THEORETICAL PHYSICS

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.
1. M.A. Nielsen, I.L. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, 2000.
2. L. Amico, R. Fazio, A. Osterloh, V. Vedral, Entanglement in many-body systems, Reviews of Modern Physics 80 (2008) 517-575.

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).
1. T. Narayanan and A. Kumar, Reentrant phase transitions in multicomponent liquid mixtures, Physics Reports 249 (1994) 135-218.
2. J. Strečka, L. Čanová, M. Jaščur, Investigation of phase separation within the generalized Lin–Taylor model for a binary liquid mixture of large hexagonal and small triangular particles, Molecular Physics 104 (2006) 3831-3839.

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 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:
[1] B. Yan, C. Felser, Topological Materials: Weyl Semimetals, Annual Review of Condensed Matter Physics 8, 337 (2017).
[2] M. Z. Hasan, C. L. Kane, Colloquium: Topological insulators, Rev. Mod. Phys. 82, 3045 (2010).
[3] S. A. Parameswaran, Y. Wan, Topological Insulators Turn a Corner, Physics 10, 132 (2017).
[4] A. A. Burkov, Topological Semimetals, Nature Materials 15, 1145–1148 (2016).

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:
[1] I. Galanakis, Ph. Mavropoulos, P.H. Dederichs, Introduction to half-metallic Heusler alloys: Electronic Structure and Magnetic Properties, J. Phys. D 39, 765 (2006).
[2] Z. Wang et al., Time-Reversal-Breaking Weyl Fermions in Magnetic Heusler Alloys, Phys. Rev. Lett. 117, 236401 (2016).

[3] R. M. Martin, Electronic Structure: Basic Theory and Practical Methods, Cambridge Press, 2004 ISBN 9780521782852.
[4] J. Kohanoff, Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods, Cambridge Press, 2006 ISBN 9780521815918.
[5] B. Yan, C. Felser, Topological Materials: Weyl Semimetals, Annual Review of Condensed Matter Physics 8, 337 (2017).

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:

J. Cardy, Scaling and Renormalization in Statistical Physics, (Cambridge University Press, 2002).
J. Zinn Justin, Quantum Field Theory and Critical Phenomena, (Oxford University Press, 1989).
A. N. Vasil'ev The Field Theoretic Renormalization Group in Critical Behavior Theory and Stochastic Dynamics, Boca Raton:Chapman & Hall/CRC (2004).
D. J. Amit and V. Martin-Mayor, Field Theory, the Renormalization Group and Critical Phenomena, World Scientific, Singapore 2005.

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.