publication list are presented in more details starting from page 3.

SU(N) Mott isulators

1. *Competing states in the SU(3) Heisenberg model on the honeycomb lattice: Plaquette valence-bond crystal versus dimerized color-ordered state*, by Corboz P., Lajkó M., Penc K., Mila F., Läuchli A.M., in Phys. Rev. B **87** 195113 (2013).

2. *Tetramerization in a SU(4) Heisenberg model on the honeycomb lattice*, by Lajkó M., Penc K. , in Phys. Rev. B **87** 224428 (2013).

3. *Order, by disorder in a four flavor Mott-insulator on the fcc lattice*, by Sinkovicz P., Szirmai G., Penc K., in Phys. Rev. B **93** 075137 (2016).

4. **Plaquette order in the SU(6) Heisenberg model on the honeycomb lattice*, by Nataf P., Lajkó M., Corboz P., Läuchli A.M., Penc K., Mila F., in Phys. Rev. B **93** 201113 (2016).

5. **Chiral Spin Liquids in Triangular-Lattice SU(N) Fermionic Mott Insulators with Artificial Gauge Fields*, by Nataf P., Lajkó M., Wietek A., Penc K., Mila F., Läuchli A.M., in Phys. Rev. Lett. **117** 167202 (2016).

6. **Generalization of the Haldane conjecture to SU(3) chains*, by Lajkó M., Wamer K., Mila F., Affleck I., in Nucl. Phys. B **924** 508-577 (2017).

7. *Linear Flavor-Wave Theory for Fully Antisymmetric SU(N) Irreducible Representations*, by Kim F.H., Penc K., Nataf P., Mila F., in Phys. Rev. B 96, 205142/1-11 (2017).

f-electron systems

1. **Scaling theory vs exact numerical results for the spinless resonant level model*, by Kiss A., Otsuki J., Kuramoto Y. , in J. Phys. Soc. Jpn. **82** 124713 (2013).

2. **Exact dynamics of charge fluctuations in the multichannel interacting resonant level model*, by Kiss A., Kuramoto Y., Otsuki J., in J. Phys. Soc. Jpn. **84** 104602 (2015).

Quantum spin models

1. *Zero-temperature Monte Carlo study of the non-coplanar phase of the classical bilinear-biquadratic Heisenberg model on the triangular lattice*, by Wenzel S., Korshunov S.E., Penc K., Mila F. , in Phys. Rev. B **88** 094404 (2013).

2. **Berry phase induced dimerization in one-dimensional quadrupolar systems*, by Hu S., Turner A.M., Penc K., Pollmann F., in Phys. Rev. Lett. **113** 027202 (2014).

3. *Interplay of charge and spin fluctuations of strongly interacting electrons on the kagome lattice*, by Pollmann F., Roychowdhury K., Hotta C., Penc K., in Phys. Rev. B **90** 035118 (2014).

4. *Chain-based order and quantum spin liquids in dipolar spin ice*, by McClarty P., Sikora O., Moessner R., Penc K., Pollmann F., Shannon N., in Phys. Rev. B **92** 094418 (2015).

5. *Subharmonic transitions and Bloch-Siegert shift in electrically driven spin resonance*, by Romhányi J., Burkard G., Pályi A., in Phys. Rev. B **92** 054422 (2015).

6. *Hall effect of triplons in a dimerized quantum magnet*, by J. Romhányi, K. Penc and R. Ganesh, in Nat. Commun. **6** 6805 (2015).

7. *Semiclassical theory of the magnetization process of the triangular lattice Heisenberg model*, by Coletta T., Tóth T.A., Penc K., Mila F., in Phys. Rev. B **94** 075136 (2016).

8. *Spin-Orbit Dimers and Noncollinear Phases in d^1 Cubic Double Perovskites*, by Romhányi J., Balents L. and Jackeli G., in Phys. Rev. Lett. **118** 217202 (2017).

Works done in collaboration with experimentalists

1. *Empirical Monod-Beuneu relation of spin relaxation revisited for elemental metals*, by Szolnoki L., Kiss A., Forró L., Simon F., in Phys. Rev. B **89** 115113 (2014).

2. *The Elliott-Yafet theory of spin relaxation generalized for large spin-orbit coupling*, by Kiss A., Szolnoki L., Simon F., in Sci. Rep. 6 22706 (2016).

3. **Magnon spectrum of the helimagnetic insulator Cu_2OSeO_3*
Portnichenko P.Y., Romhányi J., Onykiienko Y.A., Henschel A., Schmidt M., Cameron A.S., Surmach M.A., Lim J.A., Park J.T., Schneidewind A., Abernathy D.L., Rosner H., Brink J. v d and Inosov D.S., in Nat. Commun. **7** 10725 (2016).

4. **Spin excitations in the skyrmion host Cu_2OSeO_3*, by Tucker G.S., White J.S., Romhányi J., Szaller D., Kézsmárki I., Roessli B., Stuhr U., Magrez A., Groitl F., Babkevich P., Huang P., Živković I., Rønnow H.M., in Phys. Rev. B **93** 054401 (2016).

5. *Direct observation of spin-quadrupolar excitations in $Sr_2CoGe_2O_7$ by high field ESR*, by Akaki M., Yoshizawa D., Okutani A., Kida T., Romhányi J., Penc K., Hagiwara M., in Phys. Rev. B.**96**, 214406/1-16 (2017)

Detailed presentation of some selected results.

Topological excitations and Hall effect in a quantum magnet

Topology is a mathematical discipline that, remarkably, holds the answer to many of the interesting problems arising in our field of interest. Commencing with the discovery of the quantum Hall effect [1] and topological insulators [2], it has and keeps revolutionizing today's physics. The notion of topology enabled us to distinguish symmetrically identical but topologically distinct phases. Its importance has been recognized by awarding the Nobel Prize "*for discoveries of topological phase transitions and topological phases of matter*" last year. Most of topology related advances has been made in the context of weakly interacting electron systems. The weakly interacting excitations of strongly correlated insulating magnets can, however, behave similarly to the electrons of a topological band insulator. Recently, tremendous effort has been done in this direction, underlining the relevance of such parallel.

In our work we identified the analogue of topologically nontrivial bands in the magnetic excitations of the archetypal spin-gap quantum magnet $SrCu_2(BO_3)_2$. The generalization of the conventional spin-$1/2$ Dirac physics known for the noninteracting electron systems to the spin-1 case arising naturally in the triplet excitations is of particular importance [3].

$SrCu_2(BO_3)_2$ is the physical realization of the well-known Shastry-Sutherland model, a two-dimensional orthogonal dimer lattice of antiferromagnetically interacting spin-$1/2$ entities. In the exact ground state, the spin-halves form a singlet states, which unambiguously cover the lattice, not breaking any symmetry. Due to the finite spin-gap, the dimer-singlet state remains stable in low magnetic field as well. The low energy excitations corresponds to promoting a singlet into a triplet state which then propagates over the lattice. In an isotropic (spin rotational invariant) model the three different triplets are degenerate and localized. This is not however what has been observed in experiments [4, 5]. The neutron spectrum reveals propagating triplet modes that are split even in the absence of magnetic field [5]. To fully understand the physical properties of

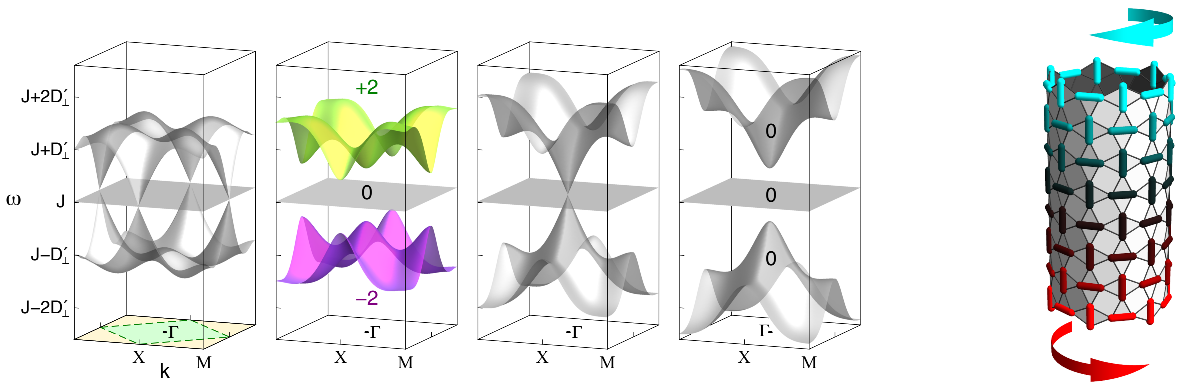

Figure 1: Left: The triplon dispersions for increasing magnetic field in the model for $SrCu_2(BO_3)_2$. The Chern number for each band is indicated. Right: Topologically protected edge-states (blue and red) at the edges of an imaginary Sr2Cu(BO3)2 layer wrapped as a cylinder. The excitation on the upper and lower edge move in opposite directions.

$SrCu_2(BO_3)_2$ therefore, one needs to extend the original Shastry-Sutherland model with anisotropies arising from a weak spin-orbit interaction. The anisotropy responsible for the experimental observations is the so called Dzyaloshinksii-Moriya interaction [6, 7].

Remarkably, the Dzyaloshinksii-Moriya is accountable for a lot more. We showed that this anisotropy term renders the triplet bands topologically nontrivial. The great advantage of topological excitations over the conventional noninteracting electron systems is that the topological properties can be tuned by magnetic field instead of the more complicated doping. Such is the case with $SrCu_2(BO_3)_2$. In zero field the triplet bands form a novel spin-1 Dirac cone, with the three bands touching at a single point. A finite field fully splits the triplets and the Chern number, the invariant characterizing the topological properties of the bands, becomes a well-defined quantity. The larger spin-1 nature of triplets is reflected in the larger $+2, 0, -2$ Chern numbers. Increasing the magnetic field, the bands undergo a band touching topological transition, above which they become topologically trivial with zero Chern numbers. This topological transition is shown in Fig. 1

As a consequence of finite Chern numbers and nontrivial topology, when the system has edge states appearing at its open boundaries. Such edge modes emerge in the gap of the Chern-bands connecting those, and are topologically protected against back-scattering, simply because there is "nowhere" to be scattered. This means that at the edges, the sample is "conducting" and the current of edge modes is unaffected by local defects or other small perturbations present in real materials. A representative propagating edge state of $SrCu_2(BO_3)_2$ is shown in Fig. 1. Beyond theoretical interest, the robust topological edge states have tremendous potential in applications. They are ideally suited for devices in which the electrons themselves are static, but the spin can be transported as in a wire. Such currents will not be dissipated by heating and the device itself can work at higher speeds. This discovery suggests new systems for spintronics and new ways to use spin currents to process and store information.

Our work has been published as: "*Hall effect of triplons in a dimerized quantum magnet*" by J. Romhányi, K. Penc and R. Ganesh in Nat. Comm. **6**, 6805/1-6, (2015)

Generalization of the Haldane conjecture to SU(3) chains

About 35 years ago, Haldane's conjecture for Heisenberg spin chains came as a surprise to both condensed matter and high energy physics communities [8,9]. Mapping the low energy degrees of freedom in the large-S limit to the 1+1 dimensional $\mathrm{O}(3)$ nonlinear sigma model, Haldane argued that integer and half-integer chains have fundamentally different behaviours: while half-integer spin chains are gapless, integer spin chains are gapped with a unique ground state. The argument hinges on the presence of a topological term in the sigma model, that has a nontrivial angle for half integer spins, while being trivial for the the integer spin case. Despite the initial controversy, Haldane's conjecture was quickly verified by numerical simulations and by experiments on quasi one dimensional antiferromagnets [10].

Extending Haldane's method to the $\mathrm{SU}(N)$ case is of interest for several reasons. Recent developments in cold atom experiments allow the realization of $\mathrm{SU}(N)$ symmetric systems using alkaline earth atoms [12,13], therefore it is very timely to provide theoretical predictions which can fuel future experiments. On the other hand, although several numerical techniques are also extended for the $\mathrm{SU}(N)$ case [14, 15], due to the increased size of the local Hilbert space and the increased correlation lengths they are often burdened with finite size effects.

In our work we extended Haldane's method to $\mathrm{SU}(3)$ spin chains in the fully symmetric representation with p boxes in the Young tableau (see Fig. 1.) In this case the low energy degrees of freedom can be mapped onto a $\mathrm{SU}(3)/[\mathrm{U}(1) \times \mathrm{U}(1)]$ nonlinear sigma model containing a topological term with a topological angle $\theta = 2\pi p/3$. Based on numerical Monte Carlo calculations on the nonlinear sigma model we argue, that the original $\mathrm{SU}(3)$ Heisenberg models must be gapped for $p = 3m$, while gapless for $p = 3m \pm 1$. The latter corresponds to an $\mathrm{SU}(3)_1$ critical point of the nonlinear sigma model at $\theta = \pm 2\pi/3$ (see Fig. 2).

This work has been published as "*Generalization of the Haldane conjecture to SU(3) chains*", by Lajkó M., Wamer K., Mila F., Affleck I., in Nucl. Phys. B **924** 508-577 (2017).

Quantum Monte Carlo simulations of Samarium based heavy electron compounds

Heavy-fermion materials with strong electron correlations play central role in solid state physics since they provide fascinating novel phenomena such as unconventional superconductivity, non-fermi liquid behavior

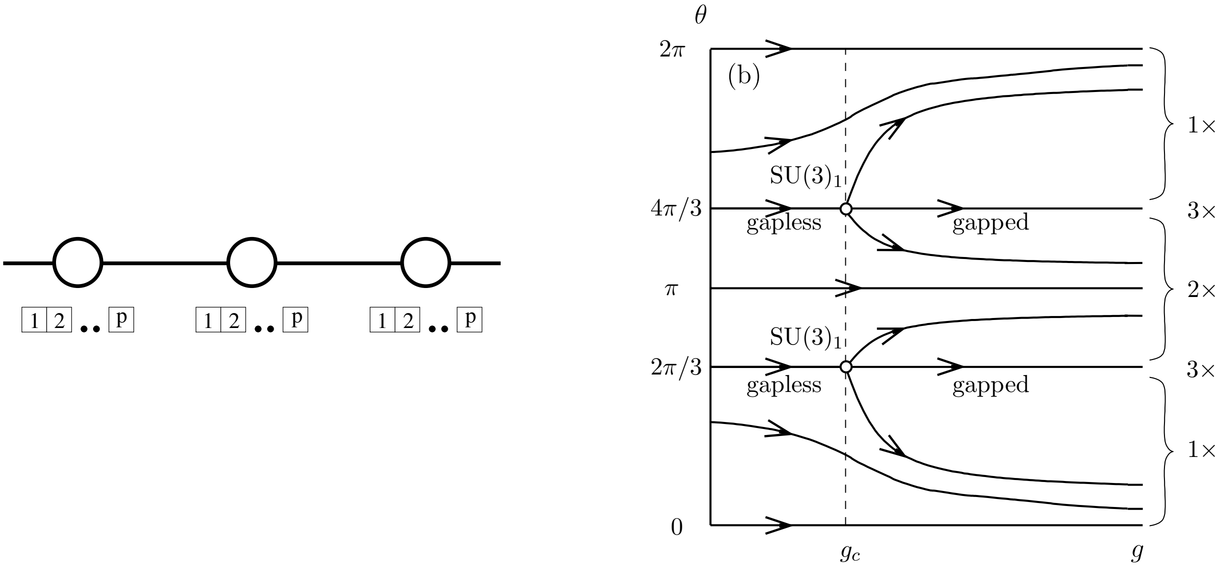

Figure 2: Left: Illustration for SU(3) spin chains with spins of the fully symmetric representation p-box representation on each site. Right: The renormalization group flow diagram for the $\mathrm{SU}(3)/[\mathrm{U}(1) \times \mathrm{U}(1)]$ nonlinear σ-model. At $\theta = 2\pi/3$ and $\theta = 4\pi/3$ the system undergoes a phase transition from a gapless phase at $g < g_c$ into a gapped phase with a spontaneously broken $\mathbb{Z}_3$ symmetry at $g > g_c$. This corresponds to a gapless to dimerized phase transition upon turning on next nearest neighbour interactions in the original spin model [11]. For $2\pi/3 < \theta < 4\pi/3$ the system is gapped with a spontaneously broken $\mathbb{Z}_2$ symmetry, while for $\theta < 2\pi/3$ and $\theta > 4\pi/3$ the system is gapped with a unique ground state for all values of g.

or anomalous Kondo effect. The main challenge in these systems is the study and understanding of interactions between the localized electrons of partly filled *f*-orbitals and conduction electrons, which led to large enhancement of the effective mass of electrons reflected in the low-temperature specific heat or resistivity.

Recently, peculiar heavy-fermion behavior has attracted attention in some samarium-based compounds with large specific heat coefficient which is insensitive to external magnetic field. The resistivity shows clear Kondo-like logarithmic anomaly in these compounds, which is, however, almost completely magnetic field independent in strong contrast to the ordinary Kondo effect based on the spin degrees of freedom. Motivated by these experimental observations we have searched for a charge fluctuation mechanism that gives rise to energy scale much smaller than the bare hybridization. As a first step, we studied numerically a modified version of the spinless Anderson model by the continuous-time quantum Monte Carlo method, and then we extended this model by the inclusion of multiple channels for the conduction electrons. In this extended model we have found that the competition of the Anderson orthogonality effect with the exciton effect gives rise to heavy fermion state with large effective mass and strong charge fluctuations, which might be responsible for the observed peculiar properties in the samarium-based compounds. Additionally, we have found an unusual double-Lorentzian lineshape for the single-particle spectra which is explained successfully by a quasi-particle perturbarion theory.

Our work has been published as "*Scaling theory vs exact numerical results for the spinless resonant level model*" by Kiss A., Otsuki J., Kuramoto Y. in J. Phys. Soc. Jpn. **82** 124713 (2013) and as "*Exact dynamics of charge fluctuations in the multichannel interacting resonant level model*" by A. Kiss, Y. Kuramoto, J. Otsuki in J. Phys. Soc. Jpn. **84** 104602 (2015)

Excitations in the magnetoelectric skyrmion host Cu_2OSeO_3

Long-range dipole interactions, magnetic frustration, or relativistic spin-orbit coupling can lead to the formation of twisting spin structures in a wide range of compounds. *Skyrmions* are probably the most prominent among them due to their nontrivial topology. These extended vortex-like spin textures can under certain conditions condense into a lattice commonly observed in the metallic helimagnets such as MnSi [16, 17], $Fe_{1-x}Co_xSi$ [18, 19], FeGe [20], and CoZnMn [21].

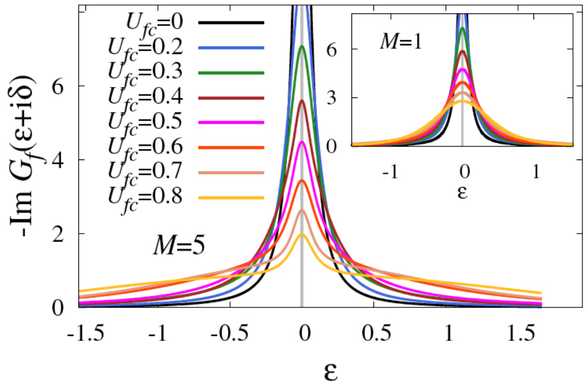

Figure 3: Energy dependence of single-particle spectra with $M = 1$ (inset) and $M = 5$ (main panel) channels for the conduction electrons. The double-Lorentzian lineshape develops with increasing Coulomb interaction U_{fc} for $M = 5$.

When additional magnetoelectric coupling is present, the topologically protected skyrmions can be controlled with the use of electric field, opening new frontiers in spintronical applications. Among the cubic helimagnets, Cu_2OSeO_3 is the only *insulator* exhibiting skyrmion lattice phase and having finite magnetoelectric coupling. Cu_2OSeO_3 offers a unique playground to explore the microscopic origins of skyrmion formation, besause its ground-state properties and low-energy excitations are fully governed by the magnetic interactions between localized spins and are not affected by the presence of itinerant carriers.

Cu_2OSeO_3 consists of alternating Cu-tetrahedra with strong and weak interactions. A suitable model thus treats the strongly interacting spins exactly, allowing for quantum mechanical entanglement between them. These Cu-tetrahedra are the elementary units of our calculations. The four spin-halves form an entangled spin-1 state on each tetrahedra, which below $T_C = 60$ K establish the helical or the skyrmion lattice phases instead of the bare Cu^{2+} spins.

Inelastic neutron scattering measurements accompanied with our theoretical calculation of magnon dispersion reveal the complete picture of magnetic excitations in Cu_2OSeO_3 over a broad range of energies in the entire Brillouin zone. We used tetrahedron-factorized multiboson method to calculate the magnon spectrum for the collinear state. Symmetrizing the time of flight data we assembled energy–momentum profiles along a polygonal path involving all high-symmetry directions in momentum space as shown in Fig. 4(a). As a test of our model, we calculated the scattering cross section (see Fig. 4(b)) demonstrating strikingly good agreement with the inelastic neutron scattering data. This proves that the tetrahedral entities are protected by a considerable gap and give rise to a rich magnetic excitation spectrum comprising a low-energy manifold and a set of weakly dispersive high-energy magnon branches. The low energy modes can be understood as classical (inter-tetrahedra) fluctuations of the effective $S = 1$ spins and the spectrum is dominated by an intense parabolic Goldstone mode associated with the spin-wave branch of ferromagnetically ordered spin-1 entities. The high-energy modes correspond to intra-tetrahedra fluctuations which involves breaking up the triplet state of a Cu-tetrahedron. The gap separating the two sets of excitations is nothing but the energy-cost of the transition to a different spin-S multiplet.

Our model is able to describe all the available experimental results (magnetization, electron spin resonance and inelastic neutron scattering data) simultaneously and may serve as a starting point for more elaborate low-energy theories to understand the complex magnetic phase diagram of Cu_2OSeO_3, including the helimagnetic order and challenging skyrmion-lattice phases.

This work has been published as "*Magnon spectrum of the helimagnetic insulator Cu_2OSeO_3*" by Portnichenko P.Y., Romhányi J., Onykiienko Y.A., Henschel A., Schmidt M., Cameron A.S., Sumach M.A., Lim J.A., Park J.T., Schneidewind A., Abernathy D.L., Rosner H., van den Brink J., Inosov D.S., Nature Commun. 7, 10725, 2016; and as "*Spin excitations in the skyrmion host Cu_2OSeO_3*" Tucker G.S., White J.S., Romhányi J., Szaller D., Kézsmárki I., Roessli B., Stuhr U., Magrez A., Groitl F., Babkevich P., Huang P., Živković I., Rønnow H.M., Phys. Rev. B 93, 054401/1-5, 2016

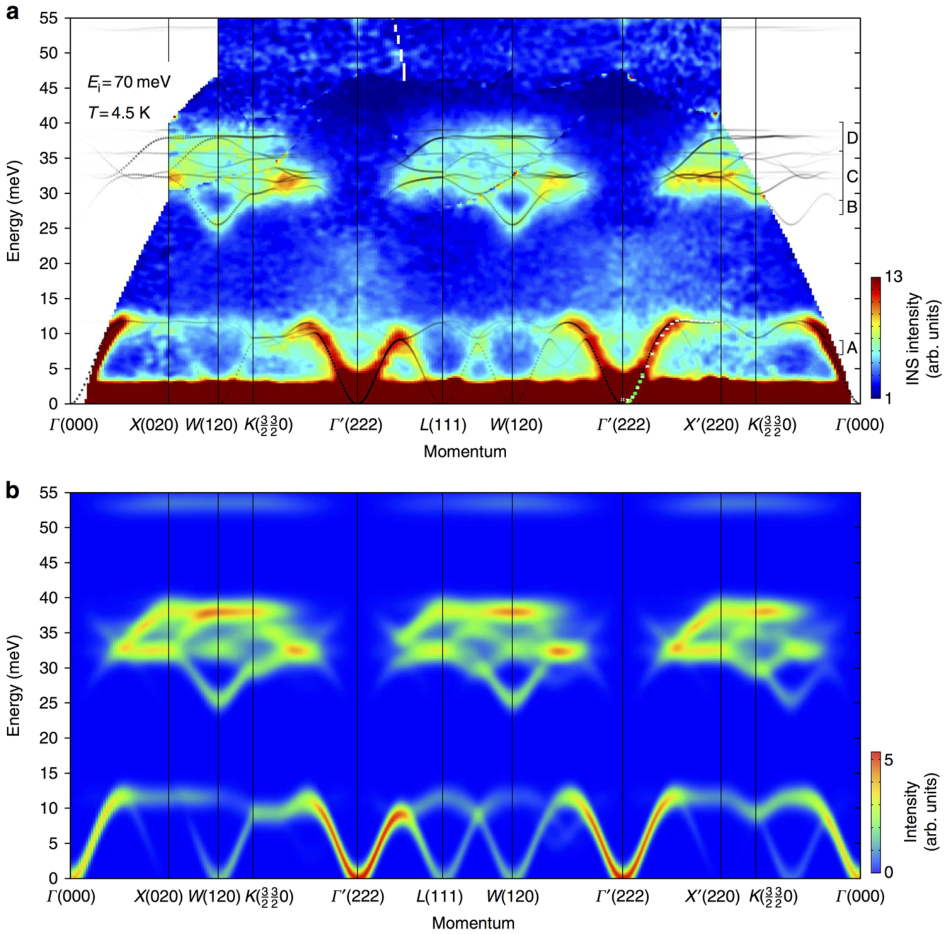

Figure 4: (a) Inelastic neutron scattering spectrum of Cu_2OSeO_3. The black lines represent the theoretically calculated spectrum. The theoretically determined intensity of the modes is shown by the opacity of the lines. (b) Dynamical spin structure factor calculated theoretically. The lines are artificially broadened with a Gaussian function to model the experimental resolution.

Spin-orbital dimer-singlet

On account of spin-orbit interaction, the lattice- and spin degrees of freedom become coupled. A weaker spin-orbit coupling, characteristic for light $3d$ transition metal compounds, gives rise to anisotropic exchange interactions. In these materials the orbital degrees of freedom order and a local Jahn–Teller distortion of the ligands surrounding the magnetic ions realizes the magnetic anisotropies. For materials with heavy transition metal ions with $4d$ and $5d$ electric configurations, the spin-orbit coupling has a more direct effect in admixing the spin and orbital degrees of freedom. The Jahn–Teller effect falls victim to the strong spin-orbit coupling and the interplay between magnetism and lattice symmetries is manifested in modulated interactions and the formation of unconventional magnetically and orbitally disordered ground states. The Mott insulating double perovskites, such as spin-$1/2$ $Ba_2B\,MoO_6$ (B=Y, Lu) and Ba_2BOsO_6 (B=Na, Li) well exemplify this physical scenario.

In these compounds the magnetic ions, Mo^{5+} or Os^{7+}, form undistorted face centered cubic (fcc) lattices. The osmium compounds Ba_2NaOsO_6 and Ba_2LiOsO_6 order magnetically [22–24], but the strong reduction of local moments is a direct fingerprint of unquenched orbital momentum and strong SOC [25–27]. The molybdenum compound, Ba_2YMoO_6 does not show any structural or magnetic transition down to 50 mK [28–30]. Based on magnetic susceptibility and muon spin rotation data, a valence bond glass state has been proposed for Ba_2YMoO_6, in which spin singlets are amorphously distributed on the fcc lattice [29]. Theoretically various exotic phases have been suggested, such as multipolar order [31] and chiral spin-orbital liquid states [32].

To elucidate the physical origins of the experimental observation in the double perovskites, we introduced a

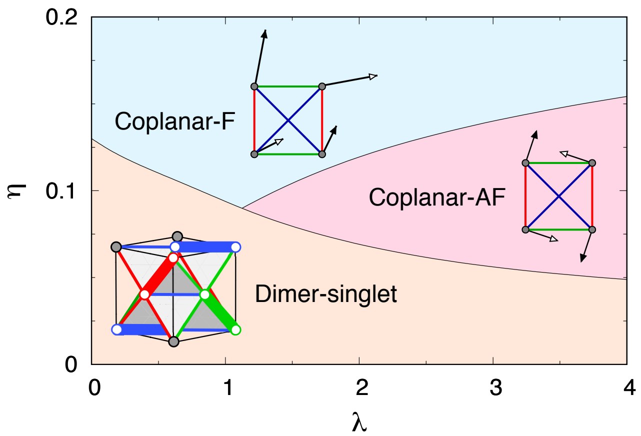

Figure 5: Phase diagram as the function of Hund's coupling η and the spin-orbit coupling λ (in units of J). For small values of η the dimer-singlet phase is stable over the entire range of the spin-orbit coupling. With increasing η, noncollinear coplanar phases with ordered moments are stabilized.

suitable spin-orbital model which encompasses the directional dependent interactions, the Hund's and spin-orbit coupling. A dimer-singlet phase, composed of random arrangement of spin-orbit dimers that do not break any symmetry nor show any type of long-range order is a natural ground state of the model. This state can account for the experimental observations in the molybdenum compound; the lack of ordering and the extensive degeneracy are consistent with the observed glassy behavior and measured residual entropy. In addition, the four-sublattice ordered states with reduced moments emerging at larger values of Hund's coupling can describe the isostructural osmium compounds [33]. In both the spin-orbital dimer and the ordered phases the spin and orbital degrees of freedom are entangled, involving the superposition of a $S = 1/2$ spin and the relevant t_{2g} orbitals. The calculated phase diagram as the function of Hund's and spin-orbit coupling is shown in Fig. 5.

Our work has been published as "*Spin-Orbit Dimers and Noncollinear Phases in d^1 Cubic Double Perovskites*" by Judit Romhányi, Leon Balents, and George Jackeli in Phys. Rev. Lett. **118**, 217202 (2017)

Berry phase induced dimerization in one-dimensional quadrupolar systems

The way quantum fluctuations melt a classical order and create novel quantum states is a fundamental question of modern condensed matter physics. Mechanisms involving topological effects [34] have been studied in great detail in one-dimensional spin chains as minimal models [35, 36]. In particular, the Berry phase [37] associated with rotation of spins discriminates between antiferromagnetic Heisenberg chains with half-integer and integer spins, making the excitations in the former gapless and in the latter gapped [38].

We studied the role of the Berry phase in the case of spin quadrupoles. Such nonmagnetic spin states appear as a mean field solution of the $S = 1$ Heisenberg model

$$\mathcal{H}_{\rm BB} = \sum_{j=1}^{L-1} \cos\theta \left(\mathbf{S}_j \cdot \mathbf{S}_{j+1}\right) + \sin\theta \left(\mathbf{S}_j \cdot \mathbf{S}_{j+1}\right)^2 \ , \tag{1}$$

where θ parameterizes the ratio of the bilinear and biquadratic terms and L is the length of the chain. It is generally agreed that the model exhibits a ferromagnetic phase, a gapped "Haldane" phase [38], a gapless trimerized phase and a gapped dimerized phase [39–41]. A long lasting debate has been going on about the possible existence of a fifth, non-dimerized phase close to the $\theta_F = -3\pi/4$ SU(3) symmetric point.

At the ferromagnetic SU(3) point θ_F the ground state is degenerate, and it has no fluctuations: any wave function where each spin is in the same state is an exact ground state. Such is the spin ferromagnet, where each spin points in the same direction, but also the

$$|\psi_{\rm FQ}\rangle = \prod_{j=1}^{L} |\psi\rangle_j = \prod_{j=1}^{L} \left(n^x |x\rangle_j + n^y |y\rangle_j + n^z |z\rangle_j\right) \tag{2}$$

wave function which describes a nonmagnetic ferroquadrupolar state. Here the coefficients are the components of the $\hat{\mathbf{n}} = (n^x,\ n^y,\ n^z)$ real unit vector. The states $|x\rangle_j = i(|1\rangle_j - |\bar{1}\rangle_j)/\sqrt{2}$, $|y\rangle_j = (|1\rangle_j + |\bar{1}\rangle_j)/\sqrt{2}$ and $|z\rangle_j = -i|0\rangle_j$ form the time-reversal invariant basis of the $S = 1$ spins at site j ($|1\rangle$, $|0\rangle$ and $|\bar{1}\rangle$ are the S^z eigenstates), so the whole wave function is time reversal invariant. The $|\psi_{\mathrm{FQ}}\rangle$ does not have the full SO(3) symmetry. The order parameter can be thought of as an ellipsoid, as shown in Fig. 6(a). It has a rotational symmetry around $\hat{\mathbf{n}}$, as well as an additional symmetry from flipping the direction axes $\hat{\mathbf{n}} \to -\hat{\mathbf{n}}$. This extra symmetry distinguishes the quadrupolar order from the ferromagnetic order. As a consequence, the "director" $\hat{\mathbf{n}}$ lives in the projective plane $\mathbb{RP}^2$ formed by identifying antipodal points of the unit sphere.

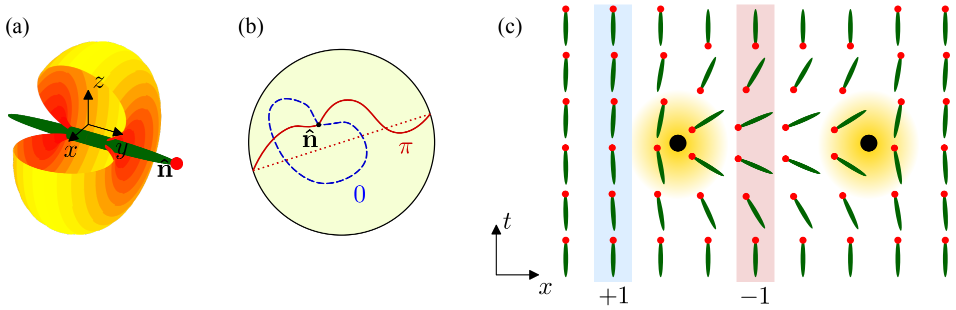

Figure 6: (a) In the quadrupolar state $|y\rangle$ the spin fluctuates over the yellow region perpendicular to the director (green) [42, 43]. (b) Rotating a director in the projective plane, a Berry phase is picked up on the red path only (the red dashed line connects equivalent points in $\mathbb{RP}^2$). (c) World lines of directors in $1 + 1$ dimensional space time. The directors tend to align with adjacent ones in space, and they can rotate in time. Rotations of a director as a function of time lead to a Berry-phase. Directors can either rotate by an angle 0 or π as shown in the two highlighted world lines, picking up a phase π in the latter case. To keep track of the total rotation, we add a red dot onto the green ellipsoid. In between domains of different windings, π-vortices appear (black dots).

Slightly away from θ_F, the nematic state of the spins described by $|\psi_{\mathrm{FQ}}\rangle$ have lower energies than other states at the mean-field level. There is no obvious reason that this state should become modulated with a period of two near this point. Could this nematic phase be the fifth phase? This question was first raised in [44, 45], where a window $\theta_F < \theta \lesssim -0.66\pi$ for the existance of the nematic was given. This idea has attracted considerable interest, and despite the progress in numerical techniques, recent simulations still are producing contradicting results [46–49]. In Refs. [50, 51] it has been argued that the Berry phase associated with quantum fluctuations of the quadrupoles dimerizes the nematic phase.

The Berry phase of a spin-quadrupole behaves differently from the Berry phase of a spin-coherent state. We can distinguish two topologically distinct classes of closed adiabatic paths of the $\hat{\mathbf{n}}$: the paths can cross the boundary of the $\mathbb{RP}^2$ an even or odd number of times [see Fig. 6(b)]. Since the Berry phase for the time reversal invariant quadrupoles is quantized to 0 or π [52], the phase on homotopic paths is equal. In the case of even number of crossings the path can be contracted to a single point, and we expect no Berry phase. For an odd number of crossings the path cannot be contracted, and the wave function acquires a Berry phase π for a spin-1 quadrupolar state.

To show that the Berry phase indeed makes the ground state dimerized, we constructed a low-energy effective description by mapping the spin-model to a quantum rotor model near θ_F and used a space-time path integral approach. Because of the continuous O(3) rotation symmetry $\hat{\mathbf{n}}$ does not have long-range order. As illustrated in Fig. 6(c), the $\hat{\mathbf{n}}$ field in the two-dimensional $(x, \tilde{t})$ space has topological defects in the form of *vortices*, characterized by the fundamental group $\pi_1(\mathbb{RP}^2) = \mathbb{Z}_2$ [53]. The vortices separate domains where worldlines of the directors have different winding numbers (and hence different Berry phases 0 and π). The sign of the path integral depends on their distance: the sign is positive (negative) if the vortices are separated by an even (odd) number of sites. This alternation leads to the dimerization. The mapping also allowed us to derive scaling predictions, which we verified using large scale density-matrix renormalization group simulations.

Additional insight into the nature of the ground state was obtained by studying the entanglement spectrum, by comparing the numerical one to the exact spectrum at the SU(3) symmetric θ_F point, which we also derived.

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Chiral phases in SU(N) Heisenberg models

With the recent progress towards achieving SU(N) symmetry with ultra-cold fermionic atoms, [12, 54–60] the investigation of the effective SU(N) Heisenberg model on various one- and two-dimensional lattices has become a very active field of research. Several remarkable ground state properties have been reported, including long-range color order [61], algebraic correlations [62], translational symmetry breaking valence-bond solid states in which groups of N atoms form local singlets on plaquettes [63, 64], and chiral ground states [65, 66]. In particular, for the SU(6) Heisenberg model on the honeycomb lattice, a mean-field calculation predicted a chiral spin one particle per site [67, 68]. However, the quite natural plaquette state in which six SU(6) spins form singlets on nonadjacent hexagons was found to lie very close in energy.

To clarify the situation, we considered the SU(6) Heisenberg model defined by the Hamiltonian

$$\mathcal{H} = \cos\theta \sum_{\langle i,j\rangle} P_{ij} + \sin\theta \sum_{\text{plaquettes}} i\left(P_{\hexagon} - P_{\hexagon}^{-1}\right) \tag{3}$$

where the operator $P_{ij} = \sum_{\alpha,\beta} |\alpha_i\beta_j\rangle\langle\beta_i\alpha_j|$ exchanges the $N = 6$ colors α and β of the atoms on neighboring sites i, j of a honeycomb lattice, and the $P_{\hexagon}$ and $P_{\hexagon}^{-1}$ ring exchange terms permute the configuration on a hexagon clockwise and anticlockwise. We studied the properties of the model as a function of θ, noting that $\theta = 0$ corresponds to the pure Heisenberg model using state-of-the-art numerical methods: variational Monte Carlo simulations based on Gutzwiller projected wave functions, exact diagonalizations, and infinite projected entangled pair states (iPEPS) simulations.

In the variational Monte Carlo method we projected out the configurations having multiple occupancy from the Fermi-sea constructed from a mean-field model. The variational parameters are the hopping amplitudes and the artificial fluxes given by their total phase around the elementary hexagons (plaquettes). An importance sampling Monte Carlo method was used to calculate the energies and correlations of the projected states. [62] Our calculations [shown in Fig. 7(a)] revealed that the lowest energy states are similar to those of Ref. [67]: (i) a configuration with uniform $2\pi/3$-flux before projection, corresponding to a chiral spin-liquid, [69] and (ii) a translation symmetry breaking configuration with 0-flux in a center plaquette surrounded by π-flux plaquettes with non-uniform hopping integrals, corresponding to a plaquette ordered phase. While the mean-field results of Ref. [67] favored the chiral phase, the plaquette-ordered phase turned out, after projection, to have a slightly lower energy. Only after turning to exact diagonalizations and iPEPS could we find compelling evidence that the ground state indeed has plaquette order. However, the chiral state is not far in parameter space, however, and it does not take a large ring-exchange term to stabilize it.

The exact diagonalization spectrum on 24 sites [Fig. 7(e)] shows a clear change of behavior between the small θ range, with a twofold excited state well separated from the rest of the spectrum, and the range above $\theta \simeq 0.2$, where a manifold of 6 singlet states becomes almost degenerate and very well separated from the rest of the spectrum. So, the ED results are clearly consistent with a phase transition between a plaquette phase and a chiral phase upon increasing the ring exchange term. This interpretation is further supported by the comparison with variational Monte Carlo calculation on 24 sites. To access the low energy spectrum and not just the ground state, we have constructed a large family of Gutzwiller projected states by changing the boundary conditions of the fermionic wave-functions. For the chiral state, this parton construction leads to 6 (and only 6) significant eigenvalues of the overlap matrix [Fig. 7(f)], which themselves lead to 6 low-lying states very close in energy. The 6-fold degeneracy of the ground state, which does not break translational nor SU(6) symmetry, is of topological origin.

Encouraged by these results, we have extended our study to the triangular lattice with nearest neighbor exchange and triangular ring-exchange terms for N=3, 4…9. We have found very similar behavior, the N-fold degenerate chiral ground state appeared for some finite values of ϑ.

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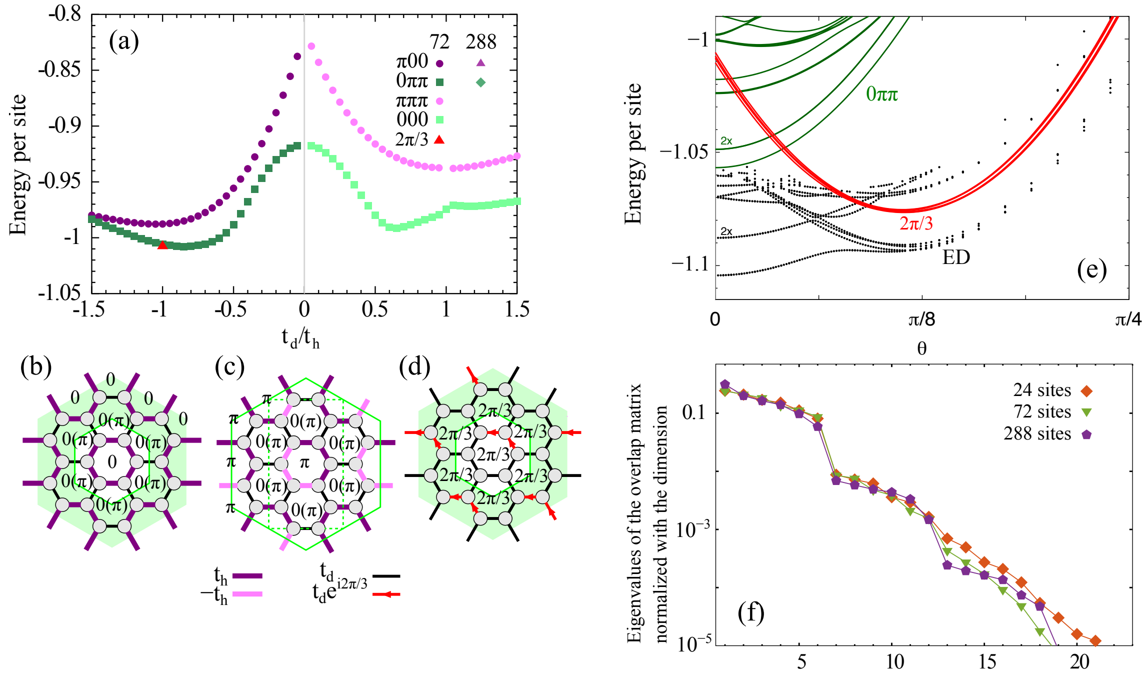

Figure 7: Energies of Gutzwiller projected wave functions (a) after projection for the different flux configurations as a function of t_d/t_h for 72 site cluster. (b)-(d) shows the flux configurations, black bonds represent hopping amplitude t_d, while dark and light purple bonds denote hopping amplitudes t_h and $-t_h$, respectively. In case of the uniform $2\pi/3$ flux configuration, red arrows represent the complex hopping amplitude $\propto e^{i2\pi/3}$. (e) Comparison of the ED spectrum (black points) of the model of Eq. (3) with the variational energies (continuous lines) based on Gutzwiller projected wave-functions for the $0\pi\pi$ plaquette phase and the $2\pi/3$ chiral phase. (f) The ordered eigenvalues λ_j of the overlap matrices of the projected states with different twisted boundary conditions before projection as a function of j. The cutoff after 6 large eigenvalues in the $2\pi/3$ case corresponds to the sixfold degenerate ground state of the chiral phase.

in "*Chiral Spin Liquids in Triangular-Lattice SU(N) Fermionic Mott Insulators with Artificial Gauge Fields*, by Nataf P., Lajkó M., Wietek A., Penc K., Mila F., Läuchli A.M., in Phys. Rev. Lett. **117** 167202 (2016).

List of the invited talks for the 'Topological properties in quantum magnets' workshop

- Didier Poilblanc (Université Paul Sabatier, Toulouse), *"Chiral spin liquid in a simple spin-1/2 frustrated Heisenberg AF on the square lattice"*
- Frank Pollmann (TU München), *"Dynamical signatures of quantum spin liquids"*
- Judit Romhányi (Okinawa Institute of Science and Technology), *"Chernful multiplet excitations in the breathing kagome model"*
- Fakher Assaad (Universität Würzburg) *"Dirac Fermions with Competing Mass Terms: Non-Landau Transition with Emergent Symmetry"*
- Christopher Mudry (Paul Scherrer Institute) *"Topological order in three spatial dimensions from coupled wires"*
- George Jackeli (Universität Stuttgart) *"Spin-orbital frustration in Mott insulators"*
- R. Ganesh (The Inst. of Mathematical Sciences, Chennai) *"The quantum spin quadrumer"*

- Frédéric Mila (EPFL, Lausanne) *"Edge states and exact zero modes in topological 1D quantum magnets"*
- Itamar Kimchi (MIT, Cambridge Boston) *"Randomness and Valence Bonds: theory and relevance to YbMgGaO4"*
- Alexei M. Tsvelik (Brookhaven National Laboratory) *"Non-Abelian analog of Kitaev model"*
- Hong-hao Tu (Ludwig-Maximilians-Universität, Munich) *"Universal entropy of conformal critical points on a Klein bottle"*
- Keisuke Totsuka (Yukawa Institute, Kyoto University) *"SU(N) cold fermions in a double-well optical potential - a realistic playground for symmetry-protected topological phases"*
- Matthias Punk (Ludwig-Maximilians-Universität, Munich) *"Deconfined criticality in triangular SU(3) antiferromagnets"*
- Miklós Lajkó (EPFL, Lausanne) *"Generalization of the Haldane conjecture to SU(3) chains"*

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