THEORETICAL PHYSICS

Effects of dimensional and spin crossovers on magnetic ordering in a superfrustrated kagome lattice Ising antiferromagnet
supervisor: doc. RNDr. Milan Žukovič, PhD.
study form: full time
Annotation: A superfrustrated kagome lattice Ising antiferromagnet (KLIA) is a spin model with a high degree of geometrical frustration. As a result the system shows no log-range ordering at any temperature. The spin correlation function decays exponentially even in the ground state, which is characterized by the highest residual entropy of all two-dimensional (2D) frustrated systems. A study of another albeit less frustrated model on a triangular lattice, which also remains disordered at any finite temperature, has shown the possibility of long-range ordering due to increase in the spin number or dimensionality by gradual stacking of the 2D planes. The goal of the present study is investigation of the possibility of the emergence, the nature and the region of the existence of long-range ordering in KLIA due to increase in the spin number or dimensionality.

Quantum entanglement in unconventional states of exactly solved models
supervisor: doc. RNDr. Jozef Strečka, PhD.
study form: full time
Annotation: Quantum entanglement belongs to the most intriguing consequences of the quantum mechanics, which is highly contra-intuitive and remains at a forefront of the current research interest. Among the most challenging issues related to this subject matter is to investigate the thermal entanglement through different measures (e.g. concurrence, negativity, von Neumann entropy, etc.), which quantify how the quantum entanglement evolves with rising temperature. The main focus of this dissertation thesis is to examine different measures of the thermal entanglement in the exactly solved lattice-statistical spin models. In particular, the considerable attention will be devoted to an open questions whether or not the thermal entanglement may coexist with a spontaneous long-range order and how it changes across quantum critical points.

Theoretical investigation of phase separation in binary and ternary liquid mixtures
supervisor: doc. RNDr. Jozef Strečka, PhD.
study form: full time
Annotation: The phase separation of binary and ternary liquid mixtures will be investigated within the framework of the lattice-statistical models such as the generalized Frenkel-Louis and Lin-Taylor models. In particular, the main emphasis will be laid by accounting for the multiparticle (e.g. three-body) interactions, which may play a crucial role in determining possible non-universal critical behavior. Besides, the dissertation thesis will focus on a problem of reentrant miscibility of some binary and ternary liquid mixtures with highly orientation-dependent forces (e.g. hydrogen bonding).

**Theoretical study of frustrated spin models on a bipartite lattices**  
supervisor: prof. RNDr. Andrej Bobák, DrSc.  
consultant: doc. RNDr. Milan Žukovič, PhD.  
study form: full time  
Annotation: Generally, the frustration is generated by the competition of different kinds of interaction and/or by the lattice geometry. As a result, in the ground state all bonds are not fully satisfied. However, a honeycomb lattice antiferromagnet like the square lattice with only nearest-neighbor exchange interactions are considered as bipartite lattice, the ground state exhibits long-range ordering. These systems become frustrated, if the next-nearest-neighbor exchange interactions are considered. Hence, it is interesting to study the magnetic properties of such lattices under frustrating interactions, which are still not well understood at present.

**Quantum properties of selected topological two-dimensional systems from first principles**  
supervisor: prof. RNDr. Michal Jaščur, CSc.  
consultant: RNDr. Martin Gmitra, PhD.  
study form: full time  
Annotation: Quantum mechanics provides description of material properties on fundamental level. Fundamental research in last years has pointed to the priority areas of innovation, material science and nanotechnology. Recently discovered and intensively studied materials like graphene, topological insulators, Weyl semimetals are examples of crystalline solids in which quantum properties results from a cooperative coupling between charge, spin and orbital momentum of electrons. Specific crystal structure and type of atoms determine topological essence of wave functions and macroscopic properties of the material like its electrical, magnetic, optical, thermal and mechanical properties. Common feature of the macroscopic manifestation is existence of the physical quantity called order parameter. The order parameter behaves like a classical quantity, however, its origin is quantum mechanical. It turned out that topological properties of the electronic states are a key concept to study quantum materials. Density functional theory (DFT) implemented in numerical methods of electronic structure calculations (also called first principles or ab-initio methods) represents a robust theoretical tool to describe properties and physical effects of known quantum materials as well as a tool in a search for new materials. Application of the DFT method in theoretical investigations shows increasing trend appreciated in many experiments as a free parameter theory.

References:
[1] see EIT RIS (European Institute of Innovation & Technology Research Regional Innovation Scheme), https://eit.europa.eu/tags/ris  
Quantum topological materials study from first principles
supervisor: prof. RNDr. Michal Jaščur, CSc.
consultant: RNDr. Martin Gmitra, PhD.
study form: full time
Annotation: Topological materials have newly been identified as quantum materials and their properties are highlighted by topology. In topology properties of objects (material properties) are invariant under smooth deformations of their Hamiltonian. Such materials are known also as topological materials. Topological insulators are insulating in bulk and conducting at surface. Topological semimetals having in their bulk semimetal character in which their valence and conduction bands touch near the Fermi level. Depending on band degeneracy (non-degenerate or doubly degenerate) topological material is called a topological Weyl semimetal or a topological Dirac semimetal. Topological Dirac or Weyl semimetals show linear dispersion around nodes, termed the Dirac or Weyl points, as the three-dimensional analogue of graphene (which is twodimensional). Most fundamental theoretical approaches to the study of the topological materials are electronic structure methods from first principles or derived tight-binding methods.
References:

Electronic, magnetic and topological properties of Heusler alloys
supervisor: prof. RNDr. Michal Jaščur, CSc.
consultant: RNDr. Martin Gmitra, PhD.
study form: full time
Annotation: The family of Heusler compounds, incorporates a huge number of magnetic members exhibiting diverse magnetic phenomena like itinerant and localized magnetism, antiferromagnetism, helimagnetism, Pauli paramagnetism or heavy-fermionic behavior. The lattice structure consists of 4 interpenetrating fcc lattices forming e.g. full-Heusler X2YZ or semi-Heusler XYZ alloz. Heusler alloys are amongst the most attractive halfmetallic systems due to the high Curie temperatures, structural similarity to the binary semiconductors and great potential for different applications such as future energy applications and for spintronics. Due to their half-metallic character, they may have a spin polarization of 100% at the Fermi level. The band gap can be tuned between 0 and 4 eV in the minoritz spin channel by the electronegativity difference of the constituents. Heusler alloys pave the way to new multifunctional materials, which have potential to revolutionize technological applications. Recently a new family of Weyl topological systems defined by broken time-reversal symmetry were predicted in Co-based magnetic Heusler materials. By means of density functional theory we can study electronic properties of the Fermi arcs and propose manipulation of the Weyl physics in these materials.
References:
Stochastic dynamics and turbulence: Calculation of relevant parameters and anomalous exponents in higher orders of perturbation theory.
supervisor: prof. Dr.h.c. RNDr. Michal Hnatič, DrSc.
consultant: RNDr. Tomáš Lučivjanský, PhD.
study form: full time

Annotation: PhD thesis will be devoted to a theoretical analysis of complex classical systems using sophisticated methods of quantum field theory. Classical systems in consideration are usually formulated in a form of stochastic models, which describe a whole class of phenomena. Most relevant models are reaction-diffusion problems, equilibrium and non-equilibrium phase transitions, turbulent flows and others. A common feature of such systems is presence of strong fluctuation effects, which precludes use of the ordinary perturbation theory. It is necessary to go beyond and apply non-trivial perturbation methods of quantum field theory, functional integrals and renormalization group. From a quantitative and experimental point of view we are interested in relevant observable parameters (e.g. Prandtl number, skewness and flatness factors, Kolmogorov constant etc.) and anomalous scaling indices, because they determine behavior of statistical correlations of random fields on large spatial scales.

Research in this area has achieved a point in which relevant parameters and anomalous scaling indices are known in the leading order of a loop expansion. Calculations of such quantities in higher orders of perturbation theory (two- and three-loop) belong to a current task in modern theoretical physics. Concrete calculations of multi-loop Feynman diagrams are very demanding and challenging problem. They require development of new numerical and symbolic algorithms, which can be implemented on computers. PhD candidate will have access to a supercomputer. Besides adequate knowledge of modern physics it is expected that a candidate is well acquainted with programming languages and techniques. Especially important will be a Monte Carlo method and its use on the evaluation of multidimensional integrals containing different types of singularities.

References:

The Graphitic Wormholes
supervisor: RNDr. Richard Pinčák, PhD. - Institute of Experimental Physics Slovak Academy of Sciences Košice
study form: full time

Annotation: A model will be formulated for the description of the electronic properties of an exotic graphene nanostructure called the graphene wormhole. This structure could arise due to
the topological as well as dopant defects in a bilayer or multilayer graphene, graphite. These structures for their extreme distortions could be widely used in a new field called STRAINTRONICS, where only through deformations of graphene nanostructures the gap varies between the valence and conduction band and thus the electronic properties of the given nanostructure are significantly affected. The Pi-orbital as well as the spin orbit interaction on the electronic spectrum of the graphene wormhole will be also derived and numerically calculated which should have significant applications in the electron microscopy.