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Dr hab. Nicholas Sedlmayr
Institute of Physics
Maria Curie-Skłodowska University
Plac Marii Skłodowskiej-Curie 1
20-031 Lublin, Poland
sedlmayr@umcs.pl

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Report on the Habilitation Application of Dr Jacek Herbrych

"Properties of orbital-selective Mott insulators within low-dimensional multiorbital systems"

Dr Jacek Herbrych is an assistant professor in the Faculty of Fundamental Problems of Technology at Wrocław University of Technology. He obtained his doctorate from the University of Ljubljana in Slovenia in 2013 on the topic of *"Finite-temperature dynamics of quantum spin chains"* under the supervision of Prof. Dr Peter Prelovsek. Following this he spent several years as a postdoctoral researcher. First in the University of Crete where he worked with Prof. Xenephon Zotos, and then jointly at the University of Tennessee and Oak Ridge National Laboratory with Dr Elbio Dagotto, before moving to his current position in Wrocław University of Technology as an assistant professor (Polish: adiunkt).

For the scientific achievement Dr Herbrych has chosen to group together six of his publications (H1 - H6) on the theme *Properties of orbital-selective Mott insulators within low-dimensional multiorbital systems.* These works consider typically one dimensional many-body systems such as chains or ladders with electronic, spin, and orbital degrees of freedom. Often the physical system under consideration can be captured by one of several paradigmatic models like the Heisenberg or Hubbard models. Here the physical models are often related to Cu and Fe based materials. Nonetheless, these models, including the various generalisations of them that Dr Herbrych considers (for example multi-orbital Hubbard models), are rich enough to show a wide range of behaviour including high-T_c superconductivity, Mott physics, orbital selective Mott phases, and a range of magnetic ordering. Along with his collaborators he has investigated magnetic order, frustration, spin dynamics, topological phase transitions, and the possible existence of Majorana zero modes. To all six of these works Dr Herbrych has made a substantial contribution which often has involved sophisticated numerical simulations, analytical work, and the development or instigation of the projects themselves.

The challenge faced in the study of these materials is the existence of various competing orders and multiple interactions between the components. The overarching aim of the collection of papers H1 - H6 is to understand the magnetic ordering and transport properties of multi-orbital low dimensional systems. These can be compared to experimental studies such as inelastic neutron scattering, particularly on $BaFe_2$-Se_3, which contains ladder structures. The results of these six papers were found using analytical methods and density matrix renormalisation group (DMRG) numerics, the latter performed mostly by Dr Herbrych.

Work H1, *Spin Dynamics of the Block Orbital-Selective Mott phase*, the dynamical spin structure factor for a three orbital one dimensional Hubbard model, and two orbital ladder Hubbard model, were calculated using DMRG. The motivation was

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to explain inelastic neutron scattering experiments on $BaFe_2$-Se_3 which not only confirmed the relevance of multi-orbital effects, but also suggested low and high energy effects which need explanation. Although exact correspondence with the experimental results was not possible, as the models do not capture correctly all features of $BaFe_2$-Se_3, several interesting results could be observed. Block spin order with a rotation of $\pi/2$ was correctly recovered in the ladder model. This is a phases where a local block of several spins behaves with a mutually fixed spin orientation. Furthermore low energy acoustic modes, comprised of excitations between the rigid magnetic blocks, and high energy dispersionless optical modes were observed, in agreement with previous experimental work. These results required pushing DMRG to its limits, and in addition to the technical accomplishment shown here the new interesting features should be applicable to a range of materials.

Taking as its starting point the block order inside the orbital-selective Mott phase seen in H1, H2 concerns *Novel Magnetic Block States in Low-Dimensional Iron-Based Superconductors*. Starting from the multi-orbital Hubbard model effective models which capture the orbital selective Mott phase are derived. These are referred to as a generalised Kondo-Heisenberg model. The effective models allow for a 'simpler' and therefore more detailed, though still accurate, investigation of the orbital selective Mott phase. Using these effective models the authors firstly demonstrate that the magnetic block phases are not confined to spin rotations of $\pi/2$. Depending on the electron filling different spin orders can be seen. The development of simpler effective models is in itself an important contribution to the field, and furthermore it is used here to demonstrate the existence of several previously unknown phases possible in several materials.

H3, *Block-Spiral Magnetism: An Exotic Type of Frustrated Order*, includes a continuation of these investigations into orbital selective Mott phases. Focusing now on purely one dimensional chains the authors discover novel exotic magnetic order. A block-spiral state is found between competing ferromagnetic and block spin phases. This new state is explained as the result of competition between Hund dominated double exchange in the multi-orbital system and the Hubbard interaction which is controlling super exchange.

In H4, *Block Orbital-Selective Mott Insulators: A Spin Excitation Analysis*, the dynamical spin structure factor is calculated for the multi-orbital Hubbard model and the generalised Kondo-Heisenberg Hamiltonian introduced in H2. By varying the electron density, interaction strength, and Hund exchange the parameter space in which different spin block orders develops were found. Excitations in these phases give rise to dispersive low energy acoustic modes, seen in the dynamical structure factor. They also find dispersionless modes generically present in all cases. By mapping out this full parameter space the authors hope to guide crystal growers to develop new materials which demonstrate this novel magnetic order in addition to the previously mentioned $BaFe_2$-Se_3, which could then be investigated by neutron scattering to confirm (or not) the predicted phases.

Work H5, *Interaction-Induced Topological Phase Transition and Majorana Edge States in Low-Dimensional Orbital-Selective Mott Insulators*, picks up on an intriguing possibility suggested by the spiral spin order seen in H3. The existence of spiral magnetic order near superconductivity raises the spectre of Majorana zero modes and topological superconductivity. The search for the non-abelian anyons known as Majorana zero modes has recently been very widely studied, and this paper makes a very interesting contribution to the field, novel in several respects. Once again the starting point is the generalised Kondo-Heisenberg model coupled to a BCS superconductor, which is reduced to the generalised Kondo-Heisenberg model with an effective s-wave pairing. In the block spin spiral phase all the usual ingredients for topological superconductivity are present, albeit in an interacting system considerably more complicated than the non-interacting topological superconductors often

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studied. Using DMRG a detailed analysis of the local density of states, triplet and singlet pairing, and spin order demonstrates the likely existence of Majorana zero modes in this system. This is interesting not only as a non trivial example of a many-body topological superconductor, but also because this is achieved in a model which retains $SU(2)$ symmetry.

The final work in the series H6, *Quantum Magnetism of Iron-Based Ladders: Blocks, Spirals, and Spin Flux*, concerns the effective generalised Kondo-Heisenberg for multi-orbital ladders, as previously in the orbital selective Mott phase. Although this is an approximate model it is stressed that the accuracy is sufficient to capture the relevant physics. By calculating the spin structure factor and chiral correlations phases with different magnetic blocks are identified. As the Hubbard interaction is increased exotic spiral phases are observed and for an appropriate electronic filling quantum spin flux is observed. Elsewhere in the phase diagram physics of Cuprates and Manganites is observed. This is a comprehensive study in which Dr Herbrych performs in the supervising role, with his doctoral student performing the numerical calculations.

In addition to the above Dr Herbrych has a *further* 26 publications since his PhD, principally in highly regarded Journals such as Physical Review Letters and Physical Review B. These include work on transport through low dimensional systems, many-body localisation and multi-orbital models. Dr Herbrych is also the principle investigator of two grants, one *OPUS 18* from NCN (2020-2022), and *Polish Returns* from NAWA (2019-2022). He has further taken part in several grants lead by other people. He has given seminars internationally at conferences and in scientific institutions. He is a member of the American Physical Society and has a varied list of international collaborators. All of these additionally speak to his development and high level as a scientist.

To summarise, Dr Jacek Herbrych chose a small collection of his articles on which to base his scientific achievements for the habilitation. The quality if these articles, and his significant contribution to each, make this in my opinion an outstanding application. This is additionally supported by the rest of his achievements. In my opinion, the scientific achievements presented for evaluation along with the other scientific achievements and activities of Dr. Jacek Herbrych meet the statutory and customary requirements for candidates to be awarded the degree of habilitated doctor in the discipline of physical sciences.

Nicholas Sedlmayr

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