HABILITATION THESIS REVIEWER'S REPORT

Masaryk University	
Applicant	Mgr. Jiří Chaloupka, Ph.D.
Habilitation thesis	Exotic Magnetismin Relativistic Transition Metal Compounds
Reviewer	Karlo Penc, DSc.
Reviewer's home unit, institution	Wigner Research Centre for Physics, Budapest

The interaction of atoms in condensed matter systems allows new phenomena to appear, which goes beyond the physics of its constituting atoms. Superconductivity and superfluidity are beautiful examples of achieving quantum coherence at macroscopic scales. Yet they are easily understood at the mean-field level. Much more exciting is the physics induced by strong interactions in materials, usually referred to as strongly correlated systems. For example, in transition-metal oxides, the strong Coulomb interactions in the d-electron shell localize the electrons and make these compounds insulators. These are the Mott insulators. The spins and the orbitals of the localized electrons combine into some effective local degrees of freedom. These are usually magnetic materials with local magnetic moments at sites, where the precise nature of the local degrees of freedom, interactions, and connectivity (lattice) determines the low-temperature phases. The inclusion of the relativistic spin-orbit coupling in systems with partially filled *4d* and *5d* shells adds further complexity to this problem, with exciting new concepts appearing, like topology and spin liquids. Dr. Chaloupka is one of the pioneers in this field. His studies about the realizability of Kitaev spin-liquids in iridium oxides and the statical and dynamical properties of the Ca_2RuO_4 were of great importance, including his contribution to the observation of a Higgs-mode in this material.

The habilitation thesis begins with a pedagogical introduction to the subject of Mott insulators. He presents the concepts of correlations and low-energy effective spin models, like Heisenberg and the Kitaev model. He continues with the discussion of the description of the physics of transition metal ions: crystal fields, exchange paths, multiplet structure, up to the introduction of the relativistic spin-orbit coupling. In chapter 3. he gives details about the realizability of Kitaev models in real compounds with a single hole in the t_{2g} orbitals (t_{2g}^5 configuration). He calculates the symmetry allowed terms in the Hamiltonian and their physical origin. By constructing a detailed phase diagram, he established the window in parameters where the Kitaev liquid may form and how the additional terms describe the experiments done on Na_2IrO_3. The final chapter discusses what happens when there are two holes in the t_{2g} orbitals (t_{2g}^4 configuration), as is the case of the Ru^{4+} ions in Ca_2RuO_4. The construction of an effective singlet-triplet model and the ground state phase diagram is described. The excitations are then treated with a generalized spin-wave approach that leads to the identification of a Higgs amplitude mode in neutron and Raman scattering experiments. In the end, the 14 papers on which the habilitation thesis is based are collected.

Dr. Chaloupka uses group theory (symmetry analysis) and perturbation techniques to establish the relevant low energy effective model for a particular compound, which he later studies by analytical (mean-field and generalized spin-wave) and numerical (exact diagonalisation at zero and finite temperatures) methods. All these procedures he applies with high proficiency, with the ultimate goal to compare the theory with experiments.

The habilitation thesis of Dr. Chaloupka encompasses research he performed in the last decade. He is coauthor of papers that appeared in renowned journals, including 2 Nature Physics, 6 Physical Review Letters, and a Physical Review X. He is the first author in seven of them. The papers are either purely theoretical with very few authors (typically 2 or 3) or written in collaboration with experimentalists. The high number of citations - over 2000 - quantifies the impact of his work in the scientific community. His work on “Kitaev-Heisenberg Model on a Honeycomb Lattice: Possible Exotic Phases in Iridium Oxides A_2IrO_3”, coauthored with G. Jackeli and G. Khaliullin, was among the ones that triggered the search for Kitaev spin liquids in iridates and received more than 600 citations. These numbers are well beyond what I would expect from a habilitation candidate and demonstrate that Dr. Chaloupka is a well-established researcher.

Reviewer's questions for the habilitation thesis defence (number of questions up to the reviewer)

1. Is there a symmetry argument why the ^1E and $^1T_2$ states are degenerate in Fig. 11?
2. The singlet-triplet model is typical for S=1/2 spin dimer systems. What are the major differences between an (anisotropic) Heisenberg model describing spin dimers and the spin-triplet model describing the t_{2g}^4 electrons?
3. After Eq. (4.26), the “dynamical Gutzwiller approximation” is employed. How does it compare to a standard multi-boson spin-wave expansion?

Conclusion

The habilitation thesis entitled “Exotic Magnetism in Relativistic Transition Metal Compounds” by Dr. Jiří Chaloupka **fulfils** the requirements expected of a habilitation thesis in the field of Condensed Matter Physics.

Date: April 11, 2021 Signature: