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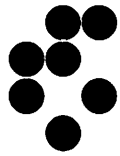

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Report on the Habilitation thesis by Jiri Chaloupka

Dr. Jiri Chaloupka, being in the procedure of habilitation at the Masaryk University, Brno, submitted the habilitation thesis: Exotic magnetism in relativistic transition metal compounds. The thesis is to my opinion an excellent introduction into the theory of transition-metal compounds. It gives a professional overview of the present status of this field, but also summarizes the contribution of Jiri Chaloupka to this subject and his most relevant publications, which are evidently very visible and cited in the community. The thesis is divided into sections, which are partly dedicated to different audience, starting with the Introduction for quite general physicists, followed by more specialized graduate-level presentation of theory of systems with correlated electrons, and finally a detailed summary of his own research, results and publications on the subject.

Sec.1 gives a quick introduction to the physics of transition-metal-oxide (TMO) compounds and to basic theoretical models which represent the starting point for further theoretical studies and calculation of various properties, which finally can be compared with relevant experimental results. Since the focus of the thesis are TMO insulators, the emphasis is on the presentation of the prototype Hubbard model and its reduction to effective spin models, following by consideration of their phase diagrams involving different ordered magnetic states, including also effects of geometrical frustration. Following is a quick introduction to Kitaev spin model on a honeycomb lattice with its intriguing topological and spin-liquid properties, as well to soft-spin systems, both being the central subject of Chaloupka's research work.

Sec.2 goes into more detail in the presentation and derivation of effective models for physics of TMO insulators. This section is quite technical, but at the same I find it very useful, since it can serve as a detailed and serious introduction for newcomers to the theory of TMO systems, i.e., as pointed out it is written on the level of graduate students or to my opinion even to more senior theorists searching for a systematic overview of quite broad range of additional effects which should be taken into account going beyond simple one-band description. Dr. Chalupka presents systematically essential elements for proper treatment of TMO insulators with the crucial role of electronic d^4 and d^5 orbitals: a) orbital crystal-field splitting in a crystal environment with the interplay of geometry of the lattice and orbital character, leading to partly quenched angular momentum, b) proper modelling and treatment of electron correlations due to Coulomb repulsion between electrons and leading to generalized multi-orbital Hubbard models, c) the role of spin-

orbit coupling becoming increasing strong for TMO materials with heavier elements, and finally e) the itinerant/hopping character of electrons between different ion sites taking into account quite complicated local orbital character. Taking these pieces properly together defines the effective model for electrons in TMO compounds. The thesis is focused on TMO insulators, so the last part of Sec.2 is the general discussion of the mechanism of Mott (repulsion-driven) mechanism to TMO insulators, the physics of corresponding metal-insulator transitions as well as the formal derivation of effective spin-type models starting from more general multi-orbital model, described above. I find this section very well written, so it can (should) become accessible to general audience as a review, to my knowledge not available so far.

Next two sections then focus on the actual research subjects and results of J. Chaloupka, i.e. so called Kitaev materials and soft-spin materials, which are detail presented in his attached publications. As presented in Sec.3, in connection with frustrated Kitaev systems his central effort and result is to derive effective very anisotropic Kitaev-Heisenberg model for the pseudospin $\tilde{S} = 1/2$ taking into account d-orbitals in realistic geometries and strong spin-orbit coupling as realized in most studied TMO Kitaev materials Na_2IrO_3 and α-$RuCl_3$. Since the model besides Kitaev terms on a heneycomb lattice involves also isotropic Heisenberg term as well some other correcting terms, the next effort is to explore very rich phase diagram for possible magnetic ground state in terms of model parameters. Clearly the experimental and theoretical goal is to find materials and regimes where the physics is as close as possible to Kitaev spin liquid. To monitor that J. Chaloupka presents also results for several static and dynamical correlation in such models which can be compared to experiments on actual materials. In more detail results, obtained in close collaboration with G. Khaliullin and other theoreticians, but also with experimental groups measuring such systems, are presented in attached papers.

In Sec.4 J. Chaloupka summarizes his work on soft-spin systems. Such physics arises when due to quasi-degeneracy of spin systems the crucial role is played by the superexchange interaction leading to soft magnetic moments and as the result to interesting spin excitation spectra. Again, main contribution of J. Chaloupka is the derivation of proper effective models for such systems, starting with local orbital structure, Hund coupling, leading via the superexchange to the singlet-triplet model and its modification due to crystal-field and lattice-geometry effects. Next goal is the analysis of such models where the main feature is the the emergence of the long-range order interpreted as macroscopic triplon condensation. Such physics leads to very interesting novel magnetic excitations calculated theoretically and compared to experimental results of the inelastic neutron and Raman scattering performed on material Ca_2RuO_4, revealing such phenomena.

The research work J. Chaloupka on Kitaev materials and soft-spin systems is published in last 10 years in 14 papers in most visible physical journals, among them 6 papers are published in prestigious Physical Review Letters, whereby in four of them he is the first author. Most of them are the result of the close collaboration with Ginyat Khalliullin, where both of them clearly found a perfect match of dealing with developing deep ideas and bringing them into contact with fascinating new materials. Staying with their theories close to experimentalists, they have produced a number of common publications, published

again in high-impact journals, two of them in Nature Physics. The impact of research achievement and publications is also impressive, as evidenced in overall more than 1500 citations (according to WS) and three papers with over 250 citations, where he is the first author.

The habilitation thesis of Dr. J. Chaloupka represents a mature overview of the theory of complex TMO materials, which exhibit fascinating new phenomena as Kitaev and soft-spin physics. The contribution of J. Chaloupka to recent development of this interesting field is evident and well known. I support fully his habilitation at the Masaryk University in Brno, and I am confident that he will play further an important role in performing and promoting top research in his local environment and also be able to convey his knowledge and enthusiasm to students and colleagues.

Conclusion

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

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