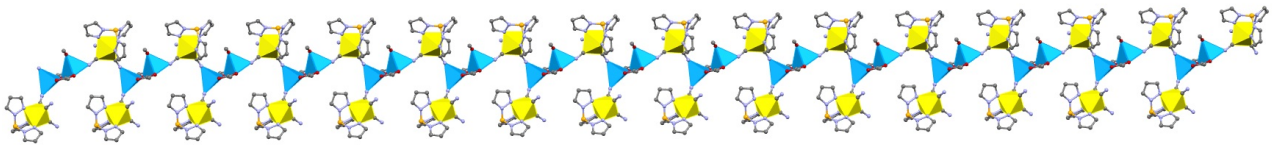

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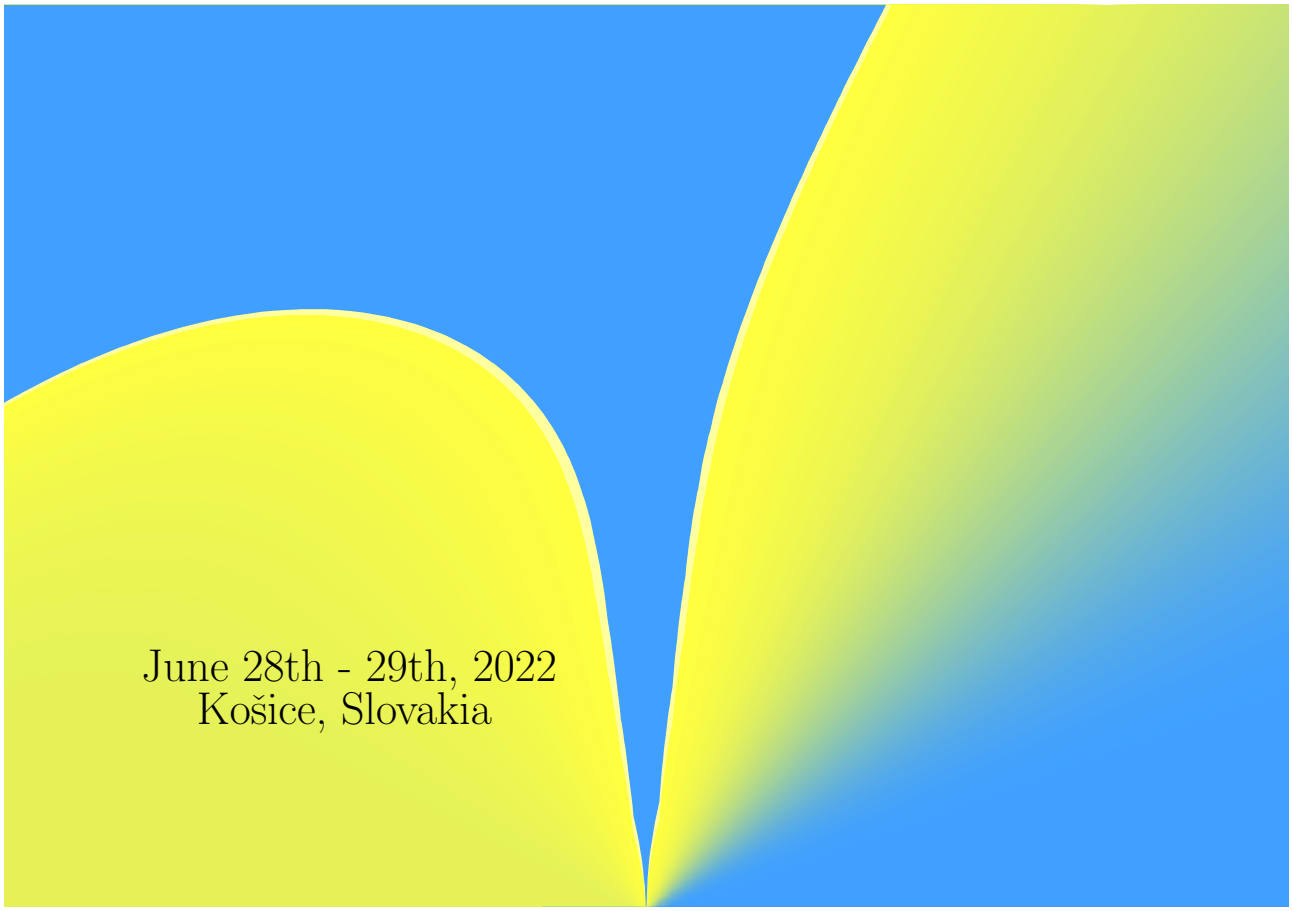
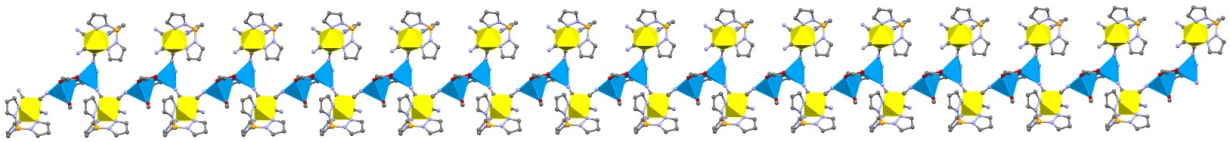


Programme & Abstracts



Pavol Jozef Šafárik University in Košice
Faculty of Science
Institute of Experimental Physics of Slovak Academy of Sciences in Košice

1st Workshop on Perspective Electron Spin Systems for Future Quantum Technologies

Jozef Strečka, Katarína Karľová (eds.)

Košice 2022

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Programme & Abstracts

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Conference email
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Conference Date and Location
The workshop will be held on June 28th - 29th, 2022 in Promatech building, Watsonova 1935/47, 040 01 Košice, Slovakia.

Conference Language
The working language of the conference is English.

Main conference topics:

1. Quantum and thermal entanglement
2. Frustrated magnetism
3. Graphene
4. van der Waals heterostructures
5. Magnetic phase transitions
6. Superconductivity
7. Skyrmions
8. Flat-band systems

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List of Invited Speakers

Oleg Derzhko	Institute for Condensed Matter Physics, L'viv, Ukraine
Andrej Gendiar	Institute of Physics, SAS, Bratislava, Slovakia Institute
Taras Verkholyak	for Condensed Matter Physics, L'viv, Ukraine
Hamid Arian Zad	Alikhanyan National Science Laboratory, Armenia
Milan Žukovič	Institute of Physics, Košice, Slovakia

Programme - Tuesday June 28th, 2022

13.00-13.30 Registration

13.30-15.20 Chair: Jozef Strečka

13.30-14.15 Keynote lecture - K1:
O. Derzhko, T. Hutak, T. Krokhmalskii, J. Schnack and J. Richter
Thermodynamics of the S=1/2 pyrochlore-lattice Heisenberg antiferromagnet

14.15-14.30 Short oral presentation - S1:
K. Karl'ová, J. Strečka and J. Richter
Towards lattice-gas description of low-temperature properties above the Haldane and cluster-based Haldane ground states of a mixed spin-(1,1/2) Heisenberg octahedral chain

14.30-14.45 Short oral presentation - S2:
T. Moško and M. Gmitra
Electronic structure of ferromagnetic intercalated α-$NbSi_2N_4$ monolayer

14.45-15.00 Short oral presentation - S3:
D. Danková and J. Strečka
Strong coupling analysis of the tetramer Heisenberg bond-alternating chain describing Cu(3-Chloropyridine)$_2$(N_3)$_2$

15.00-15.20 Contributed lecture - C1:
J. Haniš and M. Gmitra
Quasiparticle Interference in Superconducting Layered Misfit Compounds $(\mathrm{LaSe})_{1.14}$ $(\mathrm{NbSe_2})_{\mathrm{x}}, \mathrm{x} = 1, 2$

15.20-15.50 Coffee break

15.50-17.50 Chair: Martin Gmitra

15.50-16.20 Invited lecture - I1:
A. Gendiar and M. Grajcar
Photon detector: antiferromagnetic hysteresis

16.20-16.35 Short oral presentation - S4:
H. Vargová and J. Strečka
Enhancement of the quantum and thermal entanglement in the mixed spin-(1/2,S) Heisenberg dimer

17.35-17.05 Invited lecture - I2:
M. Lach and **M. Žukovič**
Phase diagrams of frustrated generalized XY model

17.05-17.20 Short oral presentation - S5:
M. Semjan and M. Žukovič
Absence of phase transition in the Ising antiferromagnet on a kagome latice with general spin-S

17.20-17.35 Short oral presentation - S6:
M. Rončík, M. Jaščur, T. Balcerzak and K. Szałowski
Generalized Spin-1/2 isotropic XY Heisenberg chain

17.35-17.50 Short oral presentation - S7:
D. Sivý
Numerical study of quantum phase transitions of the Heisenberg branched chain

18.00-21.30 Dinner

Programme - Wednesday June 29th, 2022

8.40-10.35 Chair: Milan Žukovič

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H. Arian Zad and J. Strečka
Intermediate magnetization plateaus in the spin-1/2 Ising-Heisenberg and Heisenberg models on 2D frustrated martini lattice

09.10-09.25 Short oral presentation - S8:
M. Mohylna and M. Žukovič
Nonmagnetic impurities and the skyrmion lattice phase in a frustrated Heisenberg antiferromagnet with Dzyaloshinskii-Moriya interaction

09.25-09.45 Contributed lecture - C2:
M. Gmitra
Spin-orbit coupling and magnetic exchange proximity effects in graphene within van der Waals heterostructures

09.45-10.00 Short oral presentation - S9:
J. Mnich
Electron structure in twisted bilayer graphene

10.00-10.20 Contributed lecture - C3:
M. Jaščur M. Rončík, T. Balcerzak and K. Szałowski
Spin-1/2 transverse field Ising model with a negative thermal expansion

10.20-10.35 Short oral presentation - S10:
A. Zoshki, H.Arian Zad, N. Ananikian and M. Jaščur
Robust quantum entanglement in the tetrapartite spin-1/2 square clusters: Theoretical study on the effect of a cyclic four-spin exchange

10.35-11.00 Coffee break

11.00-13.00 Chair: Katarína Karl'ová

11.00-11.30 Invited lecture - I4:
T. Verkholyak and J. Strečka
The Shastry-Sutherland model in low and high fields: perturbative treatment of XY interdimer coupling

11.30-11.50 Contributed lecture - C4:
L. Gálisová
The ground state and bipartite entanglement in $[Dy_2Cu_2]_n$: the study based on the spin-1/2 Ising-Heisenberg orthogonal-dimer chain calculations

11.50-12.10 Contributed talk - C5:
R. Krčmár, A. Gendiar and L. Šamaj
Ising ferromagnets and antiferromagnets in an imaginary magnetic field

12.10-12.30 Contributed talk - C6:
A. Ghannadan, K. Karl'ová and J. Strečka
On the concurrent bipartite entanglement of a geometrically frustrated spin-1 Heisenberg diamond cluster

12.30-12.45 Short oral presentation - S11:
V. Tkachenko, M. Mohylna and M. Žukovič
Heterostructure-based stabilization of zero-field and high-temperature skyrmion crystal in an antiferromagnetic triangular lattice

12.45-13.00 Short communication - S12:
J. Strečka, T. Verkholyak, K. Karl'ová, N. Caci, S. Wessel and A. Honecker
Phase boundary of spin-1/2 Ising-Heisenberg and Heisenberg models on a diamond decorated square lattice as magnetic analog of vapor-liquid phase border of water

13.00-13.10 Closing

13.10-15.00 Lunch

Index of Abstracts

Keynote lecture

(40 min. talk + 5 min. discussion)

K1

Thermodynamics of the S=1/2 pyrochlore-lattice Heisenberg antiferromagnet

Oleg Derzhko*[1], Taras Hutak[1], Taras Krokhmalskii[1], Jürgen Schnack[2], and Johannes Richter[3]

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Abstract

The S=1/2 Heisenberg antiferromagnet (HAF) on the pyrochlore lattice, which is a $3D$ network of corner sharing tetrahedra, is one of the most challenging problems in the field of highly frustrated quantum magnetism. There are several compounds where the magnetic atoms reside on the lattice sites of the pyrochlore lattice and the exchange interaction is antiferromagnetic. However, the S=1/2 pyrochlore-lattice HAF is in focus mainly because of huge academic interest as a candidate for a quantum spin liquid state in D=3.

While almost all numerous studies of the quantum pyrochlore-lattice HAF are focused on an interplay of frustration and quantum fluctuations in the ground state at $T = 0$, the finite-temperature properties (i.e., thermodynamics) of the model, when the thermal fluctuations come into play, are much less investigated. Since the quantum Monte Carlo method is inapplicable because of the sign problem, the toolbox to tackle the thermodynamics of the S=1/2 pyrochlore-lattice HAF is rather poor: Finite-lattice calculations (exact diagonalizations, finite-temperature Lanczos method), high-temperature expansion series, density-matrix renormalization group technique, or several uncontrolled approximations like, e.g., the rotation-invariant Green's function method.

In my talk, I will explain our recent paper on the thermodynamic properties of the S=1/2 pyrochlore-lattice HAF [1], which uses the finite-lattice calculations (N=32 sites) and high-temperature expansions series up to 13th order with respect to $\beta=1/(k_{\rm B}T)$ complemented by a simple Padé extrapolation and a cleverly designed interpolation called the entropy method. The entropy method was suggested by B. Bernu and G. Misguich in 2001 [2], however, a similar strategy can be recognized in the seminal paper by M. Planck on the energy distribution of electromagnetic radiation emitted by a black body in thermal equilibrium [3]. The main ideas of the entropy method are as follows: One has to work in the microcanonical ensemble with the entropy s as a function of the internal energy e, $s(e)$ has to be interpolated between certain low-temperature behavior around the ground-state energy $e_0<0$ and the known high-temperature behavior around $e_\infty=0$, some input about the low-temperature behavior is required

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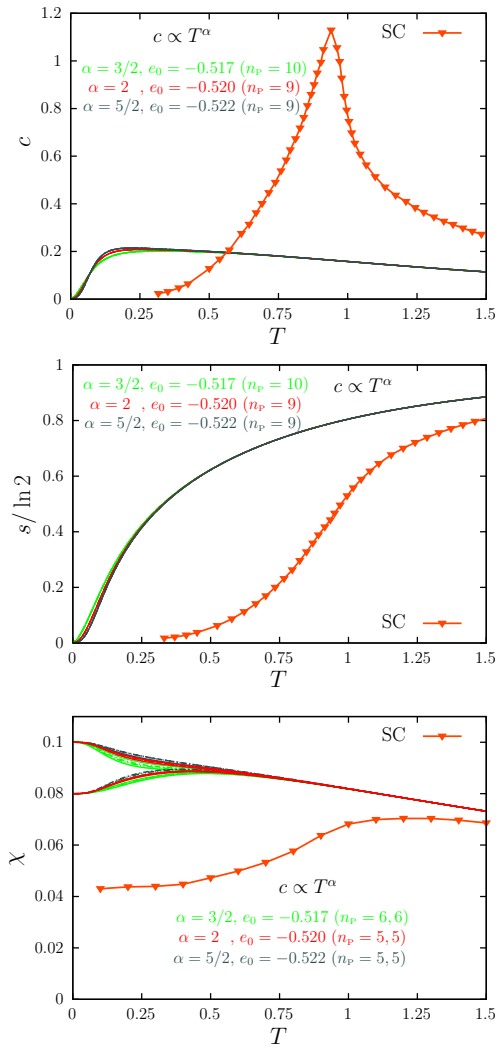

Figure 1: Specific heat c, entropy s, and uniform susceptibility χ for the S=1/2 HAF on the pyrochlore lattice (entropy method) and the simple cubic lattice with T_N≈0.946 (quantum Monte Carlo simulations).

(e_0, gapped or gapless excitations, in the latter case the exponent α>0 characterizing the power-law specific-heat decay $c(T)\propto T^\alpha$ as $T\to 0$ and the zero-temperature uniform susceptibility χ_0), an appropriate auxiliary function $G(e)$, instead of $s(e)$, has to be interpolated by two-point Padé approximants, i.e., $G(e)\to G_{\rm app}(e)$, and then all required quantities of interest like the specific heat $c(T)$, the entropy $s(T)$, or the uniform susceptibility $\chi(T)$ have to be calculated, see Fig. 1. Since the low-temperature properties of the S=1/2 pyrochlore-lattice HAF are unknown, we combine several assumptions and inspect the outcomes using the guidelines of B. Bernu with coauthors to evaluate the used input data and obtain definite conclusions on their relevance.

Our main findings for the specific heat $c(T)$ are as follows. Contrary to the two-dimensional kagome HAF, we do not find hints either for an extra low-temperature peak or an extra shoulder below the main maximum. However, the absence of an extra low-temperature feature goes hand in hand with a significant shift of the single maximum towards T≈0.25, which is much lower than for the kagome HAF, where the main maximum is at $T_{\rm max}$≈0.67. A gapless spectrum is more favorable than a gapped one, i.e., most likely there is a power-law low-temperature behavior of $c(T)$. Although best results are for the exponent α=2, other exponents (α=1, 3/2, 5/2, 3) cannot be excluded. We predict a ground-state energy $e_0\approx -0.52$. Concerning the entropy, the frustration leads to a fast increase of $s(T)$ at low temperatures: At T=0.5 the entropy already amounts to more than 50% of its maximal value. Our entropy-method data for the susceptibility $\chi(T)$ in comparison with data obtained by diagrammatic Monte Carlo provide further evidence for a gapless spectrum with a ground-state energy $e_0\approx -0.52$. The temperature profile of χ most likely does not show a maximum, rather there is a monotonous increase of χ upon decreasing of T reaching a zero-temperature value of χ_0≈0.1. For the pyrochlore lattice, similarly to the simple cubic lattice, each site has six neighbors, that is, within a mean-field picture both systems would be identical. More accurate description shows a drastical difference between both cases owing to frustration, see Fig. 1.

I will also discuss the newest findings on the S=1/2 pyrochlore-lattice HAF obtained using the numerical linked cluster expansion, the density-matrix renormalization group analysis, and the many-variable variational techniques.

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Invited lectures

(25 min. talk + 5 min. discussion)

I1

Photon detector: antiferromagnetic hysteresis

Andrej Gendiar*[1] and Miroslav Grajcar[2]

[1]*Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava, Slovakia*
[2]*Department of Experimental Physics, Comenius University, 842 48 Bratislava, Slovakia*

Abstract

An array of ferromagnetically coupled superconducting qubits inside superconducting coplanar waveguide resonator is designed. The antiferromagnetic coupling is realized by Josephson inductance. The array of the superconducting qubits is simulated by the quantum Ising model in perpendicular and longitudinal magnetic fields. The magnetization of the array can exhibit hysteretic behavior with some jumps under specific conditions. It is expected that perturbation of the coupler with an itinerant photon affects the coupling energy so as to detect changes in the magnetization. We modified density matrix renormalization group method to study the system by means of the entanglement entropy, the magnetic susceptibility and the hysteresis both in the ferromagnetic as well as the antiferromagnetic array of the qubits.

Acknowledgement

The support received from the Project APVV-20-0150, VEGA 2/0092/21, and Joint Research Project SAS-MOST 108-2112-M-002-020-MY3 is acknowledged.

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I2

Phase diagrams of frustrated generalized XY model

M. Lach[1] and M. Žukovič*[1]

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Abstract

We study the phase diagram topology evolution of the geometrically frustrated generalized XY model on a triangular lattice with the increasing order of the (pseudo)nematic term. The model is described by the Hamiltonian

$$\mathcal{H} = -J_1 \sum_{\langle i,j \rangle} \cos(\phi_{i,j}) - J_q \sum_{\langle i,j \rangle} \cos(q\phi_{i,j}), \tag{1}$$

where the summations run over the nearest-neighbor spins, $\phi_{i,j} = \phi_i - \phi_j$ is the angle between two neighboring spins at sites i and j, and $J_1 < 0$ and $J_q < 0$ are antiferromagnetic (AFM) and q-order antinematic (ANq) exchange interaction parameters. We consider $q = 3, 4, ..., 10$ and $J_1 = -\Delta$, $J_q = \Delta - 1$, with $\Delta \in [0, 1]$. We employ Monte Carlo simulations with a highly efficient parallelized implementation on graphical processing units, which allowed simulation of the system sizes $L \times L$, with $L = 384 - 1\,536$. In the model on a nonfrustrated square lattice, with both J_1 and J_q positive, it has been found that the higher-order terms lead to a qualitatively different phase diagrams than the one observed for $q = 2$ [1]. In particular, for $q \geq 4$ they revealed up to two additional ordered phases originating from the competition between the FM and Nq couplings, with the phase transitions belonging to a variety of universality classes [2,3].

In the present study of the model on the frustrated triangular lattice, with both J_1 and J_q negative, we find that for all q divisible by 3, the competition between the AFM and ANq interactions changes the ground state from the usual AFM with $2\pi/3$ relative phase angles to a peculiar canted (CAFM) state and leads to phase diagrams containing three quasi-long-range-ordered (QLRO) phases. For $q = 3$, AFM-CAFM and AN3-CAFM transitions belong to the weak Ising and weak three-state Potts universality classes, respectively, and chiralities vanish simultaneously with non-Ising critical exponents [4].

In the case of q nondivisible by 3, the well known phase diagram topology for $q = 2$ changes first at $q = 4$ and then again at $q = 7$ [5]. In particular, for $q = 4$ the AFM_0 phase with purely AFM correlations separates from the AFM_1 phase with the coexistent AFM and AN4 correlations. In the AFM_1 phase, both the magnetic and generalized nematic order parameters reach saturated values at low temperatures and the snapshots show typical AFM structure. Increasing the nematic parameter to $q = 7$ leads to the appearance of the AFM_2 phase in a part of the region previously occupied by the AFM_1 phase. This new phase still shows both the AFM and ANq orderings, however, the typical AFM spin structure disappears. Instead, for each sublattice there are $\lceil q/2 \rceil$ possible spin orientations with different weights belonging to the same half plane. The order parameter for the AFM_1-AFM_2 phase transition is $m_{\lceil q/2 \rceil}$.

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All the observed phases also display some kind of chiral LRO. In the low-temperature AFM_1 and AFM_2 phases, as well as the frustrated CAFM phase, both the standard κ_1 and the generalized κ_q staggered chiralities remain finite. κ_1 vanishes at the transition to the ANq phase from the low-temperature phases for all q so that inside the ANq phases only κ_q remains finite. On the other hand, at the transition to the AFM_0 phase from the low-temperature phases, κ_q remains nonzero for q up to 6, while starting with $q = 7$ it drops to zero together with the nematic m_q order parameter at the AFM_1-AFM_0 or AFM_2-AFM_0 transition and thus inside the AFM_0 phase only κ_1 remains finite. The resulting phase diagrams are shown in Fig. 1.

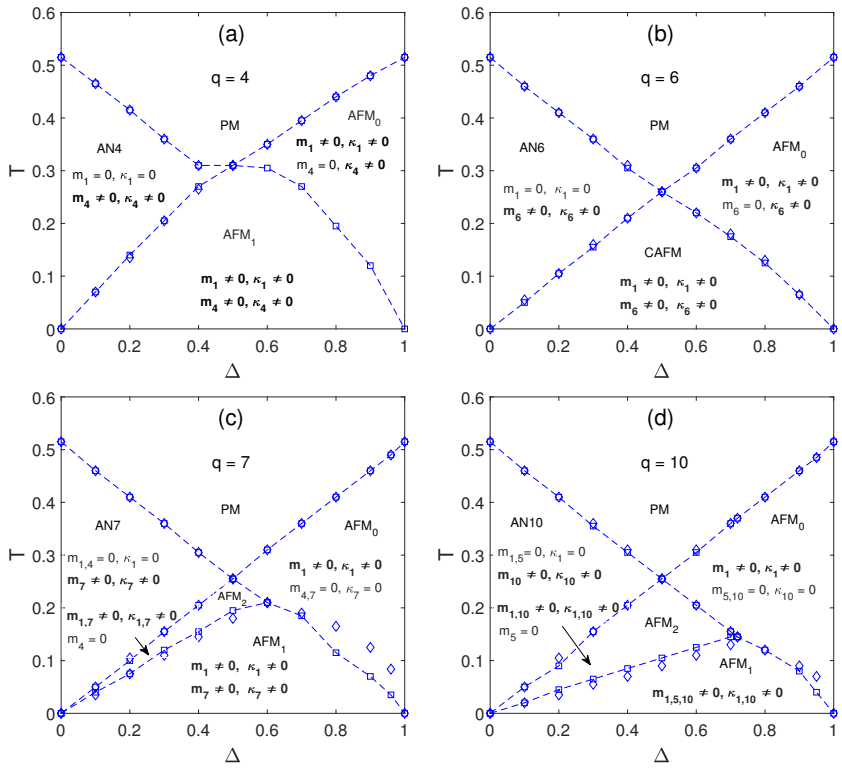

Figure 1: Phase diagrams in $\Delta - T$ parameter plane, for representative values of q. Diamond (square) symbols represent phase boundaries located from the peaks of the specific heat (generalized magnetic order susceptibility). The captions display the observed phases and the corresponding order parameters, with those taking nonzero values in the respective phases highlighted in bold.

Acknowledgement

This work was supported by the Slovak Research and Development Agency (Contract No. APVV-20-0150) and the Scientific Grant Agency of Ministry of Education of Slovak Republic (Grant No. 1/0531/19).

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I3

Intermediate magnetization plateaus in the spin-1/2 Ising-Heisenberg and Heisenberg models on 2D frustrated martini lattice

Hamid Arian Zad*[1] and Jozef Strečka[2]

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[2]*Department of Theoretical Physics and Astrophysics, Faculty of Science, P. J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovak Republic*

Abstract

We consider the spin-1/2 Ising-Heisenberg [1] and full Heisenberg models on the frustrated martini lattice in the presence of an external magnetic field. The former is exactly solved by the combination of generalized star-triangle transformation, the transfer-matrix technique and Monte Carlo (MC) simulations. The generalized star-triangle transformation establishes an exact mapping correspondence with the effective spin-1/2 Ising model on a pure Ising triangular lattice with effective temperature-dependent field, two- and three-body interactions. In fact, to get the results of the single-site magnetizations of the Ising spins m_{I} and Heisenberg spins m_{H} numerical MC simulation is adopted. Full Heisenberg XXX model on the martini lattice is investigated by utilizing the infinite projected entangled-pair state (iPEPS) [2,3] within the tensor-network framework. The Ising-Heisenberg spin model reveals in its ground-state phase diagram two unconventional dimerized and one trimerized quantum ground states together with two classical ground states. It is demonstrated that the spin frustration is responsible for a variety of magnetization scenarios with up to two or three intermediate magnetization plateaus. The total magnetization m_{T} of the Ising-Heisenberg model on the martini lattice shows fractional plateaus at 1/12, 1/6 and 1/4 of the saturation magnetization. The magnetization of full Heisenberg model manifests the same intermediate plateaus as for the Ising-Heisenberg counterpart together with stepwise increase, evidencing the existence of Luttinger-like spin liquid phase. The exact results for the total magnetization of the Ising-Heisenberg model are confronted with the corresponding results for the Heisenberg model which were derived by the tensor-network method. Although the exact ground states for the Ising-Heisenberg model does not capture the actual ground states for the pure Heisenberg model [4], the ground-state magnetization of both models is quite reminiscent, such that some insight into the ground states of the Heisenberg model can be obtained from the quantum-classical Ising-Heisenberg analogous.

Acknowledgement

H. Arian Zad acknowledge for the financial support of the National Scholarship Programme of the Slovak Republic (NŠP).

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I4

The Shastry-Sutherland model in low and high fields: perturbative treatment of XY interdimer coupling

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[2]*Institute of Physics, Faculty of Science, P. J. Šafárik University, Park Angelinum 9, 040 01, Košice, Slovakia*

Abstract

The Shastry-Sutherland model, as a highly frustrated system, poses an intricate problem for the theoretical studies. The specific structure of the lattice, as a two-dimensional array of the mutually orthogonal dimers, leads to the emergence of the flat band of triplon excitations on spin dimers. Such localized excitations are responsible for the emergence of a series of fractional plateaux in the model. Moreover, other complex quantum phases of singlet plaquettes and bound triplons arise for some particular ratio between intradimer and interdimer spin couplings for the model in the magnetic field.

We discuss the results of the perturbation theory based on the perturbative treatment of the XY part of the interdimer coupling. At first we consider the ground-state properties of the model at low fields sufficient to magnetize the system up to 1/3 magnetization plateau. Within the perturbation theory we get the effective Hamiltonian of the localized triplons excitations on dimers with the extended hard-core repulsion, where the only quantum term is provided by the correlated hopping of triplons. The latter term is essential for the intermediate values of the interdimer coupling, and it promotes the creation of the bound pairs of triplons and the corresponding quantum phase of such bound quasiparticles. The origin of this quantum phase is not well understood even by means of the numerical methods which suffer from the finite-size effects. Therefore, we consider the Shastry-Sutherland tubes as a model with a finite number of dimers in one direction and study what is the minimal width of the tube sufficient to reproduce the main features of the model.

We also considered the model at high fields leading the system from the 1/2 plateau to the saturation. Within the second-order perturbation theory, we get the effective model, which is described by a gas of magnons with the additional hard-core repulsion between the nearest-neighbor sites and anisotropic hopping terms. We study the effective model and compare the transition field to 1/2 plateau phase and the saturation field with the available numerical data.

Acknowledgement

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Contributed lectures

(17 min. talk + 3 min. discussion)

C1

Quasiparticle Interference in Superconducting Layered Misfit Compounds $(LaSe)_{1.14}$ $(NbSe_2)_x, x = 1, 2.$

Jozef Haniš*[1] and Martin Gmitra[1,2]

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Abstract

Unconventional superconductivity in transition metal dichalcogenides exhibits a special form of Ising pairing mechanism in which quasiparticle spins are firmly pinned due to symmetry [1, 2]. This enables interesting consequences where in-plane upper critical magnetic fields are far beyond the Pauli limit for superconductivity. Misfit layered systems $(LaSe)_{1.14}$ $(NbSe_2)_x, x = 1, 2$ are a stack of transition metal dichalcSogenide $NbSe_2$ layers intercalated by the LaSe layers [3]. The system is a bulk superconductor indicating a unique three-dimensional Ising superconductor and impurity scattering can reveal some features of superconducting behavior [4]. We investigate possible quasiparticle interference patterns relevant for Fourier-transform scanning tunneling spectroscopy. We discuss scalar and magnetic impurity effects in normal and superconducting states for conventional and unconventional pairing parameters using the T-matrix approach [5]. For electronic structure we employ a tight-binding model [6] fitted to the first-principles calculations.

Acknowledgement

This work was supported by the project APVV SK-PL-21-0055, VEGA Grant No. 1/0105/20, Slovak Academy of Sciences project IMPULZ IM-2021-42 and project FLAG ERA JTC 2021 2DSOTECH.

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C2

Spin-orbit coupling and magnetic exchange proximity effects in graphene within van der Waals heterostructures

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Abstract

Bare electronic structure of graphene limits its applications. Embedding it in van der Waals heterostructures [1] opens new venues for utilizing induced proximity effects [2] in novel device design [3]. In the talk we discuss induced spin-orbit coupling and exchange coupling proximity effects in graphene [4] and bilayer graphene [5] on transition metal dichalcogenides and on two dimensional magnets [6], and twisting effects [7]. Specially we analyze 1T-TaS_2 which undergoes charge density wave and spontaneous magnetic transition at low temperatures. The proximity effects on electronic states in graphene near the Dirac point will be discussed in terms of density functional theory and effective tight-binding model. An emphasis will be given to extracted model parameters relevant for realistic modeling of low energy electronic structure of graphene.

Acknowledgement

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C3

Spin-1/2 transverse field Ising model with a negative thermal expansion

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Abstract

A generalized spin-1/2 transverse field Ising model with a negative thermal expansion of the lattice is introduced and investigated using standard methods of statistical mechanics. Besides the volume-dependent magnetic energy, the static lattice energy, and anharmonic Einstein phonon energy are also considered in calculations. Analytic relations for the Gibbs free energy, magnetic moments, and equations of state are obtained, taking into account a simple volume dependence of all energy contributions. The ground-state and finite-temperature phase diagrams are discussed in detail for the strong and weak magneto-elastic coupling. It is clearly demonstrated that the generalized spin-1/2 transverse field Ising model exhibits a novel critical behavior, due to the strong negative expansion of the lattice, which is controlled by the strength of magneto-elastic coupling. The presented approach can be easily modified to study many other theoretical models in different fields of solid-state physics.

Acknowledgement

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C4

The ground state and bipartite entanglement in $[Dy_2Cu_2]_n$: the study based on the spin-1/2 Ising-Heisenberg orthogonal-dimer chain calculations

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Abstract

The possible ground-state spin arrangements of the real polymeric compound $[Dy_2Cu_2]_n$ [1] and the bipartite entanglement within its Cu^{2+}- Cu^{2+} dimers through the concurrence concept [2] are theoretically modeled by using the exactly solved symmetric isotropic spin-1/2 Ising-Heisenberg orthogonal-dimer chain [3]. The model's parameters are set to the specific values that provide the best possible theoretical fit for known experimental magnetization data of the compound [4].

It is shown that the low-temperature value of the concurrence quantifying a strength of the quantum entanglement of Cu^{2+}- Cu^{2+} dimers in $[Dy_2Cu_2]_n$ is strongly magnetic-field dependent. Besides two zero plateaus within the field range $(0.274-4.107)$ T and above the saturation field 6.366 T due to stability of the standard ferrimagnetic and saturated ground-state arrangements, respectively, it also shows nonzero plateaus at $\mathcal{C}=1$ and $\mathcal{C}\approx 0.211$. The maximum value $\mathcal{C}=1$ can be found at the fields $(0.000-0.177)$ T and $(4.107-6.366)$ T due to presence of the quantum frustrated and quantum ferrimagnetic phases, where the cooper dimers are in perfect singlet states, respectively. The nontrivial value $\mathcal{C}\approx 0.211$, appearing at $(0.177-0.274)$ T, can be ascribed to the quantum ferrimagnetic singlet-like phase. In general, the bipartite entanglement between two exchange-coupled Cu^{2+} ions gradually weakens with increasing temperature until it completely vanishes. On the other hand, the non-monotonous temperature variations of $\mathcal{C}$ clearly point to the temperature-induced strengthening of the phenomenon above the partially entangled ferrimagnetic singlet-like phase and the thermal activation of the entangled states of Cu^{2+}- Cu^{2+} dimers above the non-entangled ferrimagnetic and saturated ground states.

Acknowledgement

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C5

Ising ferromagnets and antiferromagnets in an imaginary magnetic field

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Abstract

We study classical Ising spin-$\frac{1}{2}$ models on the 2D square lattice with ferromagnetic or antiferromagnetic nearest-neighbor interactions, under the effect of a pure imaginary magnetic field. The complex Boltzmann weights of spin configurations cannot be interpreted as a probability distribution which prevents from application of standard statistical algorithms. In this work, the mapping of the Ising spin models under consideration onto symmetric vertex models leads to real (positive or negative) Boltzmann weights. This enables us to apply accurate numerical methods based on the renormalization of the density matrix, namely the corner transfer matrix renormalization group and the higher-order tensor renormalization group. For the 2D antiferromagnet, varying the imaginary magnetic field we calculate with a high accuracy the curve of critical points related to the symmetry breaking of magnetizations on the interwoven sublattices. The critical exponent β and the anomaly number c are shown to be constant along the critical line, equal to their values $\beta = \frac{1}{8}$ and $c = \frac{1}{2}$ for the 2D Ising in a zero magnetic field. The 2D ferromagnets behave in analogy with their 1D counterparts defined on a chain of sites, namely there exists a transient temperature which splits the temperature range into its high-temperature and low-temperature parts. The free energy and the magnetization are well defined in the high-temperature region. In the low-temperature region, the free energy exhibits singularities at the Yang-Lee zeros of the partition function and the magnetization is also ill-defined: it varies chaotically with the size of the system.

Acknowledgement

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C6

On the concurrent bipartite entanglement of a geometrically frustrated spin-1 Heisenberg diamond cluster

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Abstract

The bipartite entanglement of a quantum spin-1 Heisenberg diamond cluster with two different coupling constants in a presence of external magnetic field is quantified through negativity in two cases between spins on the diagonal and the spins on the sides of the diamond cluster. The drop of negativity at zero temperature is analytically calculated from the density operator of the mixed states at the transition field. Besides, kinks were detected in some of the temperature dependencies of negativity due to vanishing of some of the contributions to the negativity, while their counterparts in magnetic-field dependencies of the negativity appear due to onset of some of the contributions of the negativity at that point. The tetranuclear nickel complex $[Ni_4(\mu\text{-}CO_3)_2(\text{aetpy})_8](ClO_4)_4$ (aetpy = 2-aminoethyl-pyridine) represents the antiferromagnetic spin-1 Heisenberg diamond cluster prone to a geometric spin frustration and according to previously obtained coupling constants, it is conjectured that the bipartite entanglement exists between Ni^{2+} magnetic ions on the main diagonal of the diamond cluster.

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Short oral presentations

(12 min. talk + 3 min. discussion)

S1

Towards lattice-gas description of low-temperature properties above the Haldane and cluster-based Haldane ground states of a mixed spin-(1,1/2) Heisenberg octahedral chain

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Abstract

The mixed spin-1 and spin-1/2 Heisenberg octahedral chain with regularly alternating monomeric spin-1 sites and square-plaquette spin-1/2 sites has, in a magnetic field, an extraordinarily rich ground-state phase diagram, which includes the uniform and cluster-based Haldane phases, two ferrimagnetic phases of Lieb-Mattis type, two quantum spin liquids, two bound magnon crystals in addition to the fully polarized ferromagnetic phase [1].

In the highly frustrated parameter region the lowest-energy eigenstates of the mixed-spin Heisenberg octahedral chain belong to flat bands, which allow a precise description of low-temperature magnetic properties within the localized-magnon approach exploiting a classical lattice-gas model of hard-core monomers. Moreover, we have found a more comprehensive version of the localized-magnon approach, which extends the range of its validity down to a less frustrated parameter region involving the Haldane and cluster-based Haldane ground states.

A comparison between results of the developed localized-magnon theory and accurate numerical methods like full exact diagonalization and finite-temperature Lanczos methods convincingly evidence that the low-temperature magnetic properties above the Haldane and the cluster-based Haldane ground states can be extracted from a classical lattice-gas model of hard-core monomers and dimers, which is additionally supplemented by a hard-core particle spanned over the whole lattice representing the gapped Haldane phase.

Acknowledgement

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S2

Electronic structure of ferromagnetic intercalated α-$NbSi_2N_4$ monolayer

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Abstract

Two-dimensional materials attract significant attention as they are able to form new class of systems with diverse electronic properties. Proper layer-by-layer engineering provides novel topological, magnetic and superconducting systems. An innovative approach is to construct new atomically thin monolayers by intercalation. A specific systems are MA_2Z_4 monolayers with a septuple-atomic-layer structure [1]. Here an InSe-type monolayer A_2Z_2 is intercalated with a MoS_2-type monolayer MZ_2. In the talk we discuss ground state electronic properties of α-$NbSi_2N_4$, a specific system from the MA_2Z_4 family, by means of density functional theory calculations. We present effective tight-binding model for Nb 4*d*-orbitals describing energy dispersion of spin split bands in vicinity of the Fermi level. Using the effective model we have calculated electronic susceptibility in order to explore a possible occurrence of charge density wave phase. We also discuss non-collinear magnetic order and magnetocrystalline anisotropy.

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S3

Strong coupling analysis of the tetramer Heisenberg bond-alternating chain describing Cu(3-Chloropyridine)$_2$(N$_3$)$_2$

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Abstract

The polymeric compound Cu(3-Chloropyridine)$_2$(N$_3$)$_2$, which has been already analysed both theoretically within the simplified Ising-Heisenberg model and experimentally in an article published in 2015 [1], hints at the possible existence of a quantum spin liquid state in the close neighbourhood of the saturation magnetic field. The spin-1/2 Heisenberg model on a bond alternating tetrameric chain was considered within this work as to obtain more precise proof of the existence of a quantum spin-liquid state. A further analysis using many-body perturbation theory, also known as strong-coupling approach [2], allowed us to obtain an effective Hamiltonian from the quantum Heisenberg Hamiltonian, which formerly described the magnetic behaviour of the coordination polymer Cu(3-Chloropyridine)$_2$(N$_3$)$_2$. Results obtained from the effective Hamiltonian, which provide further proof of the existence of the quantum spin-liquid state, were compared with numerical simulations performed within the ALPS environment [3, 4].

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S4

Enhancement of the quantum and thermal entanglement in the mixed spin-(1/2,S) Heisenberg dimer

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Abstract

The concept of negativity is used to study the quantum and thermal entanglement in a generalized spin-(1/2,S) Heisenberg dimer under presence of an external magnetic field. The competition effect of interplay between the spin diversity, XXZ exchange as well as uniaxial single-ion anisotropy is additionally analysed with a goal to tune the degree and thermal stability of the pairwise entanglement. Obtained analytical results favour the antiferromagnetic spin-(1/2,S) Heisenberg dimer instead of the ferromagnetic one, where the higher degree of entanglement and higher threshold temperature are achieved at the same set of model parameters. It is demonstrated and analytically proven that the increasing magnitude of spin S in dimer with an easy-axis uniaxial single-ion anisotropy can enhance not only the thermal stability but simultaneously the degree of entanglement. It is shown additionally, that the further enhancement of entanglement can be improved in dimer with a half-odd-integer spin S as a consequence of different magnetic ground-states. In such system the low-enough thermal negativity saturates in its maximal value regardless the magnitude of half-odd-integer spin S. Because of the influence of the magnetic-field induced consecutive second-order phase transitions in dimer with $S>1$, the surprising oscillating behaviour of negativity upon the magnetic field is observed at low-enough temperature.

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S5

Absence of phase transition in the Ising antiferromagnet on a kagome latice with general spin-S

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Abstract

The Ising antiferromagnet on a kagome lattice (IAKL) is a well-known systems with huge geometric frustration, which results in an absence of LRO at any temperature including zero temperature [1], and very large value of the residual entropy ($0.5018k_B$) [2]. In case of a related Ising antiferromagnet on a triangular lattice (IATL) it was shown that the effects of frustration can be alleviated by increasing the magnitude of the spin variable S [3]. At the low temperatures the value of the correlation function exponent η decreases from $\eta = 1/2$ for $S = 1/2$ with the increasing S down to zero for S larger than some threshold value S_C, suggesting that there is LRO at zero temperature for sufficiently large and a phase transition occurs at a finite temperature.

In this Monte Carlo study is examined the possibility of the emergence of any LRO due to the increase of multiplicity of the local degrees in the IAKL model. Different values of S, including $S = \infty$, are considered, and the behavior of the critical exponent η is obtained using a finite-sized scaling analysis. It is found that the value of η depends neither on spin S, nor the temperature T and it remains constant at $\eta = 2$, suggesting that the IAKL with general spin-S exhibits no LRO at any finite temperature, unlike the IATL model, which crossovers into a partially disordered LRO phase for $S \leq S_C$. However, the presented results do not exclude a possibility of a transition into a LRO phase in the ground state, similarly to the Heisenberg antiferromagnet on the same lattice [4].

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S6

Generalized Spin-1/2 isotropic XY Heisenberg chain

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Abstract

We developed a complex theory for spin-1/2 isotropic Heisenberg XY systems with magnetoelastic interaction. This theory consists of the analytical construction of the total Gibbs free energy as the sum of magnetic energy, static lattice energy, and thermal vibrational energy. Magnetic exchange integral depends exponentially on the distance between interacting magnetic moments. Magnetic and lattice subsystems interconnect one parameter, which characterizes the relative change in the length of the crystal. In the static elastic free energy, we use Morse potential. To express the dependence of the frequency of quantum oscillators on the relative change in the length of the chain, we used Gruneisen's assumption that allows straightforward expression of all relevant thermodynamic quantities. The employed approach allows us to derive equations of state that, together with the total Gibss energy, allow a straightforward expression of all thermodynamic quantities. The principal difference to the standard Heisenberg XX model is the change in the quantum phase transition from the second kind to the first kind.

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S7

Numerical study of quantum phase transitions of the Heisenberg branched chain

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Abstract

The theoretical study of different quantum Heisenberg spin chains has its purpose not only in the academic sphere [1] but also has a practical use [2]. The aim of the submitted diploma thesis is a theoretical study of spin-1/2 Heisenberg branched chain, which was inspired by a magnetic structure of polymeric coordination compounds $[(Tp)_2Fe_2(CN)_6X(bdmap)Cu_2(H_2O)]$ [3]. We were mainly interested in the zero-temperature magnetization curves that were the base for the construction of ground-state phase diagram of the Heisenberg branched spin chain. The appropriate method for numerical simulations at zero temperature was the density-matrix renormalization group (DMRG) technique [4], which has been adapted in an open-source software library Algorithms and Libraries for Physics Simulations (ALPS) [5]. The calculated magnetization curves suggest existence of a quantum spin-liquid phase, zero magnetization plateau and also an intermediate magnetization plateau at one-half of the saturated magnetization. We were also interested in the magnetization process at finite-temperatures, in particular in the vicinity of magnetic field-driven quantum critical points. For this purpose we have used the quantum Monte Carlo method [6], which is also implemented in an open-source software library ALPS. We have also studied in detail the dependence of magnetic susceptibility on the external magnetic field, which can serve as experimentally detectable indicator of magnetic field-driven quantum phase transitions. With the combination of two different numerical approaches namely DMRG and QMC we have managed to get reliable and numerically precise data valid in a wide range of the interaction parameters of the Heisenberg branched chain.

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S8

Nonmagnetic impurities and the skyrmion lattice phase in a frustrated Heisenberg antiferromagnet with Dzyaloshinskii-Moriya interaction

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Abstract

We investigate the classical Heisenberg AFM on a triangular lattice with the following Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \sum_{\langle i,j \rangle} \vec{D}_{ij} \cdot \left[\vec{S}_i \times \vec{S}_j \right] - h \sum_i S_i^z, \quad (1)$$

where $\vec{S}_i$ is a classical unit-length Heisenberg spin at the ith site, $J < 0$ is the AFM exchange coupling constant, h is the external magnetic field applied perpendicular to the lattice plane (along the z direction) and $\langle i, j \rangle$ denotes the sum over nearest-neighbour spins. $\vec{D}_{ij}$ is the DMI vector whose orientation is chosen to point along the radius-vector $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$ between two neighbouring sites, i.e., $\vec{D}_{ij} = D \frac{\vec{r}_{i,j}}{|\vec{r}_{i,j}|}$. We implement the hybrid Monte Carlo (HMC), which combines the standard Metropolis algorithm with the over-relaxation (OR) method [1]. To perform configurational averaging we run independent simulations on 50 replicas with different configurations of randomly distributed nonmagnetic impurities for each value of the impurity concentration p. In simulations we use $2 \cdot 10^6$ MC sweeps. The lattice size in all the simulations is $L = 48$ and periodic boundary conditions are implemented. The simulations are carried out on General Purpose Graphical Processing Units (GPGPU) using CUDA.

The frustrated Heisenberg AFM with DMI has been previously intensively studied in a wide parameter space [3,4]. The phase diagram of a pure isotropic model with a moderate DMI ($0.2 < D < 1$) consists of three distinct phases: the helical (HL) phase, the skyrmion lattice (SkX) phase, which consists of three interpenetrating skyrmion lattices on each of the sublattices and the V-like (VL) phase [4]. The presence of nonmagnetic impurities (spin vacancies) is a common feature in magnetic solids and in frustrated spin systems with a ground-state degeneracy can cause a possible "order by quenched disorder" effect with a profound impact on the phase diagram [2]. Considerable effect of nonmagnetic impurities has also been observed in the nonfrustrated FM Heisenberg model on a square lattice in the field with DMI [5], which displays the SkX phase. In particular, it was found that even very tiny concentrations of the vacancie can cause the formation of bimerons and deformation of both the HL and SkX states.

To simulate the presence of nonmagnetic impurities in our system we randomly replaced $p\%$ of the sites with vacancies. The presence of the vacancies naturally results in some distortion of the HL and SkX phases. Nevertheless, there are no signs of the formation of bimerons. We believe that the present AFM system is more resilient against creation of bimerons due

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to the fact that both HL and SkX textures are formed on each of the three interpenetrating sublattices. The skyrmions have a tendency to rearrange in such way so that the vacancies stay at their outskirts, which can be expected in case of a skyrmion lattice, since it is energetically more favorable if configurations involve the whole crystal instead of isolated skyrmions.

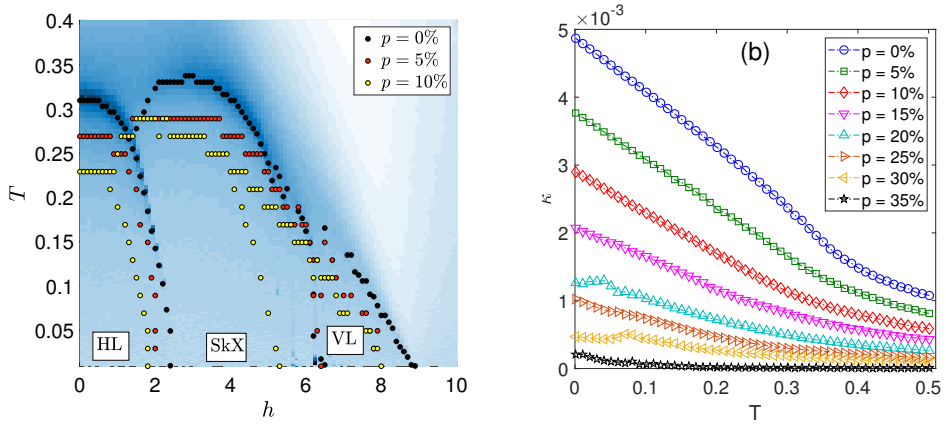

Figure 1: (a)Phase diagrams of the Heisenberg AFM model in $T-h$ plane with $D = 0.5$ and different p. (b)Temperature dependence of the chirality at $h = 3.4$, for selected values of the concentration of nonmagnetic vacancies p.

The presence of impurities leads to reduction of the magnitude of the chirality and smears out its abrupt change, particularly at the HL-SkX phase transition. The effect of the chirality reduction with the increasing concentration of the nonmagnetic impurities is demonstrated in Fig. 1(b), in which the chirality is plotted versus temperature for a wide range of the concentration p. Our rough estimate of the critical threshold of the magnetic dilution below which no skyrmions can survive even at the lowest temperatures is $p_c \approx 35\%$. This value is in a good correspondence with the value estimated for the FM model on the square lattice [5].

The phase diagrams for $p = 5\%$ (red circles) and $p = 10\%$ (yellow circles) are presented in Fig. 1(a). Their overall topology remains unchanged as compared to the case of the pure model and consists of the HL phase in the low-field region, the VL phase in the high-field region and the SkX phase sandwiched between them. However, a tendency of the SkX phase to shrink and smear with the increasing number of impurities can be noticed. Nevertheless, the area of the SkX phase still occupies a big part of a phase diagram even for $p = 10\%$.

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S9

Electron structure in twisted bilayer graphene

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Abstract

The study of twisted van der Waals heterostructures is recently a trending research field called twistronics. For a particular arrangement of layers within the multilayered solid the system can acquire unique properties, that does not posses none of the bare layer [2]. Many bilayer materials are sensitive to the relative twist angle of the individual layers and yield Moiré patterns. For particular small angles, called also "magic" angles, interesting physical properties can emerge. The computational complexity for the multilayer materials is often too high because of the large number of atoms inhabited in their supercell. We have therefore introduced effective theoretical approaches for reasonable description of the twisted bilayer systems. We have introduced commensurate supercells that can be used in calculations of electronic structure using approximative tight-binding methods [1, 2], where we have defined interlayer hopping parameter, or using density functional theory. We have also derived a continuous tight-binding model for any twist angle, which is fast and accurate even for sufficiently small twist angles. The main result of our calculations is the existence of flat bands for twist angle $\Theta = 1.05°$.

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S10

Robust quantum entanglement in the tetrapartite spin-1/2 square clusters: Theoretical study on the effect of a cyclic four-spin exchange

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Abstract

The whole entanglement measure so-called geometric Π_4 average of tangles of the antiferromagnetic spin-1/2 XXX Heisenberg model on a tetranuclear square cluster with cyclic four-spin interaction K [1, 2] is rigorously examined by the help of thermal negativity. The model comprises two nearest-neighbor exchange couplings J_1 and J_2 such that $J_1 \gg J_2$. The ground-state phase diagram of the model is studied, as well. It is demonstrated that the whole entanglement measure Π_4 nicely reproduces the ground-state phase diagram of the model including three different ground states. When the cyclic four-spin exchange is zero, the maximum value of whole entanglement Π_4 is achieved at low enough temperatures and relatively high magnetic fields ($B \approx J_1$). A nonzero value of the cyclic four-spin exchange notably enhances the whole entanglement degree [3]. The real complex $[Cu_4L_4(H_2O)_4](ClO_4)_4$ [4] as a strong antiferromagnetic tetranuclear square compound provides us an experimental representative to estimate the strength of the whole entanglement at high enough temperature.

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S11

Heterostructure-based stabilization of zero-field and high-temperature skyrmion crystal in an antiferromagnetic triangular lattice

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Abstract

Recently a three-sublattice skyrmion crystal (SkX) has been discovered in a frustrated classical antiferromagnetic (AFM) triangular lattice Heisenberg model with the Dzyaloshinskii-Moriya interaction [1]. It was stabilized at low temperatures in some window of the external magnetic field. In fact, the field required for stabilization of the SkX phase is rather high and it might be difficult or impossible to achieve it in the laboratory. For example, to access the SkX phase in the experimental realization of the present model in the compound Fe/MoS_2 the required magnetic field could be as high as 20 T [2]. High fields and very low temperatures are neither practical for technological applications. One of possible approaches to stabilization of the SkX state at much lower external fields (including zero) and ambient temperatures has been proposed by means of thoughtfully designed AFM/FM heterostructures [3].

In the present study we propose several heterostructures, which involve the SkX crystal hosting AFM layer, with the goal to decrease/eliminate the external magnetic field needed for the SkX phase stabilization or/and considerably increase the temperature window in which it appears. In particular, we show that the coupling of the AFM layer to a stiff ferromagnetic (FM) layer with strong out-of-plane anisotropy, can lead to the stabilization of the SkX phase at significantly lower, including zero, fields. In the AFM/FM bilayer structure, the effective field of the reference FM layer fully substitutes the required magnetic field for skyrmion formation. To achieve it the reference layer should be a hard ferromagnet with a sufficiently large exchange stiffness and the strong out-of-plane anisotropy, and the effective field induced by the interlayer exchange coupling should be in the range of the magnetic field required for skyrmion stabilization.

The temperature window of the SkX phase stability can be considerably broadened by ferromagnetically coupling several AFM layers on top of each other, i.e., creating a thin film. Both the increasing number of the layers as well as the increasing intralayer interaction lead to the increase of the transition temperature from the SkX to the paramagnetic phase by several times compared to the single AFM layer.

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S12

Phase boundary of spin-1/2 Ising-Heisenberg and Heisenberg models on a diamond decorated square lattice as magnetic analog of vapor-liquid phase border of water

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Abstract

Spin-1/2 Ising-Heisenberg and Heisenberg models on a diamond decorated square lattice schematically shown in Fig. 1 are investigated in a presence of the magnetic field by making use of several advanced analytical and numerical calculation schemes. The spin-1/2 Ising-Heisenberg model on the diamond decorated square lattice is exactly mapped via a generalized decoration-iteration transformation onto an effective spin-1/2 Ising square lattice with temperature-dependent nearest-neighbor interaction and field. We have found a rigorous evidence that the effective field vanishes along the line of first-order phase transitions between the classical ferrimagnetic phase and quantum monomer-dimer phase, which additionally terminates at an Ising-type critical point. This first-order phase-transition line is thus highly reminiscent of the vapor-liquid coexistence line of the water. An existence of discontinuous reentrant phase transitions observable for some range of the interaction parameters is explained in terms of the lowest-energy excitations from both considered phases. Exact results derived from the zero-field effective Ising square lattice are supplemented with classical Monte Carlo simulations in a particular subspace of the parameter region where an effective field becomes nonzero.

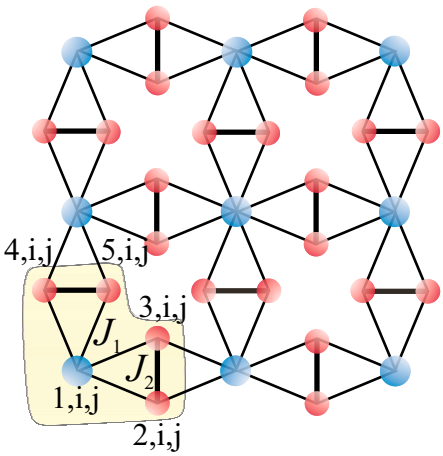

Figure 1: A part of the diamond decorated square lattice. A shaded area delimit a single unit cell.

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To compare with, the analogous spin-1/2 Heisenberg model on the diamond decorated square lattice was studied by the density-matrix-renormalization group (DMRG) technique and quantum Monte Carlo (QMC) simulations. The ground-state phase diagram of the fully quantum spin-1/2 Heisenberg model on the diamond decorated square lattice elaborated within the DMRG technique involves the Lieb-Mattis ferrimagnetic phase, the macroscopically degenerate dimer-tetramer phase, the monomer-dimer phase, the quantum spin-liquid phase and the saturated paramagnetic phase. The spin-1/2 Heisenberg model on the diamond decorated square lattice displays the line of first-order phase transitions between the Lieb-Mattis ferrimagnetic and monomer-dimer phases terminating at the Ising-type critical point quite similarly as its Ising-Heisenberg counterpart. This finding is corroborated by the advanced quantum Monte Carlo simulations performed in the dimer basis in order to avoid a notorious sign problem of this frustrated quantum spin model. The most interesting quantum spin arrangements is found within the macroscopically degenerate dimer-tetramer phase, whose low-temperature features can be explained by the effective monomer-dimer lattice-gas model.

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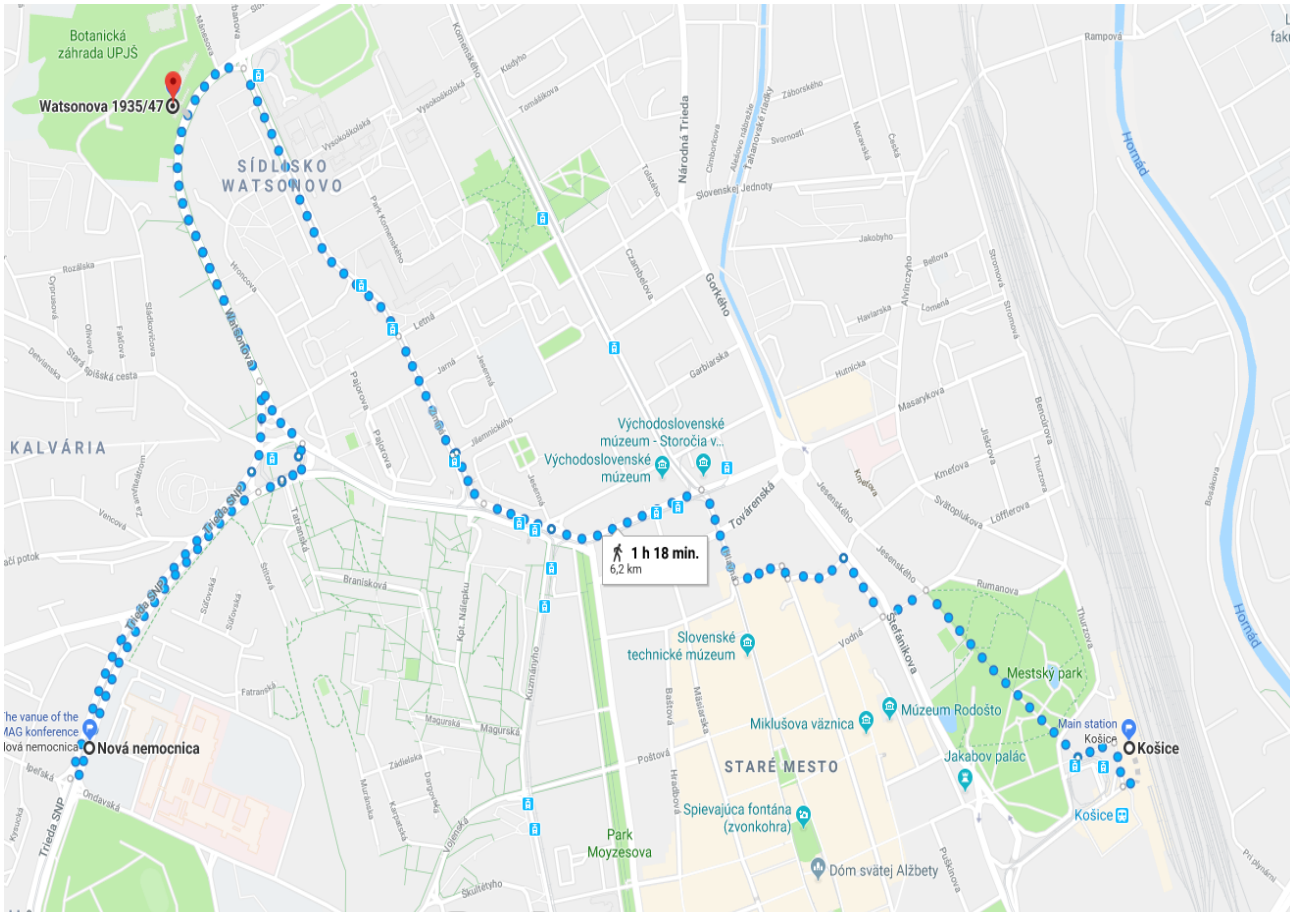

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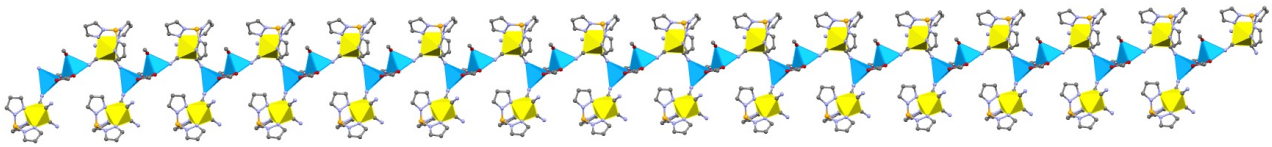

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