Summary of Professional Accomplishments

Phases and phase transitions in correlated fermion systems at and out of equilibrium

Marcin Mateusz Wysokiński

Autoreferat

Contents

1 Name:

Marcin Mateusz Wysokiński

2 Diplomas and degrees conferred in specific areas of science

- **Doctoral degree in Physics** - October 2015, Jagiellonian University in Kraków, Poland
  Title of the thesis: *Unconventional superconductivity and hybridized correlated fermion systems*,
  Supervisor: prof. dr hab. Józef Spałek,
  Secondary supervisor: dr Jan Kaczmarczyk
  The work was defended with distinction

- **Master degree in Physics** - June 2011, Jagiellonian University in Kraków, Poland
  Title of the thesis: *Properties of the liquid Helium 3 as a correlated quantum liquid*,
  Supervisor: prof. dr hab. Józef Spałek
  The work was defended with distinction

3 Information on employment in research institutes or faculties/departments

After completing my doctoral studies, I carried out my research as:

- 11/2017 - present: Postdoc (adiunkt) in the group of prof. T. Dietl,
  International Research Center MagTop, Institute of Physics of the Polish Academy of Sciences, Warszawa, Poland

- 11/2015 - 10/2017: Principal investigator of the *Mobilność Plus* project in the group of prof. M. Fabrizio,
  International School for Advanced Studies (SISSA), Trieste, Italy

- 1 - 31/10/2015: Contractor of the grant *Maestro* in the group of prof. J. Spałek,
  Jagiellonian University in Kraków, Poland

4 Description of the achievements, set out in art. 219 para 1 point 2 of the Act

4.1 Title of the scientific achievement

Phases and phase transitions in correlated fermion systems at and out of equilibrium

4.2 Publications constituting the scientific achievement

[p1] **M. M. Wysokiński**
Scientific Reports **9**, 19461 (2019)
Mechanism for transitions between ferromagnetic and antiferromagnetic orders in d-electron metallic magnets

[p2] G. Cuono, C. Autieri, **M. M. Wysokiński**
Physical Review B **104**, 024428 (2021),
Spatially modulated orbital-selective ferromagnetism in $La_5Co_2Ge_3$

[p3] **M. M. Wysokiński**
Physical Review B: Rapid Communication **97**, 041107 (2018),
Microscopic mechanism for the unusual antiferromagnetic order and the pressure-induced transition to ferromagnetism in USb_2

[p4] **M. M. Wysokiński**, M. Fabrizio
Physical Review B: Rapid Communication **94**, 121102 (2016),
Many-body breakdown of indirect gap in topological Kondo insulators

[p5] **M. M. Wysokiński**, M. Fabrizio
Physical Review B: Rapid Communication **95**, 161106 (2017),
Mott physics beyond the Brinkman-Rice scenario

[p6] **M. M. Wysokiński**, M. Fabrizio
Physical Review B: Rapid Communication **96**, 201115 (2017),
Interplay of charge and spin dynamics after an interaction quench in the Hubbard model

[p7] M. Płodzień, **M. M. Wysokiński**
Physical Review B: Rapid Communication **100**, 041116 (2019),
Rabi-resonant behavior of periodically-driven correlated fermion systems

4.3 Description of the scientific achievement

4.3.1 Introduction

The emergent behavior of correlated fermions leading to the appearance of various complex phases, e.g. magnetism or superconductivity, focuses attention of physicists, both experimentalists and theorists, for decades. Despite the increasingly precise investigations of materials under extreme conditions of low temperatures, high pressures, controllable doping as well as non-equilibrium excitation, a complete theoretical understanding of the microscopic mechanisms governing phase formation is still, to say the least, incomplete. The difficulties begin at the stage of phase definition. Many phase transitions can be described in the language of the well-established Landau theory and concepts such as spontaneous symmetry breaking and the order parameter. However, it has recently become clear that it is important to extend apparatus for the phase transition analysis to include topological order[1] as well as non-equilibrium phenomena [2].

Phase transitions occurring in systems close to the equilibrium state are subject to certain universal laws in the vicinity of special points on the phase diagram. The situation changes dramatically when we study systems in non-equilibrium conditions. The analysis of strongly interacting systems is then particularly difficult. Additional issues arise when interacting systems with topological order are studied. Therefore, the investigation of emergent phenomena in quantum matter, such as the formation of phases, the characterization of transformations between them, and predicting their properties in response to nonequilibrium perturbations, often requires special models and adequate methods of their analysis. For these reasons, in the research constituting the basis of the scientific achievement *Phases and phase transitions in correlated fermion systems at and out of equilibrium*, I propose a theoretical insight into the nature of selected phases (also topological) and phase transitions (also dynamic) observed experimentally or realized by simplified many-body models in systems of correlated fermions in and out of equilibrium.

According to the logic of usually consecutive research stages, the research areas of the scientific achievement can be divided into three groups presented in Fig. 1. For natural reasons, the implementation of particular stages listed in Fig. 1 (e.g. model selection/construction) is somehow automatically known in some works from the subject literature (e.g. the choice of the Hubbard model in order to address Mott physics in **[p5-p7]**), and in others it is a key achievement (e.g. proposing the *d-p* model to describe itinerant ferromagnetism in metallic magnetic compounds in **[p1]**). On the other hand, a clearer picture of my scientific achievement can be obtained by following the motivation of the research carried out in the works **[p1-p7]**.

Research in **[p1-p3]** was motivated by ongoing experiments suggesting phase transitions induced by pressure change between ferromagnetic (FM) and antiferromagnetic (AFM) phases (or, in general, spatially modulated magnetic phase) in $LaCrGe_3$ [3], USb_2 [4] and $La_5Co_2Ge_3$ [5]. Aim of these works was to provide a convincing microscopic understanding of the observed phenomena. In achieving this goal, it turned out to be crucial to define the minimum set of elements characterizing the behavior of correlated electrons in the d or f shells in the mentioned compounds, as well as to prove that the

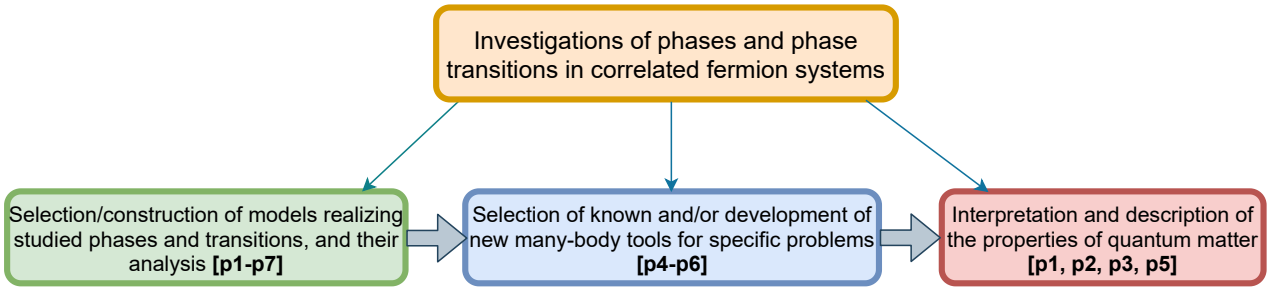

Figure 1: Schematic division of consecutive research stages concerning my investigations on phases and phase transitions in correlated fermion systems constituting the presented scientific achievement.

models constructed on this basis lead to a consistent interpretation of the experimental results.

Next, a partial motivation of the research undertaken in the works **[p4-p6]** was the development of new, numerically efficient many-body methods that can capture detailed description of selected phases and phase transitions in models of correlated fermions. The most accurate many-body methods for describing correlated fermions usually require enormous computing power to capture the properties of only the simplest systems[6]. The problem is even more complicated in the case of dynamic phenomena. This is because many-body tools, numerically accessible for description of equilibrium systems, in case of nonequilibrium conditions allow only for very short simulation times of correlated fermions (e.g. dynamic mean field theory [7]). For these reasons, it is very important to develop alternative tools that allow for numerically efficient analysis of the properties of many-body models with an accuracy close to recognized rigorous methods.

Finally, the research in **[p4-p7]** was motivated by the challenge of understanding the unique properties of selected correlated fermion systems under both equilibrium and non-equilibrium conditions that can be attributed to specific features of many-body interactions. In this perspective, in the work **[p4]** I focused on phenomena related to non-local correlation effects [1]. On the other hand, in **[p5-p7]** my research focused on understanding the behavior of high-energy quantum fluctuations [2] (leading to the exchange spin interaction [8]) in connection with Mott physics in both equilibrium and non-equilibrium situations.

Following detailed description of scientific achievement is organized as follows. Chapter 4.3.2 discusses the minimal many-body models analyzed in the works **[p1, p3-p7]** for the description of particular phases and phase transitions in correlated fermion systems. Chapter 4.3.3 introduces the classification of many-body numerical methods on the level of the single-particle Green's function. This classification is useful for describing the methods developed, generalized, or used in **[p1, p3-p6]**. Chapter 4.3.4 provides a detailed description of the results of works **[p1-p7]**. The description of the achievement ends with a summary in Chapter 4.3.5.

[1] Non-local correlation effects are manifested as the dependence of self-energy on momentum in a single-particle Green's function - for details see Section 4.3.3

[2] Their effect on the single-particle level is incorporated in the self-energy via full dependence on frequency - for details see Section 4.3.3

4.3.2 Models of correlated fermions

An important example of correlated fermion systems on a lattice are compounds with electrons on partially filled d or f shells. The localized nature of these orbitals provides that the leading effect of the Coulomb repulsion between electrons is a strong onsite interaction called the Hubbard interaction. In the Hamiltonian, describing the system in the language of the second quantization, this interaction takes a following form

$$H_{int} = U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow\alpha} n_{\mathbf{i}\downarrow\alpha}, \tag{1}$$

where $n_{\mathbf{i}\sigma\alpha}$ is a number operator of fermions with spin $\sigma = \{\uparrow, \downarrow\}$ on the α orbital and $\mathbf{i}$ lattice site, and U parametrizes the amplitude of interaction.

The presence of strong interaction of this type is a challenge for the theoretical description. This is because the popular and effective methods of the density functional theory (DFT), which allow to capture the complex crystal and orbital structure of chemical compounds, do not handle well the full effects of strong interaction. Even the combination of the DFT approach with many-body method that takes into account the complex effects of interactions (such as, for example, the spin exchange interaction) for the price of involving huge computational resources, suffer from the infamous, still unsolved problem of double counting of correlation effects [9]. At the same time, it should be noted that, despite some problems, DFT methods provide valuable insight into understanding of correlated fermions systems, e.g. as it is the case in the work **[p2]**.

For these reasons, often, in order to understand the properties of d or f electron materials, it is important to study minimal, but accounting for Hubbard interaction, models that capture the essential features of the particular system. Limiting the number of degrees of freedom in a given situation allows for a relatively accurate and transparent theoretical analysis of the mechanisms leading to a particular behavior. The simplest model, which describes the repulsive d electrons moving on the crystal lattice, is the single orbital Hubbard model:

$$H_{HM} = H_T + H_{int} = \sum_{\mathbf{ij}\sigma} t_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \tag{2}$$

where operators $c^{\dagger}_{\mathbf{i}\sigma}$ and $c_{\mathbf{i}\sigma}$, respectively, create and annihilate fermion with a spin σ on $\mathbf{i}$ lattice site (hence $n_{\mathbf{i}\sigma} \equiv c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma}$), and $t_{\mathbf{ij}}$ is the hopping integral. Although, this model has a relatively simple structure, there is no exact solution in arbitrary number of dimensions. Nevertheless, many approximate (and even accurate in the limit of the infinite number of dimensions [10]) numerical many-body methods have been developed allowing for fairly precise prediction of the properties of the Hubbard model [6] (see Chapter 4.3.3), in particular regarding the realized Mott insulator state and emergent broken symmetry states such as magnetism or superconductivity. Worth mentioning is that phase diagram obtained for this model allows for semi-quantitative interpretation of observation of all mentioned phases in hole-doped high temperature copper-based superconductors (e.g. [11]).

Experiments with cold fermion atomic gases trapped in optical lattices showing that these can simulate Hubbard model opened up a completely new perspective for research. Namely, high control over microscopic parameters such as e.g. interaction strength opened the possibility to study non-equilibrium properties of the system in response to time-dependent changes. As a result, many studies are focused on the experimental implementation of driven fermion systems [12, 13], but also on purely theoretical, basic considerations [14, 15]. One of the key directions of research is the so-called Floquet engineering, when in response to periodic modulation of microscopic parameters over time, a system of correlated fermions on a certain time scale is described by a new, often exotic, effectively time-independent Hamiltonian [16, 17]. Another direction of research is the analysis of the dynamics of the system after a rapid change in microscopic parameters at a certain point in time (quantum quench). Post-quench dynamics in Hubbard model revealed the spectacular phenomenon of the dynamical Mott transition [14].

The properties of the correlated fermions described by the Hubbard model were analyzed in **[p5-p7]** in the context of Mott's physics. Namely, in the work **[p5]** I proposed a new method for describing the metal - Mott insulator transition, which I then generalized to the time domain in **[p6]** where it allowed to describe the dynamical Mott transition. Additionally, in the work **[p7]** I analyzed the behavior of the Mott insulator subjected to periodic modulation of the interaction amplitude.

A slightly more complicated model that allows to describe some properties of f-electron materials is the Anderson lattice model (ALM):

$$\mathcal{H}_{ALM} = \sum_{\mathbf{k}\sigma} \epsilon_f f^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} n^f_{\mathbf{i}\uparrow} n^f_{\mathbf{i}\downarrow} + \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \left(V_{\mathbf{k}} f^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \text{H.c.} \right), \tag{3}$$

where f operators refer to the f orbital states, and the c operators refer to the ligand band states. The key feature of f-electron systems, large spatial separation between atoms with partially filled f shell entails absence of direct hopping integral, property captured by the above model with the non-dispersive energy level ϵ_f. The f-electrons, however, often delocalize by hybridizing ($V_{\mathbf{k}}$) to the conductance band ($\epsilon_{\mathbf{k}}$). Hamiltonian (3) is a minimal model for the description of f-electron systems allowing for consistent explanation of the formation of many interesting phases observed in these materials, such as heavy-fermion Fermi liquid [18], Kondo insulator [18, 19], heavy-fermion superconductor [20] or tricritical ferromagnet [21–23]. In the work **[p3]** I analyzed the Anderson lattice model in the context of the phase transition between antiferromagnetism and ferromagnetism. On the other hand, in **[p4]** the Anderson lattice model with spin-dependent hybridization was considered in the context of topological phase transitions and metal-insulator transitions. Although nominally proposed to describe f electron systems, the Anderson lattice model extended to include non-zero dispersion of correlated fermions [$\epsilon_f \to \epsilon^f_{\mathbf{k}}$ in Eq. (3)] as discussed in the work **[p1]**, can capture essential properties of many d-electron metallic ferromagnets (then the f operators describe d-electron states).

4.3.3 Numerical many-body methods and related approximations

A great challenge in describing the properties of models with the Hubbard interaction is the correct choice of the most effective many-body method offering a well-chosen type of approximation suited to the problem under consideration. Probably the most commonly used classification of methods for the problems of strongly correlated fermions is based on the imposed approximation at the level of a single-particle Green's function depending on the momentum $\mathbf{k}$ and the frequency ω, $G_{\mathbf{k}}(\omega)$. In the following, for demonstration purposes, the Hubbard model is considered. The correlation effects in a single-particle Green's function through the Dyson equation are accounted for by the physical quantity called self energy $\Sigma_{\mathbf{k}}(\omega)$,

$$G_{\mathbf{k}}(\omega) = \Big(\omega - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega)\Big)^{-1}, \tag{4}$$

where $\epsilon_{\mathbf{k}}$ is the kinetic energy of fermions obtained, for example, from the tight-binding approximation [i.e. for a square lattice with a hopping integral only to the nearest neighbors $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$]. Calculating the dependence of self energy on both the frequency and the momentum in arbitrary number of dimensions is an extremely complex task and most often requires approximations. For this reason, two qualitative approximations are often imposed, either separately or in combination, to simplify the calculations. The first is the assumption of the locality of the correlation effects (which is formally exact in an infinite number of dimensions [24]), which boils down to the independence of self energy on the momentum,

$$\Sigma_{\mathbf{k}}(\omega) \simeq \Sigma(\omega). \tag{5}$$

This approximation characterizes all (non-cluster) mean-field theories. The second widely used approximation is accounting for only coherent low-energy quantum fluctuations

$$\Sigma_{\mathbf{k}}(\omega) \simeq \Re\Sigma_{\mathbf{k}}(0) + \omega \frac{\partial \Re\Sigma_{\mathbf{k}}(\omega)}{\partial \omega}\Big|_{\omega\to 0}, \tag{6}$$

and requires only determination of $\Re\Sigma_k(0)$ and $\frac{\partial \Re\Sigma_{\mathbf{k}}(\omega)}{\partial \omega}\Big|_{\omega\to 0}$. This approximation leads to a quasiparticle description of fermions, what is immediately manifested in a single-particle Green's function,

$$G_{\mathbf{k}}(\omega) \simeq \frac{z_{\mathbf{k}}}{\omega - z_{\mathbf{k}}[\epsilon_{\mathbf{k}} - \Re\Sigma_{\mathbf{k}}(0)]} \tag{7}$$

where $z_{\mathbf{k}} \equiv (1 - \partial\Re\Sigma_{\mathbf{k}}/\partial\omega|_{\omega\to 0})^{-1}$ is a quasiparticle weight. From the above form of a single-particle Green's function it follows that in this approximation fermions behave as if they do not interact, but only have a normalized dispersion. This approximation is in heart of Landau's theory of Fermi liquid as well as diagrammatic expansion of Gutzwiller wave function method [25]; I will discuss the latter method in more details in the next section. In the following, I will present a short analysis of the variational methods based on the Gutzwiller wave function used in most of my works **[p1, p3-p6]** on the example of the Hubbard model in relation to the introduced classification. Table 1 presents a list of selected, popular many-body methods (methods used in my research in Table 1 are marked in blue) that implement specific approximations on their self energy.

The Gutzwiller wave function is constructed from the Slater determinant $|\psi_0\rangle$ modified by local (on $\mathbf{i}$ lattice site) linear operators $P_{\mathbf{i}}$,

$$|\psi_G\rangle = \prod_{\mathbf{i}} P_{\mathbf{i}} |\psi_0\rangle. \tag{8}$$

Linear operator $P_{\mathbf{i}}$ acts in local Fock space spanned by four possible configurations $|\Gamma\rangle_{\mathbf{i}} \in \{|0\rangle_{\mathbf{i}}, |\uparrow\rangle_{\mathbf{i}}, |\downarrow\rangle_{\mathbf{i}}, |\uparrow\downarrow\rangle_{\mathbf{i}}\}$,

$$P_{\mathbf{i}} = \sum_{\Gamma} \lambda_{\Gamma} |\Gamma\rangle_{\mathbf{i}\,\mathbf{i}} \langle\Gamma|. \tag{9}$$

$\Sigma_{\mathbf{k}}(\omega) \simeq$	$\Sigma_{\mathbf{k}}(\omega)$	$\Sigma(\omega)$	$\Re\Sigma_{\mathbf{k}}(0) + \omega \frac{\partial \Re\Sigma_{\mathbf{k}}(\omega)}{\partial \omega}\Big\vert_{\omega\to 0}$	$\Re\Sigma(0) + \omega \frac{\partial \Re\Sigma(\omega)}{\partial \omega}\Big\vert_{\omega\to 0}$
Metoda	cDMFT, DCA,VMC	DMFT, GA+SWT	DE-GWF	GA

Table 1: List of many-body methods that implement specific approximations on a self-energy. The methods used, extended or developed in the works being the subject of the *scientific achievement* are marked in blue. Abbreviation list: cDMFT - cellular dynamical mean-field theory [26], DCA - dynamical cluster approximation [26], VMC - variational Monte Carlo with Jastrow correlator [27], DMFT - dynamical mean-field theory [10], GA+SWT - Gutzwiller approximation + Schrieffer-Wolff transformation **[p4]**, DE-GWF - diagrammatic expansion of Gutzwiller wave function [25], GA - Gutzwiller approximation.

The idea behind the Gutzwiller wave function is a selection of an operator $P_{\mathbf{i}}$ in such a way that a single variational parameter optimizes the probability of double occupations, which due to increasing interactions should naturally decrease. A useful choice is the operator satisfying

$$P_{\mathbf{i}}^{\dagger} P_{\mathbf{i}} = 1 + x d_{\mathbf{i}}. \tag{10}$$

where x is a variational parameter and

$$d_{\mathbf{i}} = \big(n_{\mathbf{i}\uparrow} - \langle\psi_0|n_{\mathbf{i}\uparrow}|\psi_0\rangle\big)\big(n_{\mathbf{i}\downarrow} - \langle\psi_0|n_{\mathbf{i}\downarrow}|\psi_0\rangle\big). \tag{11}$$

For example, the expectation value of a local operator on the site $\mathbf{i}$ (e.g. Hubbard interaction) with respect to the Gutzwiller wave function can be expressed in a following manner [25]

$$\langle\psi_G|\mathcal{O}_{\mathbf{i}}|\psi_G\rangle = \sum_{k=0}^{\infty} \frac{x^k}{k!} \sum_{\mathbf{l}_1,\ldots,\mathbf{l}_k}{}' \langle\psi_0|P_{\mathbf{i}}^{\dagger}\mathcal{O}_{\mathbf{i}}P_{\mathbf{i}}\, d_{\mathbf{l}_1}\ldots d_{\mathbf{l}_k}|\psi_0\rangle, \tag{12}$$

where primed sum denotes, $\mathbf{l}_1 \neq \mathbf{l}_k \neq \mathbf{i}$.

Despite the simplicity of the expression, the calculation of the right side of the equation (12) is not possible in the thermodynamic limit, due to the summation of an infinite number of terms. However, this summation can be executed for a finite lattice, which results in a natural truncation at infinite sums in (12) and the effective optimization of the expectation values can be done using the Monte Carlo method (a method known as *variational Monte Carlo*, VMC). Check of the accuracy of the calculations accounts for the convergence test of the results with the increasing size of the finite system. On the other hand, truncation in infinite sums as in the Diagrammatic Expansion of the Gutzwiller Wave Function (DE-GWF) method [25] can be introduced by assuming vanishing of the expectation values of single-particle operators with site indices $\mathbf{i}$ and $\mathbf{j}$ separated by a particular distance (e.g. $|\mathbf{i}-\mathbf{j}| > l$), and by taking into account the finite number of sum of k elements in (12). In this case, checking the accuracy of the calculations comes down to the convergence test of the results depending on l and k. It turns out that some properties are already very well described even in the zeroth order of expansion, $k =$ called the Gutzwiller approximation (GA). This approximation is very effective as it leads to concise analytical results for expectation values. Formally, the Gutzwiller approximation takes into account only the local effects of the interaction and becomes variationally exact in the infinite number of dimensions [24].

Regardless of the considered order of expansion, both GA and DE-GWF methods reduce the problem of interacting fermions to the effective Hamiltonian describing free fermions with renormalized characteristics. For example, for the Hubbard model methods lead to the following effective Hamiltonian,

$$H_{\text{eff}} \sim \sum_{\mathbf{k},\sigma} q_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \tag{13}$$

where $q_{\mathbf{k}}$ is the Gutzwiller band narrowing factor, and in particular for GA is momentum independent, $q_{\mathbf{k}} = q$. The single-particle Green's function for such an effective Hamiltonian indicates that the

variationally determined factor $q_{\mathbf{k}}$ can be identified with the quasiparticle weight $z_{\mathbf{k}}$ in eq. (7). For this reason, both methods (GA and DE-GWF) are consistent with the approximation (6), and GA additionally realizes assumption of the local (independent of the momentum) self-energy (5). In the context of the Gutzwiller wave function method, the remark concerning the VMC method is in place here. Nowadays, the VMC method accounts for the use of the variational Gutzwiller wave function extended by the Jastrow correlator [27], which is able to take into account the properties of the system beyond the quasiparticle approximation (6). Hence, in the table 1, the VMC method, although limited by the finite size of the considered system, is classified as the one that takes into account the full self energy of the correlated fermions.

For the Hubbard and related models, very important, though not explicitly falling into introduced classification, is the method of canonical transformation. In the limit of strong interactions $U \gg t$ in the Hubbard model there can be singled out low-energy subspace (LES) without double occupations and high-energy subspace (HES) with double occupations. Hopping operator $T_{\mathbf{ij}} \equiv \sum_{\sigma}(c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + \text{H.c.})$ on the bond $\langle \mathbf{ij} \rangle$ can be divided into acting within LES and HES as well as subspace mixing parts. Mixing terms can be formally defined as $\tilde{T}_{\mathbf{ij}} \equiv \mathrm{P}_{20}T_{\mathbf{ij}}\mathrm{P}_{11}$ and $\tilde{T}^{\dagger}_{\mathbf{ij}} \equiv \mathrm{P}_{11}T_{\mathbf{ij}}\mathrm{P}_{20}$ where $\mathrm{P}_{nm} \equiv \mathcal{P}_{\mathbf{i};n}\mathcal{P}_{\mathbf{j};m} + (1-\delta_{nm})\mathcal{P}_{\mathbf{i};m}\mathcal{P}_{\mathbf{j};n}$, δ_{nm} is Kronecker delta and $\mathcal{P}_{\mathbf{i};n}$ is a projector on a site $\mathbf{i}$ with a configuration with $n \in \{0,1,2\}$ fermions. The method of canonical transformation accounts for removing the mixing between subspaces in the leading order, what leads to an effective description in low-energy subspace within the so-called $t-J$ Hamiltonian [8],

$$H_{t-J} = -t\sum_{\mathbf{ij}\sigma}(1-n_{\mathbf{i}\bar{\sigma}})c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma}(1-n_{\mathbf{j}\bar{\sigma}}) + J\sum_{\mathbf{ij}}\mathbf{S}_{\mathbf{i}}\cdot\mathbf{S}_{\mathbf{j}}, \tag{14}$$

in which the spin exchange interaction with amplitude $J = 4t^2/U$ is the key feature. This interaction originates from high-energy quantum fluctuations (virtual processes generated by mixing LES and HES subspaces). These are automatically incorporated in the incoherent part of the self-energy (in contrast to coherent quasiparticle part) when its full dependence on the frequency is included [as in the dynamical mean-field theory (DMFT) and its extensions: DCA, cDMFT [3] [26]]. As we have shown in **[p5, p6]**, high-energy quantum fluctuations can be also directly accounted for in the Gutzwiller wave function by means of variational canonical transformation (method that we named Gutzwiller approximation + Schrieffer-Wolff transformation, GA + SWT). This is an alternative approach to that offered by the VMC method, where the Jastrow correlator emulates the appearance of doublon-holon pairs [4] created by high-energy quantum fluctuations [27].

Similar type of transformation applied to the Anderson lattice model in the limit of the infinite U leads to a low-energy Kondo lattice model,

$$H_{KLM} = \sum_{\mathbf{k},\sigma}\epsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + J_K\sum_{\mathbf{i}}S_{\mathbf{i}}\cdot s_{\mathbf{i}} \tag{15}$$

where spins of the states forming the uncorrelated band at each node interact with a single spin of a localized electron in the f orbital. This interaction is called Kondo interaction.

A completely new challenge for numerical methods is a description of the evolution of the system of correlated fermions in response to the non-equilibrium change of microscopic parameters such as strength of interactions. In this case, methods computationally accessible for equilibrium problems, often allow to simulate only relatively short system's evolution times. This turned out to be a problem for the analysis of non-equilibrium properties of systems realizing Mott insulator state. Namely, a numerically exact description of the Mott insulator at equilibrium is offered by DMFT applied to the Hubbard model on an infinitely coordinated Bethe lattice. Extension of the method to the non-equilibrium situation, due to increasing numerical complexity, allows for a description of an excited, closed system only on short time scales [14]. For this reason, there is a great need

[3] DCA - dynamical cluster approximation, cDMFT - cellular dynamical mean-field theory

[4] A doublon is simply a double occupancy on a node, while a holon is lack of occupancy on a node. The doublon-holon pair occurs when an electron from a single occupied node jumps to the other already single occupied node.

for methods with lower computing power requirements, in order to capture much longer evolution times. One of such methods was developed in a series of two papers **[p5, p6]** which are part of the my *scientific achievement*. Namely, we proposed to combine the Gutzwiller wave function describing the quasiparticle properties of the system with the variational canonical transformation that takes into account high-energy fluctuations. On the example of the Mott's transition realized in infinite dimensional Hubbard model we have shown that the method compares very well to the exact in considered limit results **[p5]**. On the other hand, the method extended to non-equilibrium situations allowed us to study the system on virtually unlimited time scales **[p6]**.

4.3.4 Detailed description of the results obtained in works [p1-p7]

This chapter discusses in detail the results obtained in the works **[p1-p7]**. The description of each work is supplemented with a box with a short list of the most important results. Additionally, at the end of each description, there is information about my individual contribution to the creation of a given work, as well as about the conference activity related to the given work, if any.

[p1] Pressure-induced transitions between ferromagnetic and antiferromagnetic phases in *d*-electron metallic magnetic compounds

- I proposed a microscopic mechanism for phase transitions between itinerant ferromagnetism (FM) and antiferromagnetism (AFM) in *d*-electron metallic magnetic compounds.
- I demonstrated that with increasing pressure both transition sequences, FM/AFM or AFM/FM, can be realized in *d*-electron metallic magnetic compounds. The potential achievability of a particular transition depends in particular on the principal quantum number of the *d* shell and the oxidation state.
- The mechanism provided consistent interpretation to the recent observation of FM/AFM transition in $LaCrGe_3$ [3, 28]

Itinerant magnetism in elements, such as ferromagnetism in iron, is fairly well theoretically described. On the other hand, itinerant ferromagnetism in a wide range of compounds such as $ZrZn_2$, UGe_2, MnSi czy $LaCrGe_3$, still challenges theory [29]. The key feature of these systems is the observation, while lowering the temperature and increasing the applied pressure, of the change in the nature of the magnetic transition from continuous to discontinuous (e.g. $ZrZn_2$, UGe_2, MnSi [29]) or a transition to a spatially modulated phase (e.g. $LaCrGe_3$ [3, 28], CeRuPO [30]). For the first group of compounds, experiments with the magnetic field have shown that the boundaries of ferromagnetic and paramagnetic phases form a characteristic structure of the so-called *tricritical wings* [29] (Fig.2). For the second group of ferromagnetic compounds, for which a transition to the antiferromagnetic phase is observed, the appearance of *tricritical wings* is no longer typical. For that reason phase diagram of $LaCrGe_3$ [3, 28] (Fig.2), where spatially modulated phase appears between *wings* is exceptional.

From a theoretical point of view, itinerant magnetism in models of correlated fermions is usually quite well described already at the level of the mean field approximation. This approximation, however, breaks down near the quantum phase transition, where the quantum fluctuations in the order parameter strongly affect the properties of the system. In this case, with the help come theories based on Stratonovich-Hubbard transformation. It has been shown that taking into account quantum fluctuations of the order parameter in the saddle point approximation leads to disappearance of the quantum critical point in favor of the first order transition [31] (and in consequence *tricritical wings* [32]) or appearance of spatially modulated phase [31, 33]. Therefore this approach is frequently referred to as *quantum criticality avoidance theory* (QCA). It should be emphasized, however, that the QCA approach is based on the quasi-phenomenological assumption that the system, in the absence of quantum fluctuations of the order parameter, would realize a quantum critical point. The natural question arises whether, in a wide variety of ferromagnetic compounds, quantum fluctuations always determine observations such as *tricritical wings* or the appearance of a spatially modulated phase, or there is an alternative explanation that would apply to at least some of these materials.

In works [21–23] being part of my doctoral dissertation, on the example of a specific compound UGe_2, we proposed that both, the first order transition at zero temperature and *tricritical wings* can be interpreted without invoking quantum fluctuations if one takes into account the typical situation of mixing of correlated electrons with the ligand states in the vicinity of the Fermi level. In the presented story on metallic ferromagnets, there are two problems that were solved by the work **[p1]**.

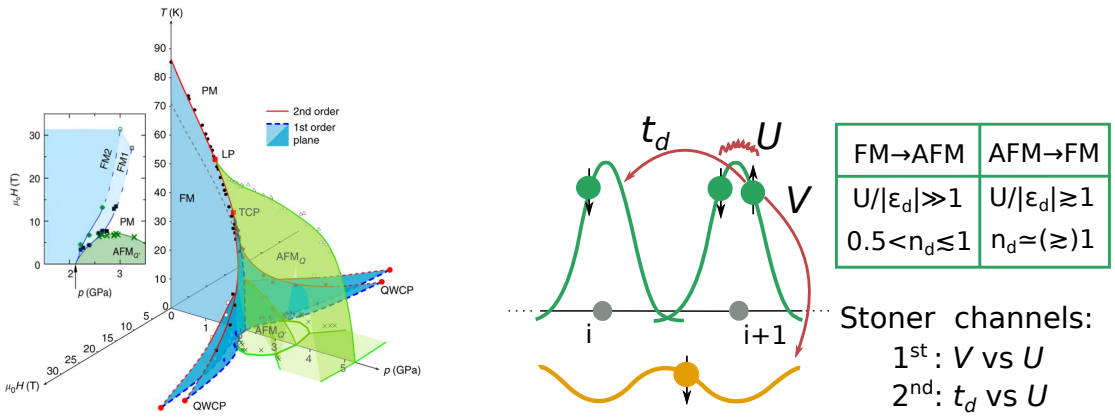

Figure 2: (Left panel) Phase diagram of metallic ferromagnet $LaCrGe_3$ with respect to pressure, temperature and magnetic field demonstrating characteristic shape of ferromagnetic/paramagnetic phase boundaries called tricritical wings, together with the inset with a cut for $T = 2K$ (borrowed from Ref. [28]). (Right panel) Schematic cartoon showing relatively well-localized d-electron states (green color) hybridizing with extended ligand states (yellow color). The figure illustrates the necessary components of the model implementing the two-channel Stoner mechanism proposed in the work **[p1]**. The table contains the necessary conditions for the parameters describing the nature of d-orbital states (U - interaction, ϵ_d - atomic level, n_d - filling) suggesting the possibility of a ferromagnetic/antiferromagnetic or antiferromagnetic/ferromagnetic transition with an increase pressure.

The first is whether the appearance of the antiferromagnetic phase with increasing pressure in the ferromagnet can also be explained without invoking quantum fluctuations. The second problem is whether only the transition FM/AFM with increasing pressure is possible in metallic magnets or the opposite, AFM/FM transition can be also expected. This point is relevant, among others, in the context of recent research with phenomenological Landau's theory analyzing mutual interplay of FM and AFM orders [34].

In the work **[p1]**, relying on the available first principles calculations for many itinerant ferromagnetic materials, I noticed that a common feature of some of them ($LaCrGe_3$, $ZrZn_2$, UIr, UGe_2) is the mixing of correlated f or d orbital states with uncorrelated ligand states in the vicinity of the Fermi level. When including nominal itinerant antiferromagnets, it turned out that the band structure of the CrAs compound has the same character. Based on this very general property, I constructed a microscopic *two-channel Stoner mechanism* that predicts phase transitions between FM and AFM in d-electron materials. Minimal description of mixing of correlated d states with uncorrelated ligand states is possible within the two-band d-p model (extended model (3))

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \epsilon^d_{\mathbf{k}} \hat{d}^\dagger_{\mathbf{k}\sigma} \hat{d}_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} \hat{n}^d_{\mathbf{i}\uparrow} \hat{n}^d_{\mathbf{i}\downarrow} + \sum_{\mathbf{k}\sigma} \epsilon^c_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \left(V_{\mathbf{k}} \hat{d}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \text{H.c.} \right). \tag{16}$$

In above, operators $\hat{d}$ and $\hat{c}$ refers to correlated d and uncorrelated ligand, orbital states respectively. The considerable electron correlations between the d states are accounted for by the Hubbard interaction with the amplitude U. It should be emphasized that the d-p Hamiltonian considered in **[p1]** is not intended to model a realistic electronic structure, but rather serves to illustrate the situation of mixing states with different degrees of correlation. For this reason, a simple model parameterization was chosen with momentum-independent hybridization $V_{\mathbf{k}} = V$ and with intra-orbital kinetic energy $\mathcal{E}_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}}$ for correlated and uncorrelated subsystems respectively with a dispersion proportional to $\xi_{\mathbf{k}} \equiv -2(\cos k_x + \cos k_y)$, i.e. $\epsilon^{\alpha\in\{c,d\}}_{\mathbf{k}} = \epsilon_\alpha + t_\alpha \xi_{\mathbf{k}}$ with arbitrarily chosen $\epsilon_c = 0$ and $t_d \ll t_c$.

Relying on model (16), I proposed that magnetism in a system of mixed correlated and uncorrelated orbitals may appear as a Stoner-type instability due to competition between the interaction energy on d-orbital states, U and two different types of kinetic energy: the one originating from

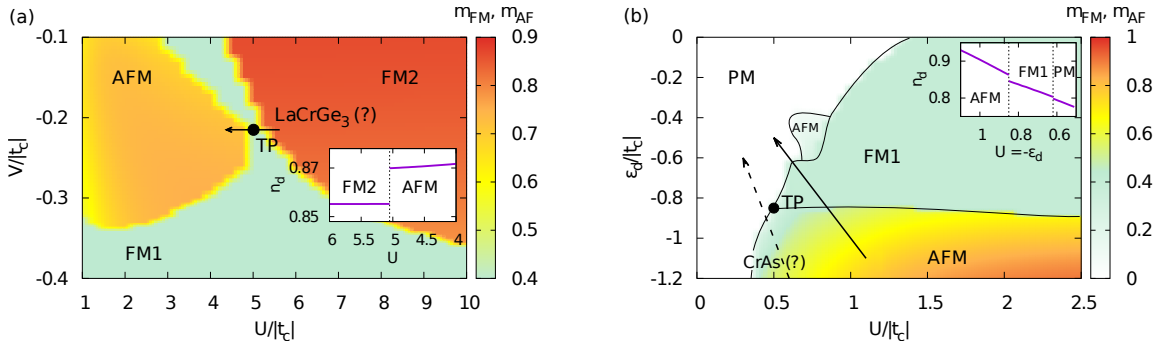

Figure 3: Magnetic phase diagrams on a plane (a)interaction - hybridization (U-V) for $\varepsilon_d = -0.95$ and (b) interaction - atomic d-orbital level (U-ε_d) for $V = -0.25$ (in both cases $n_t = 1.6$). Color scale refers to total magnetic moment (either uniform or staggered) in each phase. The arrows indicate the potential direction of the transition associated with an increase of pressure. Insets present change of d orbital filling along solid arrows through transitions (a) FM/AFM and (b) AFM/FM.

hybridization, V (first Stoner channel) and that originating from direct hopping between d orbitals, t_d (second Stoner channel) - see the right panel of Figure 2.

The seemingly subtle distinction between the two Stoner channels has considerable consequences for the realized magnetic state. In **[p1]** I solved the d-p model using the Gutzwiller approximation method, that accounts for (5) and (6) approximations on self-energy (cf. Chapter 4.3.3). These approximations are justified by choosing total filling of the bands $n_t = 1.6$, which is far from the integer value - regime allowing to ignore the incoherent effects associated with Mott or Kondo physics. The obtained results show that the type of favored magnetic order may be different because the first Stoner channel is controlled with a total filling of both bands while the second Stoner channel with filling only of d-orbital. In both cases, filling near the integer value favors the AFM phase and far from the integer value leads to FM. While the total filling of both bands is fixed in a given situation, the d-orbital filling can change drastically in response to even small changes in the microscopic parameters of the system, e.g. due to pressure. As a result, I determined the parametrization of the model (compare with the table in Fig. 2), which, according to the proposed mechanism and the physical expectation of changes in microscopic parameters with increasing pressure, predicts the existence of both FM/AFM and AFM/FM phase transitions (Fig. 3). I formulated general rules which, based on easily accessible information about the material, such as oxidation states, qualify a given compound as a potential candidate for the realization of the two-channel Stoner mechanism. A very promising result is that the compound $LaCrGe_3$, in which the FM/AFM transition has recently been observed [3, 28], has the appropriate properties for which the two-channel Stoner mechanism predicts a correct FM/AFM phase transition. In addition, for this material, the two-channel Stoner mechanism is able to theoretically describe both the appearance of two ferromagnetic phases and the triple point. On the other hand, I showed that the properties of the itinerant CrAs antiferromagnet indicate, according to the two-channel Stoner mechanism, a possible transition in this material to the ferromagnetic phase under pressure. This behavior is also suggested by recent first principle calculations [35].

From the experimental point of view, the determination of the modulation vector $\mathbf{q}$ in AFM phase emerging from FM due to pressure in $LaCrGe_3$ could suggest which mechanism is realized in this material. A short vector ($|\mathbf{q}| \sim 0$) would indicate a mechanism based on quantum fluctuations, while a long vector ($|\mathbf{q}| \sim \pi$) close to Néel order would suggest the mechanism proposed in **[p1]** and based on the characteristic band structure. Recent experimental report is not conclusive [36] as it indicates the existence of antiferromagnetically coupled ferromagnetic domains under pressure.

Individual contribution:

The work **[p1]** is entirely done by me.

Conference activity related to the results of work **[p1]***:*

- In may 2019 on conference "Quantum Ferromagnetism and Related Phenomena"(Max Planck Institute for Complex Systems, Dresden, Germany) **at the invitation of the organizers** (D. Belitz, M. Brando i A. Huxley) I gave a talk entitled "Two-channel Stoner mechanism for ferromagnetic/antiferromagnetic phase transitions in metallic magnets"

  [see `https://www.pks.mpg.de/qfm19`]

- In June 2019, on conference "Superstripes 2019" (Rome International Center for Materials Science of Superstripes, Ischia, Italy) **at the invitation of the organizer** (A. Bianconi) I gave a talk entitled "Two-channel Stoner mechanism for ferromagnetic/antiferromagnetic phase transitions in metallic magnets"

  [see `https://www.superstripes.net/superstripes-2019/invited-speakers`]

- In September 2018, on conference "From Spins to Cooper Pairs: Fundamental Aspects of Superconductivity" (Zakopane) **at the invitation of the organizer** (J. Spałek) I gave a talk entitled "Mechanisms of phase transitions between ferro- and antiferro- magnetic orderings in itinerant d and f electron materials"

  [see `http://th-www.if.uj.edu.pl/ztms/pl/conference2018/speakers.php`]

[p2] Orbital-selective, spatially modulated ferromagnetism in $La_5Co_2Ge_3$ and its evolution under pressure

- We showed that ferromagnetism in $La_5Co_2Ge_3$ derives from two different orbitals on crystallographically inequivalent cobalt atoms Co1 and Co2 .
- We showed that the difference between the magnetic moment on Co1 and Co2 atoms, initially small, increases dramatically with increasing pressure.
- We proposed a toy model which demonstrates that spatial modulation of magnetization allows for the interpretation of anomalies in resistance measurements in $La_5Co_2Ge_3$ [5].

Studies of transport and magnetization in the metallic ferromagnet $La_5Co_2Ge_3$ suggested that with increasing pressure a new magnetic state appears [5] (see Fig. 4a), possibly spatially modulated. For this reason, it has been suggested that this material may be another example of an FM/AFM transition in a metallic magnet with increasing pressure. In the context of the theories described

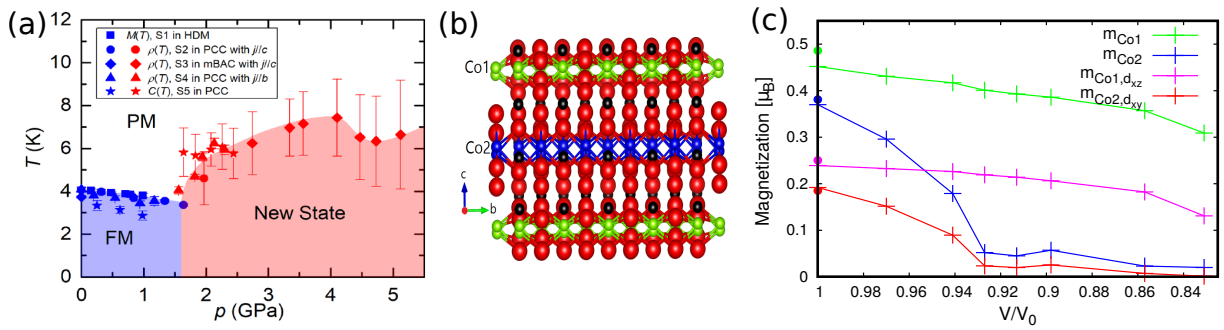

Figure 4: (a) Phase diagram of $La_5Co_2Ge_3$ from work [5]. (b) Crystal structure of $La_5Co_2Ge_3$ in c-b plane. Green spheres denote cobalt atoms Co1 i Co2, and red and black spheres La and Ge atoms. (c) Obtained in the work **[p2]** magnetic moment evolution on atoms Co1 and Co2, both total as well as this coming from leading orbitals d_{xz} on Co1 and d_{xy} on Co2.

in the previous section on the work **[p1]**, the authors of the experiment pointed to the interpretation consistent with the *quantum criticality avoidance* theory. In order to shed more light on the appearance of the new state, as well as to check the potential application of the two-channel Stoner mechanism, in **[p2]** we analyzed the band structure $La_5Co_2Ge_3$ obtained by the density functional theory (DFT) within the local density approximation (LDA).

Our analysis showed that $La_5Co_2Ge_3$ is a quasi-one-dimensional orbital-selective ferromagnet. Namely, we found that different d orbitals on crystallographically inequivalent cobalt, Co1 and Co2 atoms are responsible for ferromagnetism emergence. As a result, the magnetic moment on Co1 and Co2 atoms may be different, which, given the structural arrangement of atoms (see Fig. 4b), causes spatial modulation of the magnetization along the c axis. In our work we showed that the modulation amplitude, initially small, increases dramatically with increasing pressure (see Fig. 4c). Using a toy model, we demonstrated that such modulation can be responsible for anomaly in resistance that in experiment has been linked to the emergence of a new state.

Our interpretation suggests that the new state is the same phase as this realized at ambient pressure, except that it has a much larger difference between the magnetic moments on Co1 and Co2 atoms. This raises the question what behavior can be expected for pressures greater than the up to date measured 5GPa. Since the correlated d states do not mix with the weakly correlated s and p states around the Fermi level, it means that $La_5Co_2Ge_3$ does not meet the basic requirement by the two-channel Stoner mechanism. For this reason, for pressures greater than 5GPa if T_c would go down towards zero, effects related to quantum fluctuations can be expected.

Individual contribution:

In the work **[p2]** I proposed a research topic, I was the main author of the interpretations of the DFT results obtained by G. Cuono and C. Autieri and I was the author of the toy model describing the obtained magnetic order in explaining the appearance of anomalies in resistance. I was also the author of the text of the publication, except for chapter II of the publication on the details of DFT calculations.

Seminar activity related to the results of work **[p2]***:*

In April 2021 I was invited by professor P. Canfield to give an online seminar talk at Ames Laboratory (USA) on the results obtained in work **[p2]**.

[p3] Unconventional antiferromagnetic order ↑↓↓↑ and pressure-induced transition to ferromagnetic state in USb_2

- I proposed a microscopic model based on orbital-selectivity that interprets a non-standard antiferromagnetic order of the ↑↓↓↑ type observed in USb_2.
- I proposed explanation of the phase transition from antiferromagnetism to ferromagnetism under pressure in USb_2.
- Orbital-selectivity in USb_2 has been later observed in two experiments [37, 38].

Antiferromagnetic/ferromagnetic phase transition with increasing pressure has recently been discovered in the compound USb_2 [4] (see Fig. 5a). The magnetic properties of this material are very interesting already at ambient pressure. Namely, USb_2 realizes a non-standard antiferromagnetic order of the type ↑↓↓↑ along the crystallographic axis [001] [39] (see the schematic drawing of a magnetic unit cell in Fig. 5b).

Experimental observations in USb_2 suggest different atomic levels of crystallographically inequivalent antimony atoms [41] (Sb(I) and Sb(II) atoms - see Fig. 5b). In this manner, localized f states

at uranium atoms may hybridize with states coming from Sb(I) and Sb(II) in a different manner, i.e. yielding different quasiparticle picture in each case. In the work **[p3]** I show that both the non-standard antiferromagnetic order of the ↑↓↓↑ type and its transition under pressure to ferromagnetism can be consequence of such orbital-selectivity. Namely, additionally relying on weak Fermi surface dispersion along the z-axis [42], I proposed that the properties of USb_2 are determined by the physics of two, bipartite, two-dimensional in the x-y plane, subsystems (compare with braces in Fig. 5b). On the other hand, the coupling between subsystems is present only because they share one of the sublattices of f orbitals derived from uranium atoms. As a result, I proposed that the minimal description of each of the subsystems is offered by the Anderson lattice model (3). Due to the crystallographic equivalence of uranium atoms, the filling and the magnetic moment of f orbitals should be the same for each of the subsystems. At the same time, the lower atomic level of antimony Sb(II) [41] indicates that subsystem 2 should have a greater total filling than subsystem 1. On the other hand, the magnetic order realized in the Anderson lattice model can be very schematically presented in the phase diagram in Fig. 5c where the control parameter is the complete filling, n_t. From this perspective, consistently with the consideration of the two weakly coupled subsystems, it can be imagined that the difference in the total filling in both subsystems causes the realization of ferromagnetism in subsystem 1 and antiferromagnetism in subsystem 2 (compare with arrows in Fig. 5c). In work **[p3]** I presented the numerical results of the magnetic properties of two self-coupled Anderson lattice models solved with the Gutzwiller approximation method, confirming that the described scenario may indeed lead to a non-standard magnetic structure observed in USb_2 (cf. Fig. 5b).

The proposed interpretation of the magnetic properties of USb_2 at ambient pressure also allowed for a potential explanation of the phase transition to ferromagnetism under pressure (see Fig. 5a). The effect of pressure in the Anderson lattice is most often accounted for by an increase in hybridization and an increase in the atomic level of the f states. The change of these parameters, as shown with numerical calculations in the work **[p3]**, leads to transition in the second subsystem from

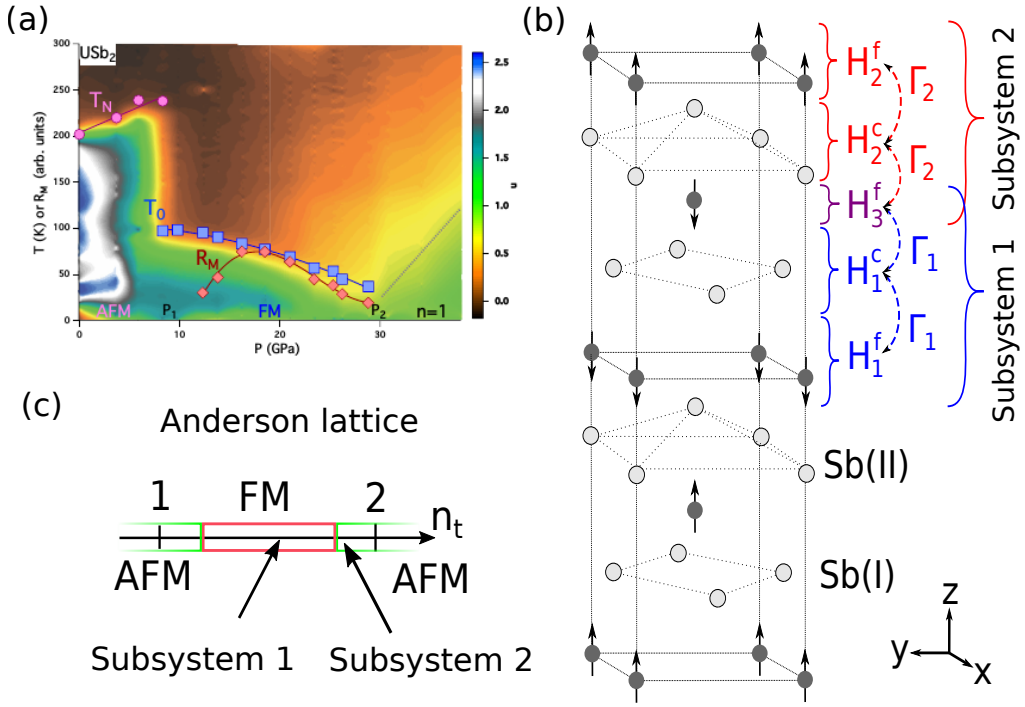

Figure 5: (a) Phase diagram of USb_2 with respect to pressure and temperature from Ref. [4]. (b) Structure of magnetic elementary cell of USb_2 together with marked subsystems. (c) Schematic, mean-field magnetic phase diagram realized by Anderson lattice model (compare with e.g. Ref. [40]).

antiferromagnetism to ferromagnetism. Therefore, as a result of increasing pressure, the proposed model predicts a transition from the antiferromagnetic state ↑↓↓↑ to the ferromagnetic state ↑↑↑↑ in accordance with the observations for USb_2 [4] (Fig. 5a).

Recent experiments [37, 38] showed the presence of two f orbital subsystems with different nature of mixing with the conduction bands, what suggests correctness of the proposed in the work **[p3]** idea of understanding the interesting properties of USb_2 based on orbital selectivity. On the other hand, other recent experiment has shown that the phase transition from antiferromagnetism to ferromagnetism in USb_2 is structural in origin [43] in contrast to the mechanism proposed in the work **[p3]**.

Individual contribution:

The work **[p3]** is entirely done by me.

Conference activity related to the results of work **[p3]***:*

- In June 2019, on conference "Superstripes 2019" (Rome International Center for Materials Science of Superstripes, Ischia, Italy) **at the invitation of the organizer** (A. Bianconi) I gave a talk entitled "Two-channel Stoner mechanism for ferromagnetic/antiferromagnetic phase transitions in metallic magnets"

  [see `https://www.superstripes.net/superstripes-2019/invited-speakers`]

- In September 2018, on conference "From Spins to Cooper Pairs: Fundamental Aspects of Superconductivity" (Zakopane) **at the invitation of the organizer** (J. Spałek) I gave a talk entitled "Mechanisms of phase transitions between ferro- and antiferro- magnetic orderings in itinerant d and f electron materials"

  [see `http://th-www.if.uj.edu.pl/ztms/pl/conference2018/speakers.php`]

[p4] Phases in topological Kondo insulators incorporating non-local effects of correlations

- We analyzed the influence of non-local correlation effects on the state of topological Kondo insulator: the obtained phase diagram encompasses transitions between phases of different topology as well as between insulator and metal.
- Non-local correlation effects are responsible for the appearance of an indirect gap in the topological Kondo insulator with non-dispersive f states.

Since the discovery of the quantum Hall effect [44] and other topological phenomena, it has become clear that it is necessary to extend the phase transition analysis apparatus to the concept of topological order. In this context, one of the widely described systems are topological insulators [1]. These are systems in which the sample volume is an insulator (it has a band gap), while at the edges there are states whose existence is guaranteed by the band structure topology. Non-trivial topology in materials is usually associated with the presence of relativistic effects, such as a strong spin-orbit coupling.

One of the most interesting materials, whose potentially topological properties have electrified the community of condensed matter physics, is SmB_6. This compound is one of the first known Kondo insulators - semiconductors with a narrow gap resulting from the hybridization of localized highly correlated f orbital states with the weakly correlated band states [45]. The physics behind this class of materials is extremely rich, and despite over 50 years of research history, it is still actual today. The state of the topological Kondo insulator, potentially realized by SmB_6, has been

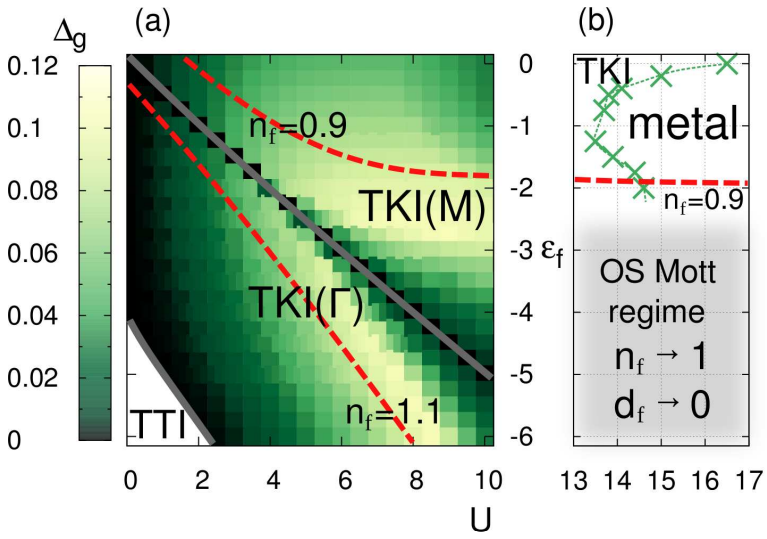

Figure 6: (a,b) Phase diagram of tALM model (17) on an interaction U - atomic f-level ϵ_f plane with a color scale in (a) denoting size of an indirect gap in unit of direct conduction states hopping. Diagram encompasses two topological Kondo insulator (TKI) phases, trivial insulator phase and metal phase. The region in (b) where the f occupancy locks at $n_f = 1$ with negligible fluctuations, $d_f \to 0$, is denoted as an orbital selective (OS) Mott regime.

proposed relatively recently [46]. This state occurs in the presence of a strong spin-orbit coupling leading to inversion of bands with opposite parity. However, as we noted in the work **[p4]**, there is a reasoning loophole when considering SmB_6 as potential topological Kondo insulator. Due to significant spatial separation of Sm atoms, the direct hopping between adjacent f orbitals is zero. On the other hand, the hybridization, due to the imposed symmetries, disappears at the time reversal invariant momenta. These two properties, when the interaction is neglected, regardless of the other parameters of the band structure or the number of bands taken into account, leads to a zero indirect gap. To open an indirect gap, the most common practice is the not rationalized assumption of the f state dispersion. In the work **[p4]** we showed that this commonly used assumption has a microscopic justification. Namely, we demonstrated that non-local correlation effects can generate an effective f state dispersion leading to the opening of the indirect gap.

The minimal model describing the inversion of the bands in the f-electron systems is the topological Anderson lattice model (tALM), for simplicity defined below on the square lattice

$$\mathcal{H}_{tALM} = \sum_{\mathbf{i}} \epsilon_f f^\dagger_{\mathbf{i}} f_{\mathbf{i}} + U \sum_{\mathbf{i}} n^f_{\mathbf{i}\uparrow} n^f_{\mathbf{i}\downarrow} + \sum_{\mathbf{ij}} t_{\mathbf{ij}} c^\dagger_{\mathbf{i}} c_{\mathbf{j}} + \sum_{\langle \mathbf{i},\mathbf{j}\rangle, \alpha=x,y} \left[iV(f^\dagger_{\mathbf{i}} \sigma_\alpha c_{\mathbf{j}} + c^\dagger_{\mathbf{i}} \sigma_\alpha f_{\mathbf{j}}) + \text{H.c.} \right]. \quad (17)$$

where two-component spinors, $f^\dagger_{\mathbf{i}} \equiv (f^\dagger_{\mathbf{i}\uparrow}, f^\dagger_{\mathbf{i}\downarrow})$ and $c^\dagger_{\mathbf{i}} \equiv (c^\dagger_{\mathbf{i}\uparrow}, c^\dagger_{\mathbf{i}\downarrow})$ describe localized f states and conduction states respectively, $\sigma_{(\alpha=x,y)}$ are Pauli matrices and $\langle \mathbf{i},\mathbf{j}\rangle_\alpha$ are pair of nearest neighboring lattice sites in direction $\alpha = x, y$. When neglecting interactions, the above model is identical to the one proposed by Bernevig, Hughes and Zhang for HgTe quantum wells [47]. A characteristic feature of most f-electron systems (including SmB_6) taken into account by model (17) is the lack of a direct hopping between the nearest neighbors (ϵ_f does not depend on momentum). As described in the previous paragraph, this yields a problem in describing the state of the insulator as such, i.e. indirect gap opening when inversion of bands with opposite parity occurs.

We have proposed that the effective direct hopping between f-states can be generated by non-local correlation effects manifested by the dependence of self-energy on momentum (compare with Eq. (7) in Chapter 4.3.3). To demonstrate our idea, we have generalized the DE-GWF method to systems with the spin-dependent hybridization. The obtained solution of tALM confirmed our expectations. Namely, we found a wide range of parameters in which non-local correlation effects actually lead to

the opening of the indirect gap (cf. Fig. 6a). It also turns out that the effective dispersion of f electrons induced by non-local correlation effects can also lead to the closure of the indirect gap. In that manner, we obtained an interesting result showing the existence of an insulator-metal transition induced by increasing interactions (Fig. 6b).

Individual contribution:

In work **[p4]** I generalized the DE-GWF method to the systems with spin-dependent hybridization, I did all the numerical calculations and I was the main author of the interpretation and the text of the publication.

Conference activity related to the results of work **[p4]***:*

- In June 2017, at the conference "Superstripes 2017" (Rome International Center for Materials Science of Superstripes, Ischia, Italy) **at the invitation of the organizer** (A. Bianconi) I gave the talk entitled "Topological Kondo semimetals"
  [zob. `https://www.superstripes.net/superstripes-2017/confirmed-invited-speakers?start=2`]
- In July 2016, at the conference "Condensed Matter in the City" (Royal Holloway University of London, Great Britain) I gave a talk entitled "Correlation driven failed topological Kondo insulators"
- In October 2016, at the conference "The New Generation in Strongly Correlated Electron Systems" (International Center for Theoretical Physics, Trieste, Italy) I gave a talk entitled "Many-body breakdown of the indirect gap in topological Kondo insulators"

[p5] Numerically efficient variational method for a description of Mott physics

- We developed a new many-body method that allows for a variational description of the Mott transition by minimizing the analytical functional depending only on two parameters.
- The method tested on the infinitely coordinated Bethe lattice has an accuracy comparable to the numerically exact results.

The localization of the charge degrees of freedom driven by the increasing interactions is called the Mott metal-insulator transition. This is one of the key phenomenon in the physics of strongly correlated fermion systems, among others due to a series of experiments suggesting a close relationship between Mott insulating state and the occurrence of unconventional superconductivity in the phase diagram of a wide range of compounds. However, quantitative research on the Mott transition began only with the recognition of the nontrivial limit of the infinite number of dimensions [24]. This laid the foundations for the numerically exact method in this limit - dynamical mean field theory (DMFT) [10]. The solution of the Hubbard model with DMFT allowed for a very detailed analysis of the nature of this transition. Additionally, the numerical complexity of the method allows for convenient study of many correlated problems, although strictly speaking defined only in the rather unrealistic limit of an infinite number of dimensions. Diagrammatic developments of the DMFT that can take into account non-local correlation effects strongly manifested in the 2nd and 3rd dimensions are numerically much more demanding [26]. For this reason, it is necessary to develop new numerical methods with lower numerical complexity, allowing to achieve accuracy comparable to DMFT in an infinite number of dimensions. Then, possible extensions to a finite number of dimensions can be very promising in the context of possibly low computational requirements.

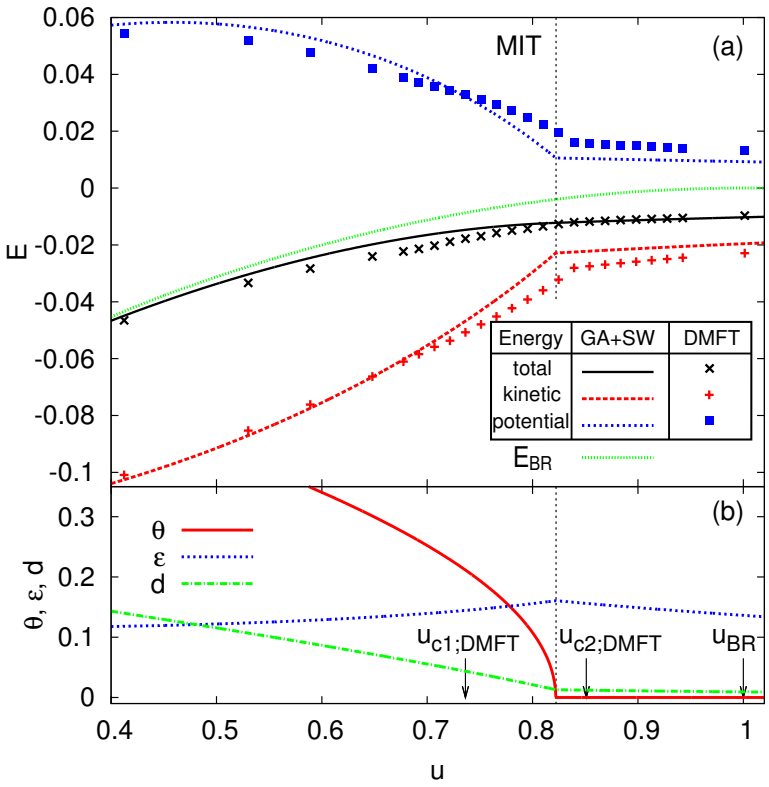

Figure 7: (a) Energy balance around the metal-Mott insulator transition in the Hubbard model on the infinitely coordinated Bethe lattice obtained using the variational wave function (18). For comparison, we also plotted the points from the numerically exact in this limit DMFT. Additionally, we also present the energy ($E_{\rm BR}$) corresponding to the Brinkman-Rice transition obtained with the bare Gutzwiller wave function [48]. (b) Variationally determined values of θ (Gutzwiller coefficient), ϵ (transformation parameter) and d (expectation value of double occupancy) around metal - Mott insulator transition. We marked the critical values of the interactions for the Brinkman-Rice transition ($u_{\rm BR}$) and those obtained from DMFT: at $u_{\rm c1;DMFT}$ both, metallic and insulating, solutions begin to coexist. Similarly as DMFT, our method predicts a non-zero value of double occupations in the Mott insulator phase. Note that u is interaction amplitude in reduced units, $u = U/8T_0$, where $T_0 = 8t/3\pi$.

In the work **[p5]** we proposed a new variational wave function which is a combination of the Gutzwiller wave function (8) and parametrized canonical transformation, often called Schrieffer-Wolff transformation (SWT),

$$|\,\Psi\rangle = \mathcal{U}(\epsilon)\,|\,\psi_G\rangle \tag{18}$$

where

$$\mathcal{U}(\epsilon) = \exp\left(\epsilon \sum_{\langle \mathbf{ij}\rangle} \left(\mathrm{P}_{20} T_{\mathbf{ij}} \mathrm{P}_{11} - \mathrm{P}_{11} T_{\mathbf{ij}} \mathrm{P}_{20}\right)\right), \tag{19}$$

$\mathrm{P}_{nm} \equiv \mathcal{P}_{\mathbf{i};n}\mathcal{P}_{\mathbf{j};m} + (1-\delta_{nm})\mathcal{P}_{\mathbf{i};m}\mathcal{P}_{\mathbf{j};n}$, δ_{nm} is Kronecker delta, and $\mathcal{P}_{\mathbf{i};n}$ is projection operator on the $\mathbf{i}$ site and configuration with $n \in \{0,1,2\}$ fermions and $T_{\mathbf{ij}} = \sum_\sigma (c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma})$. For $\epsilon = t/U$ transformation $\mathcal{U}$ applied to Hubbard model reduces to this yielding t-J model [8]. While the Gutzwiller wave function takes into account low-energy quantum fluctuations leading to a quasiparticle description, the transformation $\mathcal{U}(\epsilon)$ takes into account high-energy quantum fluctuations which give rise to the spin exchange interaction.

The strategy of calculations with the wave function (18) is such that first we determine the analytical form of the expectation value from the Hamiltonian, ignoring terms of a higher order than

the a priori selected order of expansion in ϵ. Then, the energy functional obtained in this way is minimized with respect to two variation parameters, ϵ and the Gutzwiller coefficient θ. A posteriori we check whether the equilibrium value of ϵ is small enough to justify neglecting term of higher-order in ϵ. In work **[p5]** we have shown that including terms up to the 3rd order and neglecting the higher, $\mathcal{O}(\epsilon^4)$ for an infinitely coordinated Bethe lattice leads to the desired convergence. As a result, by minimizing the simple, two-dimensional analytical functional, we described the Mott transition with an accuracy comparable to the DMFT method (cf. Fig. 7). Additionally, the developed method allows for direct insight into the effect of non-coherent high-energy quantum fluctuations even before the Mott transition in the correlated metal state.

Individual contribution:

In work **[p5]** I have done all analytical and numerical calculations and I was a main author of the result analysis and text of the publication.

Conference activity related to the results of work **[p5]***:*

- In October 2017, at the conference "FisMat" (International Center for Theoretical Physics, Trieste, Italy) I gave a talk entitled "Variational Schrieffer-Wolff transformation: Mott physics at and far from equilibrium"
- In September 2018, at the conference "The New Generation in Strongly Correlated Electron Systems" (Donostia International Physics Center, San Sebastian, Spain) I gave a talk entitled "Efficient variational approach to strongly correlated fermions at and far from equilibrium"

[p6] Coupling of charge and spin degrees of freedom in a vicinity of a dynamical Mott transition

- We developed a variational method describing unitary evolution in the non-equilibrium Hubbard model on very long time scales.
- We analyzed coupling of charge and spin degrees of freedom in the vicinity of the dynamical Mott transition.
- We suggested the existence of a dynamical crossover transition in the spin sector due to a sudden and strong change in interaction strength.

Recently, time-resolved spectroscopic experiments (including *pump and probe* measurements) have become increasingly important in investigations of correlated fermion systems [49]. Such experiments provide access to new information on the properties of correlated systems beyond the capabilities of conventional time-independent spectroscopy, e.g. on the properties of phases and phase transitions. Current non-equilibrium studies of correlated fermions mainly focus on three trends: (*i*) time-resolved spectroscopy as a selective probe for specific degrees of freedom (e.g. [50]); (*ii*) obtaining non-equilibrium selective strengthening of specific orders or the realization of long-lived metastable states (e.g. [51]); (*iii*) dynamically inducing exotic interactions within Floquet's engineering in periodically driven systems (e.g. [13]). This rapidly growing field of research, however, face critical challenges such as the development of both an apparatus for accurate experimental measurements and effective numerical methods for describing the time evolution of correlated fermions out of equilibrium.

In the context of general theoretical considerations, a very interesting problem is the study of the non-equilibrium (with time-dependent amplitude of the interaction) Hubbard model,

$$\mathcal{H}(t) = V \sum_{\langle \mathbf{ij} \rangle, \sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U(t) \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}. \tag{20}$$

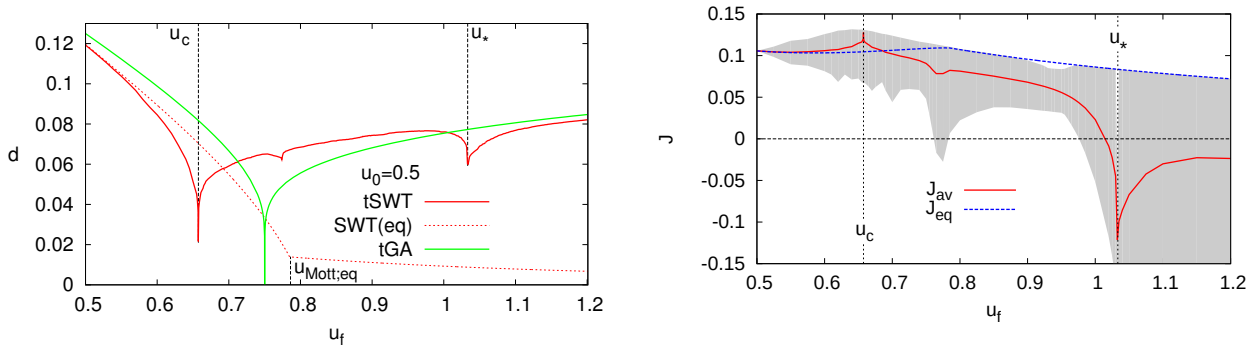

Figure 8: (Left panel) Average double occupancy after an interaction quench from $u_0 = 0.5$ to u_f for $|\Psi(t)\rangle$ (red solid line) and, for comparison, for $|\psi_G(t)\rangle$ (green solid line). We also show the equilibrium results for $|\Psi(t)\rangle$ (red dotted line). (Right panel) Time average value J_{av} of $J(t)$. In gray, we indicate the region covered by the time fluctuations of $J(t)$. For comparison we marked also equilibrium value of spin interaction J_{eq} (blue dashed line).

The initial question asked in the pioneering work [14] was about the nature of the unitary evolution in this model if the magnitude of the interaction is abruptly increased from the initial value $U_0 = 0$ to the final $U_f > 0$. Using DMFT generalized to the time domain, authors found the existence of a sharp change in characteristics (e.g. in the double occupancy) for a certain critical value of final interaction U_f. This phenomenon, despite the possibility of simulating only short evolution times, has the hallmarks of a dynamical phase transition. This observation suggests lack of thermalization in the model, because the possible temperature achieved by a rapid energy increase in the system is much higher than the critical endpoint of the Mott transition at equilibrium on the temperature vs interaction diagram [10]. However, subsequent studies with a simpler method [52] that takes into account only charge degrees of freedom, suggested that the transition is adiabatically linked to an equilibrium Mott transition [53]. This is an important argument that the found anomaly in Ref. [14] is indeed a true dynamical phase transition.

In the work **[p6]** we decided to deepen the understanding of this phenomenon. For this purpose, we extended the variational function developed in **[p5]** to the non-equilibrium situation,

$$| \Psi(t)\rangle = \mathcal{U}\Big(\epsilon(t), \epsilon^*(t)\Big) \mid \psi_G(t)\rangle \tag{21}$$

where $| \psi_G(t)\rangle$ is a time-dependent Gutzwiller wave function [52] and

$$\mathcal{U}\Big(\epsilon(t), \epsilon^*(t)\Big) = \exp\left(\sum_{\langle \mathbf{ij}\rangle}\Big(\epsilon(t)\mathrm{P}_{20}T_{\mathbf{ij}}\mathrm{P}_{11} - \epsilon^*(t)\mathrm{P}_{11}T_{\mathbf{ij}}\mathrm{P}_{20}\Big)\right). \tag{22}$$

The dynamics of the model is determined by the saddle point of the action

$$S = \int dt\, \langle \Psi(t) \mid i\frac{d}{dt} - \mathcal{H}(t) \mid \Psi(t)\rangle. \tag{23}$$

Here, the variational principle extended to the time domain yields that we find the variational wave function to be as close as possible to the true solution at each moment of time. Consequently, the Euler-Lagrange equations for the variational parameters ϵ and those defining the Gutzwiller wave function should be solved.

The developed method, thanks to the relatively low numerical complexity, allowed us to study the unitary evolution after a rapid change in the interaction in the Hubbard model on a practically arbitrarily long time scale, with transparent incorporation of the dynamics of both charge (controlled by the dynamics of Gutzwiller coefficients) and spin (controlled by the dynamics of ϵ) degrees of

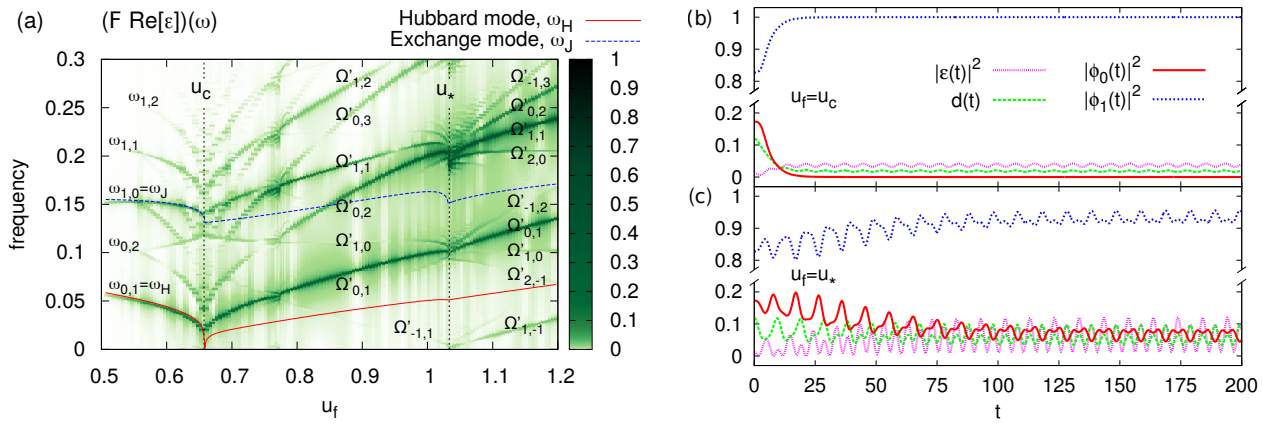

Figure 9: (a) The spectrum of the real part of a parameter ϵ with respect to final interaction u_f. The found modes have the following structure, $\omega_{n,k} = n\omega_J + k\omega_H$ and $\Omega'_{n,k} = n(\omega_J - \omega_H) + 2k\omega_H$. Evolution of Gutzwiller variational parameters $\phi_{\{1,0\}}(t)$, parameter $\epsilon(t)$ and double occupancy $d(t)$ for (b) dynamical Mott transition at $u_f = u_c$ and (c) dynamical crossover transition at $u_f = u_*$.

freedom. Similarly as time-dependent DMFT, for a certain critical final value of the interaction (U_c), our method captured a dynamical Mott transition where the system very quickly relaxes to a metastable state characterized by a residual average double occupancy (see the red solid line on the left panel in Fig. 8). Here we use reduced units, i.e. $u = U/8T_0$ and $\tau = V/8T_0$, where $T_0 = 8V/3\pi$. Our method additionally allowed for the analysis of the value of the spin exchange interaction, the mean value of which is presented in the right panel in Fig. 8. Exactly for the value of the final interaction $u_f = u_c$ the oscillations completely disappear and the value of the spin interaction is $J_c = 4\tau^2/u_c$. This is a surprising result as the Mott insulator at equilibrium has the same functional form depending on the value of the interaction U. The obtained result indicates that the metastable state achieved after fast relaxation for the final value of the interaction u_c has hallmarks of an equilibrium Mott insulator state, which, however, is achievable for a lower value of interactions.

Quite unexpectedly, for very high values of the final interaction, in the vicinity of u_* (cf. left panel Fig. 8), we obtained the characteristics of the average double occupancy very similar to this near dynamical Mott transition. The plot of average value of the spin exchange interaction in the right panel in Fig. 8, shows that for interaction slightly smaller than u_* there is an abrupt change of the J_{av} sign from antiferromagnetic to ferromagnetic, suggesting a strong relationship between the transition and the spin degrees of freedom. In order to investigate the nature of the dynamical transition at u_*, we performed a Fourier analysis of the dynamics of the ϵ parameter (see Fig. 9a). For a dynamical Mott transition at u_c most mods become soft, signaling a true phase transition character. It turns out that the transition at u_* is also accompanied by a soft mod. In addition, the dynamics of the variational parameters and double fillings are characterized with a similar relaxation for both the dynamical Mott transition (see Fig. 9b) and the u_* transition (see Fig. 9c). Despite these similarities, careful analysis of the mod structure showed that the anomaly at u_* is caused by the intersection of two different mods, $\Omega'_{-1,1}$ and $\Omega'_{1,-1}$ (Fig. 9a) at zero frequency. For this reason, the anomaly in the postquench dynamics for $u_f = u_*$ has been characterized as a dynamic crossover transition associated with a sharp change in the value and sign of the spin exchange interaction.

Individual contribution:

In work **[p6]** I have done all analytical and numerical calculations and I was a main author of the result analysis and text of the publication.

Conference activity related to the results of work **[p6]***:*

- In September 2019, at the conference "45 Zjazd Fizyków Polskich" in Kraków, Poland **at the**

invitation of the organizer (J. Spałek) I gave a talk entitled "Correlated fermions out-of-equilibrium".

- In October 2017, at the conference "FisMat" (International Center for Theoretical Physics, Trieste, Italy) I gave a talk entitled "Variational Schrieffer-Wolff transformation: Mott physics at and far from equilibrium"
- In September 2018, at the conference "The New Generation in Strongly Correlated Electron Systems" (Donostia International Physics Center, San Sebastian, Spain) I gave a talk entitled "Efficient variational approach to strongly correlated fermions at and far from equilibrium"

[p7] Explanation of a resonant energy absorption by a periodically driven Mott insulator

- We found that periodic modulation of the interaction amplitude in the Mott insulator couples the Hubbard bands in a similar fashion as the classical field with transverse and longitudinal components couples to a two-level atom.
- Relying on the analysis of the Hubbard dimer we proposed detailed multi-photon interpretation of found resonances in a driven Mott insulator.

Most of the non-equilibrium problems in systems with modulated microscopic parameters require complex numerical calculations to accurately trace characteristics such as a total energy. The problem is somewhat simplified when the system is periodically driven. In these cases, a perturbative approach based on the Floquet theory becomes helpful. Namely, for periodically modulated systems, the inevitable heating is prevented on a relatively long time scale, where the system is described by analytically determined time-independent effective model [16, 17]. The correctness of such description was confirmed in experiments on cold atomic gases in optical lattices [12, 54]. However, there are

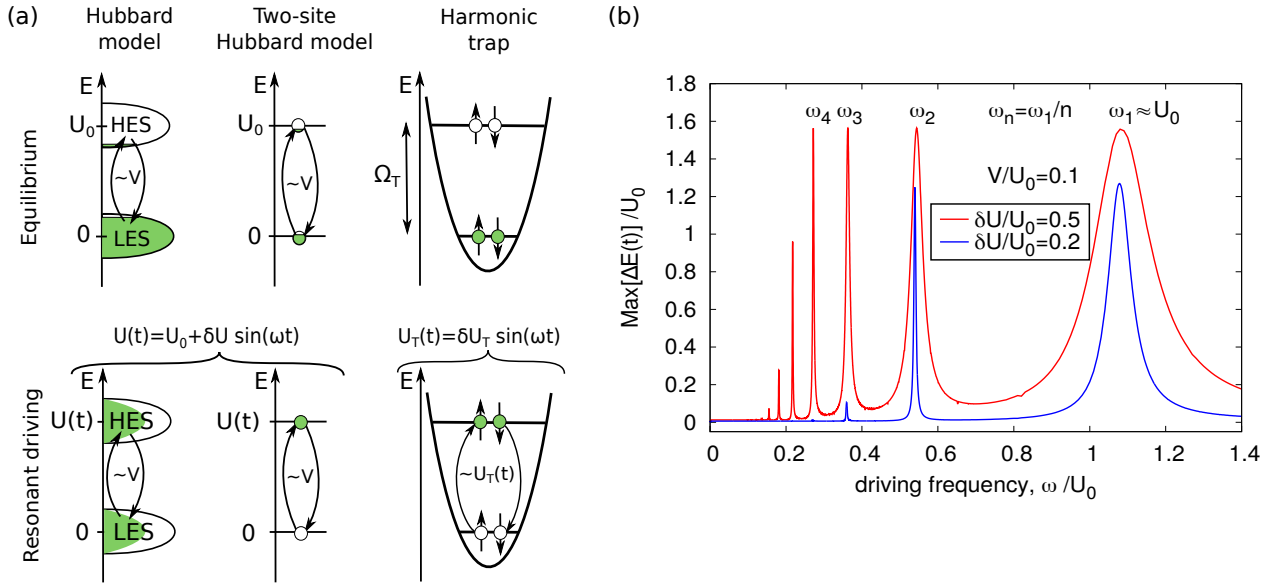

Figure 10: (a) Schematic visualization of the energy scales in the Hubbard model, the two-site Hubbard model and the two-level harmonic trap. (b) Maximum energy absorbed by the Hubbard dimer at time $tU_0 < 500$ with respect to the modulation frequency of the interaction ω for $V/U_0 = 0.1$ and two selected values of modulation amplitude $\delta U/U_0 = \{0.5, 0.2\}$.

some characteristic modulation frequencies for which energy is rapidly absorbed and the perturbative approach based on Floquet theory breaks down.

In the work [15] it has been found that the non-equilibrium Hubbard model (cf. (20)) with a periodically modulated interaction value, $U(t) = U_0 + \delta U \sin \omega t$, exhibits a resonant energy absorption for modulation frequencies approximately being submultiples of the average interaction amplitude, $\omega_R \simeq U_0/n$ where $n \in \mathbb{Z}$. However, in the work [15], there is missing detailed understanding of microscopic mechanism leading to observed in simulation phenomenon. In order to provide better understanding, in the work **[p7]** we investigated in detail resonant energy absorption in the Mott insulator.

With the help of equilibrium perturbation theory with respect to the small parameter V/U_0, we obtained the following model in a high-energy (with double occupations) and low-energy (without double occupations) subspace,

$$\mathcal{H} = \begin{pmatrix} \frac{V^2}{U_0}\big(1 - \frac{\delta U \sin \omega t}{U_0}\big) \sum\limits_{\langle \mathbf{ij} \rangle} \mathbb{J}^H_{\mathbf{ij}} & \frac{V \delta U}{U_0} \sin \omega t \sum\limits_{\langle \mathbf{ij} \rangle} \tilde{T}_{\mathbf{ij}} \\ \frac{V \delta U}{U_0} \sin \omega t \sum\limits_{\langle \mathbf{ij} \rangle} \tilde{T}^\dagger_{\mathbf{ij}} & \frac{V^2}{U_0}\big(\frac{\delta U \sin \omega t}{U_0} - 1\big) \sum\limits_{\langle \mathbf{ij} \rangle} \mathbb{J}^L_{\mathbf{ij}} \end{pmatrix}, \tag{24}$$

where $\mathbb{J}^L_{\mathbf{ij}} \equiv \mathrm{P}_{11}\, T^2_{\mathbf{ij}}\, \mathrm{P}_{11} \simeq -4\mathbf{S_i}\cdot\mathbf{S_j}$ and $\mathbb{J}^H_{\mathbf{ij}} \equiv \mathrm{P}_{20}\, T^2_{\mathbf{ij}}\, \mathrm{P}_{20}$. Superscript L and H refers to low energy and high energy subspaces respectively. The resulting structure of the derived model in these subspaces suggests that modulation of the interaction couples the Hubbard bands, just like the classical electric field with a transverse and longitudinal components, couples to a two-level atom (cf. Fig. 10a). The latter situation is well known in quantum optics and is described by the Rabi model,

$$H_R = \frac{1}{2}\big(\Omega_0 + \Omega_z \sin \omega t\big)\ \sigma_z + \Omega_x \sin \omega t\ \sigma_x, \tag{25}$$

where $\sigma_{x,y,z}$ are Pauli matrices, Ω_0 is the energy difference between the levels of the atom, and Ω_x and Ω_z are the transverse and longitudinal components of the classical field, respectively. Additionally, in the work [**p7**] we demonstrated the equivalence between the Rabi model and the considered nonequilibrium Hubbard model on two sites with the following parametrization $\Omega_0 = -\sqrt{U_0^2 + 16V^2}$, $\Omega_z = \frac{\delta U U_0}{\Omega_0}$, $\Omega_x = -\frac{2\delta U V}{\Omega_0}$. Similarity between a non-equilibrium Mott insulator and a two-level atom coupled to a classical field, is further confirmed by the fact that driven Hubbard dimer is equivalent to Rabi model, and yields virtually the same resonant behavior for frequencies $\omega_R \simeq U_0/n$ where $n \in \mathbb{Z}$ (cf. Fig. 10b) as it is the case for driven Mott insulator [15]. In order to further interpret resonances in Mott insulator next we focus on the analysis of the driven Hubbard dimer (provided in the supplement to the work **[p7]**) within the popular Rotating Wave Approximation (RWA) method.

The RWA approximation for the Rabi model with only a transverse field predicts the resonant behavior when the frequency ω is synchronized with Ω_0 which leads to filling of the high energy level (HEL) according to the probability

$$P_{HEL}(t) = \sin^2(\Omega_R t/2) \tag{26}$$

where $\Omega_R = \Omega_x$ is the Rabi frequency. For strong field $\Omega_x/\Omega_0 > 1$, solution of the model is expected to yield, elusive in RWA, multi-photon resonances at $\omega^{(p)} = \Omega_0/(2p+1)$, where $p \in \{1, 2, 3, ...\}$. However, when $\Omega_x \ll \Omega_0$ as it is the case for the Hubbard dimer, only single-photon ($p = 0$) resonance is manifested on the time scale corresponding to simulation from the work [15].

On the other hand, the existence of a sizable longitudinal field component leads to new multi-photon resonances with the structure $\omega = \Omega_0/(1+k)$, where again $k \in \{1, 2, 3, ...\}$ [55, 56]. The notation $1{+}k$ means that the multi-photon resonances have a single-photon character in the transverse field and k-photon character in the longitudinal field. The large value of the longitudinal field component in the Hubbard dimer $\Omega_0 < \Omega_z \ll \Omega_x$ suggests its key role in the formation of the resonances shown in Fig. 10b. In RWA approximation, the Rabi frequency for one photon from the transverse field and k-photons from the longitudinal field has the form,

$$\Omega_R = |\Omega_x J_k(\Omega_z(k+1)/\Omega_0)| \tag{27}$$

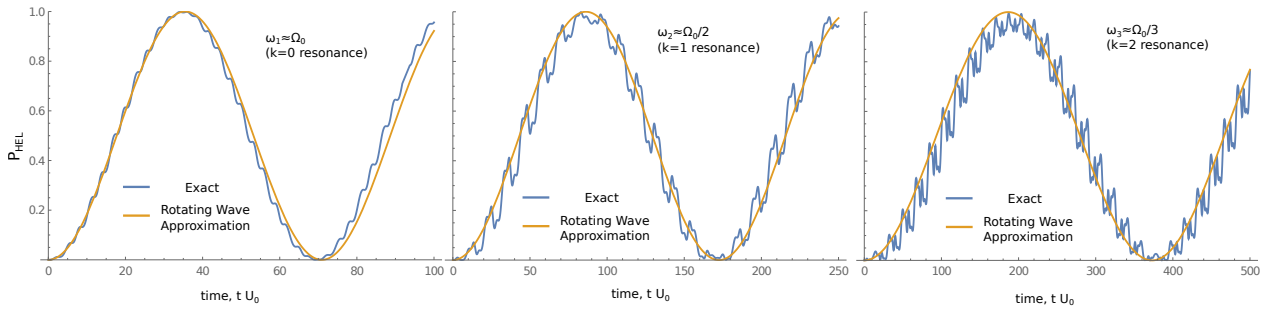

Figure 11: Numerically exact and approximate (obtained with RWA) time evolution of the probability of filling HEL in the Hubbard dimer.

where J_k is Bessel function of k-order. In Figure 11 we showed an excellent agreement of the P_{HEL} probability resulting from the aforementioned specific multi-photon nature of the resonances (seen in Figure 10b) and the exact numerical solution for three consecutive resonances. Our full analysis of the problem is a solid base under the interpretation that the periodically modulated interaction for the Mott insulator couples the Hubbard bands like a classical field with a transverse and longitudinal component couples the levels of the atom.

Thanks to a thorough understanding of the nature of resonant energy absorption in the Hubbard model, co-author of the publication, Dr. Marcin Płodzień proposed a different system of correlated fermions in which the same physics can be observed. Namely, he proposed that ultra-cold fermions confined in a one-dimensional harmonic trap, driven by periodically-modulated contact interaction, also exhibit multi-photon absorption with the same structure (Fig. 10a), proved in a numerical simulation.

Individual contribution:

The work **[p7]** is clearly divided into two parts: (*i*) considerations on the Mott insulator, Hubbard dimer and the multiphoton nature of the resonances observed in these systems and (*ii*) simulation of several fermions in a harmonic trap. In this perspective, I am the author of the part (*i*) on the Mott insulator and Hubbard dimer. The idea of the research hypothesis is the result of a joint discussion. I was also the main author of the text of the publication with the exception of the section on several fermions in a harmonic trap.

Conference activity related to the results of work **[p7]***:*

In September 2019, at the conference "45 Zjazd Fizyków Polskich" in Kraków, Poland **at the invitation of the organizer** (J. Spałek) I gave a talk entitled "Correlated fermions out-of-equilibrium".

4.3.5 Summary

In the series of works **[p1-p7]** constituting the scientific achievement, I considered the equilibrium and non-equilibrium properties of the systems of correlated fermions. Particular emphasis has been put on investigations of equilibrium phases with broken symmetry and transitions between them **[p1-p5]** as well as non-equilibrium phenomena leading to sharp changes in the nature of the system evolution, such as dynamic phase transitions, crossover transitions or multi-photon resonances **[p6-p7]**. In part of works, the key achievement was the development of a new numerical method for the investigations of a particular phases and phase transitions **[p4-p6]**. On the other hand, in other works I focused rather on an in-depth analysis of the microscopic mechanisms leading to: broken symmetry states such as magnetism and superconductivity **[p1-p3]** or resonant energy absorption in a periodically driven Mott insulator **[p7]**.

The presented theoretical research may contribute to a better understanding of the properties of very specific experimentally studied materials. Here, my greatest achievements are: providing interpretation **[p1]** for ferromagnetic-antiferromagnetic transition observed in $LaCrGe_3$ [3, 28], the discovery of the source of spatial modulation of magnetization in $La_5Co_2Ge_3$ **[p2]**, proposing the orbital selectivity of f-electrons in USb_2 **[p3]** later observed in two experiments [37, 38] as well as explaining the opening of the band gap in SmB_6 if it realizes topological Kondo insulator state **[p4]**.

4.3.6 Bibliography

[p1] **M. M. Wysokiński**, Scientific Reports **9**, 19461 (2019), *Mechanism for transitions between ferromagnetic and antiferromagnetic orders in d-electron metallic magnets*

[p2] G. Cuono, C. Autieri, **M. M. Wysokiński**, Physical Review B **104**, 024428 (2021), *Spatially modulated orbital-selective ferromagnetism in $La_5Co_2Ge_3$*

[p3] **M. M. Wysokiński**, Physical Review B: Rapid Communication **97**, 041107 (2018), *Microscopic mechanism for the unusual antiferromagnetic order and the pressure-induced transition to ferromagnetism in USb_2*

[p4] **M. M. Wysokiński**, M. Fabrizio, Physical Review B: Rapid Communication **94**, 121102 (2016), *Many-body breakdown of indirect gap in topological Kondo insulators*

[p5] **M. M. Wysokiński**, M. Fabrizio, Physical Review B: Rapid Communication **95**, 161106 (2017), *Mott physics beyond the Brinkman-Rice scenario*

[p6] **M. M. Wysokiński**, M. Fabrizio, Physical Review B: Rapid Communication **96**, 201115 (2017), *Interplay of charge and spin dynamics after an interaction quench in the Hubbard model*

[p7] M. Płodzień, **M. M. Wysokiński**, Physical Review B: Rapid Communication **100**, 041116 (2019), *Rabi-resonant behavior of periodically-driven correlated fermion systems*

References

[1] M. Z. Hasan and C. L. Kane, "Colloquium: Topological insulators," Rev. Mod. Phys. **82**, 3045–3067 (2010).

[2] Markus Heyl, "Dynamical quantum phase transitions: a review," Reports on Progress in Physics **81**, 054001 (2018).

[3] V. Taufour, U. S. Kaluarachchi, R. Khasanov, M. C. Nguyen, Z. Guguchia, P. K. Biswas, P. Bonfà, R. De Renzi, X. Lin, S. K. Kim, E. D. Mun, H. Kim, Y. Furukawa, C.-Z. Wang, K.-M. Ho, S. L. Bud'ko, and P. C. Canfield, "Ferromagnetic quantum critical point avoided by the appearance of another magnetic phase in $LaCrGe_3$ under pressure," Phys. Rev. Lett. **117**, 037207 (2016).

[4] J. R. Jeffries, R. L. Stillwell, S. T. Weir, Y. K. Vohra, and N. P. Butch, "Emergent ferromagnetism and t-linear scattering in USb_2 at high pressure," Phys. Rev. B **93**, 184406 (2016).

[5] Li Xiang, Elena Gati, Sergey L. Bud'ko, Scott M. Saunders, and Paul C. Canfield, "Avoided ferromagnetic quantum critical point in pressurized $La_5Co_2Ge_3$," Phys. Rev. B **103**, 054419 (2021).

[6] J. P. F. LeBlanc, Andrey E. Antipov, Federico Becca, Ireneusz W. Bulik, Garnet Kin-Lic Chan, Chia-Min Chung, Youjin Deng, Michel Ferrero, Thomas M. Henderson, Carlos A. Jiménez-Hoyos, E. Kozik, Xuan-Wen Liu, Andrew J. Millis, N. V. Prokof'ev, Mingpu Qin, Gustavo E. Scuseria, Hao Shi, B. V. Svistunov, Luca F. Tocchio, I. S. Tupitsyn, Steven R. White, Shiwei Zhang, Bo-Xiao Zheng, Zhenyue Zhu, and Emanuel Gull (Simons Collaboration on the Many-Electron Problem), "Solutions of the two-dimensional Hubbard model: Benchmarks and results from a wide range of numerical algorithms," Phys. Rev. X **5**, 041041 (2015).

[7] Hideo Aoki, Naoto Tsuji, Martin Eckstein, Marcus Kollar, Takashi Oka, and Philipp Werner, "Nonequilibrium dynamical mean-field theory and its applications," Rev. Mod. Phys. **86**, 779–837 (2014).

[8] K. A. Chao, J. Spałek, and A. M. Oleś, "Kinetic exchange interaction in a narrow s-band," J. Phys. C **10**, L271 (1977).

[9] G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, "Electronic structure calculations with dynamical mean-field theory," Rev. Mod. Phys. **78**, 865–951 (2006).

[10] Antoine Georges, Gabriel Kotliar, Werner Krauth, and Marcelo J. Rozenberg, "Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions," Rev. Mod. Phys. **68**, 13–125 (1996).

[11] G. Sordi, P. Sémon, K. Haule, and A.-M. S. Tremblay, "Strong coupling superconductivity, pseudogap, and Mott transition," Phys. Rev. Lett. **108**, 216401 (2012).

[12] Michael Messer, Kilian Sandholzer, Frederik Görg, Joaquín Minguzzi, Rémi Desbuquois, and Tilman Esslinger, "Floquet dynamics in driven Fermi-Hubbard systems," Phys. Rev. Lett. **121**, 233603 (2018).

[13] Frederik Görg, Kilian Sandholzer, Joaquín Minguzzi, Remi Desbuquois, Michael Messer, and Tilman Esslinger, "Realization of density-dependent Peierls phases to engineer quantized gauge fields coupled to ultracold matter," Nature **15**, 1161 (2019).

[14] Martin Eckstein, Marcus Kollar, and Philipp Werner, "Interaction quench in the Hubbard model: Relaxation of the spectral function and the optical conductivity," Phys. Rev. B **81**, 115131 (2010).

[15] Francesco Peronaci, Marco Schiró, and Olivier Parcollet, "Resonant thermalization of periodically driven strongly correlated electrons," Phys. Rev. Lett. **120**, 197601 (2018).

[16] Dmitry Abanin, Wojciech De Roeck, Wen Wei Ho, and François Huveneers, "A rigorous theory of many-body prethermalization for periodically driven and closed quantum systems," Communications in Mathematical Physics **354**, 809–827 (2017).

[17] Marin Bukov, Luca D'Alessio, and Anatoli Polkovnikov, "Universal high-frequency behavior of periodically driven systems: from dynamical stabilization to Floquet engineering," Advances in Physics **64**, 139–226 (2015).

[18] M. M. Wysokiński, J. Kaczmarczyk, and J. Spałek, "Gutzwiller wave-function solution for Anderson lattice model: Emerging universal regimes of heavy quasiparticle states," Phys. Rev. B **92**, 125135 (2015).

[19] Marcin M. Wysokiński and Michele Fabrizio, "Many-body breakdown of indirect gap in topological Kondo insulators," Phys. Rev. B **94**, 121102 (2016).

[20] M. M. Wysokiński, Jan Kaczmarczyk, and J. Spałek, "Correlation-driven d-wave superconductivity in Anderson lattice model: Two gaps," Phys. Rev. B **94**, 024517 (2016).

[21] M. M. Wysokiński, M. Abram, and J. Spałek, "Ferromagnetism in UGe_2: A microscopic model," Phys. Rev. B **90**, 081114(R) (2014).

[22] M. M. Wysokiński, M. Abram, and J. Spałek, "Criticalities in the itinerant ferromagnet UGe_2," Phys. Rev. B **91**, 081108(R) (2015).

[23] M. Abram, M. M. Wysokiński, and J. Spałek, "Tricritical wings in UGe_2: A microscopic interpretation," J. Mag. Mag. Mat. **400**, 27 – 30 (2016).

[24] Walter Metzner and Dieter Vollhardt, "Correlated lattice fermions in $d = \infty$ dimensions," Phys. Rev. Lett. **62**, 324–327 (1989).

[25] J. Bünemann, T. Schickling, and F. Gebhard, "Evaluation techniques for Gutzwiller wave functions in finite dimensions," Eur. Phys. Lett. **98**, 27006 (2012).

[26] Thomas Maier, Mark Jarrell, Thomas Pruschke, and Matthias H. Hettler, "Quantum cluster theories," Rev. Mod. Phys. **77**, 1027–1080 (2005).

[27] Manuela Capello, Federico Becca, Michele Fabrizio, Sandro Sorella, and Erio Tosatti, "Variational description of Mott insulators," Phys. Rev. Lett. **94**, 026406 (2005).

[28] U. S. Kaluarachchi, S. L. Bud'ko, P. C. Canfield, and V. Taufour, "Tricritical wings and modulated magnetic phases in $LaCrGe_3$ under pressure," Nat. Comm. **8**, 546 (2017).

[29] M. Brando, D. Belitz, F. M. Grosche, and T. R. Kirkpatrick, "Metallic quantum ferromagnets," Rev. Mod. Phys. **88**, 025006 (2016).

[30] E. Lengyel, M. E. Macovei, A. Jesche, C. Krellner, C. Geibel, and M. Nicklas, "Avoided ferromagnetic quantum critical point in CeRuPO," Phys. Rev. B **91**, 035130 (2015).

[31] D. Belitz, T. R. Kirkpatrick, and T. Vojta, "Nonanalytic behavior of the spin susceptibility in clean Fermi systems," Phys. Rev. B **55**, 9452–9462 (1997).

[32] D. Belitz, T. R. Kirkpatrick, and Jörg Rollbühler, "Tricritical behavior in itinerant quantum ferromagnets," Phys. Rev. Lett. **94**, 247205 (2005).

[33] U. Karahasanovic, F. Krüger, and A. G. Green, "Quantum order-by-disorder driven phase reconstruction in the vicinity of ferromagnetic quantum critical points," Phys. Rev. B **85**, 165111 (2012).

[34] D. Belitz and T. R. Kirkpatrick, "Quantum triple point and quantum critical end points in metallic magnets," Phys. Rev. Lett. **119**, 267202 (2017).

[35] Carmine Autieri and Canio Noce, "First principles study of structural, magnetic and electronic properties of CrAs," Philosophical Magazine **97**, 3276–3295 (2017).

[36] Elena Gati, John M. Wilde, Rustem Khasanov, Li Xiang, Sachith Dissanayake, Ritu Gupta, Masaaki Matsuda, Feng Ye, Bianca Haberl, Udhara Kaluarachchi, Robert J. McQueeney, Andreas Kreyssig, Sergey L. Bud'ko, and Paul C. Canfield, "Formation of short-range magnetic order and avoided ferromagnetic quantum criticality in pressurized $LaCrGe_3$," Phys. Rev. B **103**, 075111 (2021).

[37] Ioannis Giannakis, Justin Leshen, Mariam Kavai, Sheng Ran, Chang-Jong Kang, Shanta R. Saha, Y. Zhao, Z. Xu, J. W. Lynn, Lin Miao, L. Andrew Wray, Gabriel Kotliar, Nicholas P. Butch, and Pegor Aynajian, "Orbital-selective Kondo-lattice and enigmatic f-quasiparticles emerging from inside the antiferromagnetic phase of a heavy fermion," Science Advances **5**, 9061 (2019).

[38] Q. Y. Chen, X. B. Luo, D. H. Xie, M. L. Li, X. Y. Ji, R. Zhou, Y. B. Huang, W. Zhang, W. Feng, Y. Zhang, L. Huang, Q. Q. Hao, Q. Liu, X. G. Zhu, Y. Liu, P. Zhang, X. C. Lai, Q. Si, and S. Y. Tan, "Orbital-selective Kondo entanglement and antiferromagnetic order in USb_2," Phys. Rev. Lett. **123**, 106402 (2019).

[39] J. Leciejewicz, R. Troć, A. Murasik, and A. Zygmunt, "Neutron-diffraction study of antiferromagnetism in USb_2 and UBi_2," Phys. stat. sol. (b) **22**, 517–526 (1967).

[40] R. Doradziński and J. Spałek, "Antiferromagnetic heavy-fermion and Kondo-insulating states with compensated magnetic moments," Phys. Rev. B **56**, R14239–R14242 (1997).

[41] M.F. Beaux, T. Durakiewicz, L. Moreschini, M. Grioni, F. Offi, G. Monaco, G. Panaccione, J.J. Joyce, E.D. Bauer, J.L. Sarrao, M.T. Butterfield, and E. Guziewicz, "Electronic structure of single crystal UPd_3, UGe_2, and USb_2 from hard x-ray and angle-resolved photoelectron spectroscopy," Journal of Electron Spectroscopy and Related Phenomena **184**, 517 – 524 (2011).

[42] Dai Aoki, Piotr Wiśniewski, Kousaku Miyake, Narumi Watanabe, Yoshihiko Inada, Rikio Settai, Etsuji Yamamoto, Yoshinori Haga, and Yoshichika Onuki, "Crystal growth and cylindrical fermi surfaces of USb_2," J. Phys. Soc. Jpn. **68**, 2182–2185 (1999).

[43] Z. E. Brubaker, Y. Xiao, P. Chow, C. Kenney-Benson, J. S. Smith, H. Cynn, C. Reynolds, N. P. Butch, R. J. Zieve, and J. R. Jeffries, "Valence instability across the magnetostructural transition in USb_2," Phys. Rev. B **101**, 085123 (2020).

[44] K. v. Klitzing, G. Dorda, and M. Pepper, "New method for high-accuracy determination of the fine-structure constant based on quantized Hall resistance," Phys. Rev. Lett. **45**, 494–497 (1980).

[45] P. S. Riseborough, "Heavy fermion semiconductors," Advances in Physics **5649**, 257–320 (2000).

[46] Maxim Dzero, Kai Sun, Victor Galitski, and Piers Coleman, "Topological Kondo insulators," Phys. Rev. Lett. **104**, 106408 (2010).

[47] B. Andrei Bernevig, Taylor L. Hughes, and Shou-Cheng Zhang, "Quantum spin Hall effect and topological phase transition in HgTe quantum wells," Science **314**, 1757–1761 (2006).

[48] W. F. Brinkman and T. M. Rice, "Application of Gutzwiller's variational method to the metal-insulator transition," Phys. Rev. B **2**, 4302–4304 (1970).

[49] Claudio Giannetti, Massimo Capone, Daniele Fausti, Michele Fabrizio, Fulvio Parmigiani, and Dragan Mihailovic, "Ultrafast optical spectroscopy of strongly correlated materials and high-temperature superconductors: a non-equilibrium approach," Adv. Phys. **65**, 58–238 (2016).

[50] S. Dal Conte, L. Vidmar, D. Golež, M. Mierzejewski, G. Soavi, S. Peli, F. Banfi, G. Ferrini, R. Comin, B. M. Ludbrook, L. Chauviere, N. D. Zhigadlo, H. Eisaki, M. Greven, S. Lupi, A. Damascelli, D. Brida, M. Capone, J. Bonča, G. Cerullo, and C. Giannetti, "Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in cuprates," Nature Physics **11**, 421 (2015).

[51] M. Mitrano, A. Cantaluppi, D. Nicoletti, S. Kaiser, A. Perucchi, S. Lupi, P. Di Pietro, D. Pontiroli, M. Riccò, S. R. Clark, D. Jaksch, and A. Cavalleri, "Possible light-induced superconductivity in K3C60 at high temperature," Nature **530**, 461–464 (2016).

[52] Marco Schiró and Michele Fabrizio, "Time-dependent mean field theory for quench dynamics in correlated electron systems," Phys. Rev. Lett. **105**, 076401 (2010).

[53] Matteo Sandri, Marco Schiró, and Michele Fabrizio, "Linear ramps of interaction in the fermionic Hubbard model," Phys. Rev. B **86**, 075122 (2012).

[54] Rémi Desbuquois, Michael Messer, Frederik Görg, Kilian Sandholzer, Gregor Jotzu, and Tilman Esslinger, "Controlling the Floquet state population and observing micromotion in a periodically driven two-body quantum system," Phys. Rev. A **96**, 053602 (2017).

[55] Jian Li, M.P. Silveri, K.S. Kumar, J.-M. Pirkkalainen, A. Vepsäläinen, W.C. Chien, J. Tuorila, M.A. Sillanpää, P.J. Hakonen, E.V. Thuneberg, and G.S. Paraoanu, "Motional averaging in a superconducting qubit," Nature Communications **4**, 1420 (2013).

[56] Yiying Yan, Zhiguo Lü, JunYan Luo, and Hang Zheng, "Effects of counter-rotating couplings of the Rabi model with frequency modulation," Phys. Rev. A **96**, 033802 (2017).

5 Presentation of significant scientific activity carried out at more than one university or scientific institution, especially at foreign institutions

- Jagiellonian University, Kraków, Poland
  - 1/10/2011 - 30/09/2015: doctoral studies under supervision of prof. Józef Spałek (secondary supervisor: dr. Jan Kaczmarczyk). During doctoral studies I was doing research on:
    a) generalizing DE-GWF method for a description of unconventional superconductivity in the Anderson lattice model
    b) ferromagnetism and critical points in UGe_2
    c) properties of liquid He^3 in magnetic field
    d) thermoelectric properties of superconducting tunel junctions, also based on graphene.
  - 1/10/2015 - 31/10/2015: postdoctoral training in the group of prof. J. Spałek. During training I was studying properties of superconducting state realized in Anderson lattice model.
- Institute of Science and Technology (IST Austria), Klosterneuburg, Austria
  - 24/11/2014 - 7/12/2014: scientific training during which together with dr. J. Kaczmarczyk we work on the formulation of the DE-GWF method for description of normal state of Anderson lattice model
  - 12/01/2015 - 24/01/2015: scientific training during which together with dr. J. Kaczmarczyk we work on the formulation of the DE-GWF method for description of superconducting state of Anderson lattice model
- International School for Advanced Studies (SISSA), Trieste, Italy
  - 1/11/2015 - 31/10/2017: realization of project *Non-equilibrium dynamics of strongly correlated fermions with the use of the Gutzwiller wave function* within MOBILNOŚĆ PLUS program in the group of prof. Michele Fabrizio. During this time, I was conducting theoretical research on:
    a) the development of the time-dependent Gutzwiller approximation in order to incorporate high-energy quantum fluctuations.
    b) the state of topological Kondo insulator
    c) the superconducting state in the Hubbard model
- International Research Center MagTop, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland
  - 1/11/2017 - present: Postdoc (adiunkt) in the group of prof. Tomasz Dietl. During employment at MagTopie I am conducting research on:
    a) topological states in topological crystalline insulator in SnTe material class.
    b) leveraging geometrical phases for the quantum computations on defects that can be characterized with effective spin 3/2 localized in semiconductor structure in the presence of QED cavity.
    c) mechanisms leading to transitions between ferromagnetism and antiferromagnetism in correlated metallic compounds
    d) nonequilibrium properties of correlated fermion systems

6 Presentation of teaching and organizational achievements as well as achievements in popularization of science

6.1 Teaching

- Institute of Physics, Polish Academy of Sciences, Warszawa, Poland
  - winter semester 2020/2021: I conducted a **monographic lecture for PhD students** in English at the Institute of Physics of the Polish Academy of Sciences (Warszawa) entitled "Condensed Matter Theory" (30h)
  - winter semester 2018/2019: I conducted a **monographic lecture for PhD students** in English at the Institute of Physics of the Polish Academy of Sciences (Warszawa) entitled "Condensed Matter Theory" (30h)
    Plan of the course may be found at [`http://www.ifpan.edu.pl/msdifpan/wyklady2018_19/Condensed_matter_theory_winter_2018-19.pdf`]
- Jagiellonian University, Kraków, Poland
  - 1-31/07/2015 - I was a tutor of a month-long summer internship for a third-year physics student
  - summer semester 2014: I was a tutor at the first physics laboratory (45h)
  - winter semester 2013/2014: I conducted exercises for the lecture "Physics" for the Geology at the Jagiellonian University (30h)
  - winter semester 2012/2013: I conducted exercises for the lecture "Physics" for the Geology at the Jagiellonian University (30h)
  - academic year 2011/2012 i 2012/2013: I co-conducted classes on behalf of the Jagiellonian University, preparing high school students for the physical Olympiad. Our pupils reached the finals and became laureates of the national Olympiad in physics and astronomy.
  - 1-31/07/2011 - I was the tutor of a month-long summer internship for a third-year physics student

6.2 Organization of conferences

- 05/01/2018 one-day long scientific conference "Symposium on the physics of Majorana bound states", Warszawa, Poland - together with prof. A. Wiśniewski I was responsible for all technicalities concerning organization of the conference.
- 22-26/09/2014 conference "From spins to Cooper pairs: New physics of the spins", Zakopane, Poland - I was a member of the local organizing committee
- 7-12/10/2013 conference "XVI Narodowej Konferencji Nadprzewodnictwa" Zakopane, Poland - I was a member of the local organizing committee

6.3 Popularization of science

- 23/10/2010 - I took part in the organization of the "Małopolskiej Nocy Naukowców", Kraków, Poland
- 14-16/05/2009 - I took part in the organization of the Science Festival in Kraków, Poland

7 Other information about professional career

7.1 A short description of the works published after obtaining PhD degree, which are not part of the scientific achievement

- **M. M. Wysokiński**, J. Kaczmarczyk, Journal of Physics: Condensed Matter **29**, 085604 (2017), *Unconventional superconductivity in generalized Hubbard model: Role of electron-hole symmetry breaking terms*

  In this work, we investigated the effect of the particle-hole symmetry-breaking charge-bond interaction on the properties of superconducting instability in the Hubbard model considered on the square lattice. The amplitude, K of this interaction, even for the nearest neighbors, is considered much smaller than amplitude U parameterizing the Hubbard interaction, and hence often neglected. However, if the amplitude U is much greater than the hopping integral to the closest neighbors, t, it is likely that the amplitude K, although small in relation to U and t, will be comparable to the hopping integral to the next nearest neighbors, t', that also breaks particle-hole symmetry. Consequently, both terms, hopping to the next nearest neighbors and the charge-bond interaction can have a significant impact on the asymmetry of the superconducting state with respect to doping.

  In our work, we investigated this problem by analyzing the properties of the superconducting state in the doped Hubbard model with the DE-GWF method, depending on the mentioned terms breaking the particle-hole symmetry on a square lattice. The obtained results showed that the effect on the asymmetry of the gap of each term separately for the investigated mechanism of superconductivity is opposite. Namely, a non-zero parameter t' leads to a larger gap for hole doping, while $K \neq 0$ leads to a larger gap for electron doping. The combined effect of both terms, however, leads to a larger gap in the hole doping region and a significant asymmetry in the function of doping. In order to further characterize the obtained superconducting state depending on the doping, we examined to what extent the analyzed d symmetry is consistent with the $d_{x^2-y^2}$ symmetry typically expected for the Hubbard model. We found that long-range superconducting correlations cause a significant deviation from the $d_{x^2-y^2}$ symmetry.

- W. Brzezicki, **M. M. Wysokiński**, T. Hyart, Physical Review B: Rapid Communication **100**, 121107 (2019), *Topological properties of multilayers and surface steps in the SnTe material class*

  In our work, we thoroughly investigated the properties of low-energy states appearing on the atomic steps on the surface of the $Sn_{1-x}Pb_xTe_{1-y}Se_y$. Using the approximate symmetries found in this structure, we constructed topological invariants such as mirror and spin Chern numbers. On their basis, we have shown that the boundary states appear on the step when the invariants are different on both sides of the step. Due to accumulation in the density of states, the system is susceptible to various types of instabilities. In our work, we considered ferromagnetism as a realistic possibility. We have shown that magnetic domain walls give rise to low energy bound states because regions with opposite magnetization are topologically different in the presence of non-symmorphic chiral and mirror symmetries. The obtained results allow for a potential explanation of the observation of the zero-voltage peak in conductivity in the considered class of materials [Mazur et al., Phys. Rev. B **100**, 041408(R) (2019)].

- **M. M. Wysokiński**, M. Płodzień, M. Trif, Physical Review B: Letter **104**, L041402 (2021), *Berry phase induced entanglement of hole-spin qubits in a microwave cavity*

  In our work, we investigated the potential of spin 3/2 holes located in semiconductor structures for fault-tolerant quantum computing. Namely, we considered two holes interacting with a common photonic field originating from the microwave cavity. The spin 3/2 hole can serve as a platform for quantum computations, with the use of both, spectrum split by a magnetic field and degenerate Kramers doublets in the presence of an electric field only. In the latter case, the

operation is performed by the non-Abelian Berry phase generated by a time-varying electric field. Although, due to the absence of magnetic field it is believed to be a very efficient and energetically undemanding method of performing quantum calculations, reading such a qubit is impossible with a traditional spectroscopic methods. In our work, we proposed a new method for a readout of the considered qubit. We have shown that in the presence of a microwave cavity, the non-Abelian Berry phase is imprinted into the photonic field through a frequency shift that depends on the initial qubit configuration, what allows for a qubit readout. In addition, we have shown that the non-Abelian Berry phases of two independently manipulated holes interact with each other through a shared photonic field, what allows them to become entangled. Owing to its geometrical structure, such a scheme is more robust against external noises than conventional hole-spin qubit implementations.

7.2 Awards, scholarships and research grants

- 2019: 3-year (2020-2022) scholarship of the Minister of Science and Higher Education in Poland for outstanding young scientists
  `https://www.gov.pl/attachment/29cf556e-78f0-452e-a624-dae2c57db3db`

- 2017: START award of the Foundation for Polish Science (FNP) for young, talented scientists in Poland
  `https://www.fnp.org.pl/laureaci-start-2017/`

- 2017: winning a grant from the National Science Center SONATINA 1; second place in the ST panel - Exact and Technical Sciences. I **resigned** from realization of the grant because for formal reasons - it could not be combined with the position of postdoc (that I got at the same time) at the International Research Center MagTop financed by the Foundation for Polish Science.

  `https://ncn.gov.pl/konkursy/wyniki/2017-08-03-sonatina1`

- 2015: winning the "MOBILNOŚĆ PLUS" grant of the Ministry of Science and Higher Education; 9th place on the ranking list covering all areas of science. As part of the grant, for two years 1/11/2015-31/10/2017 I conducted research at the International School for Advanced Studies in Trieste, Italy
  `https://www.gov.pl/documents/1068557/1069061/Laureaci_IV_edycji_Mobilno%C5%9Bci_Plus.pdf/555893c7-1ab1-f6c9-6d3a-e331500bbf7e`

- 2012: 3-year (2013-2015) scholarship "DOCTUS - Małopolska Scholarship Fund for PhD students" of the Małopolska Center of Entrepreneurship based in Kraków, Poland.

7.3 Conference and seminar talks

7.3.1 Invited talks

1. 10/05/2019 "Quantum Ferromagnetism and Related Phenomena", Max Planck Institute for Complex Systems, Dresden, Germany. At the invitation of the organizers D. Belitz, M. Brando, A. Huxley I gave a talk entitled *Two-channel Stoner mechanism for ferromagnetic/antiferromagnetic phase transitions in metallic magnets*
   `https://www.pks.mpg.de/qfm19`

2. 26/06/2019 "Superstripes 2019", Ischia, Italy. At the invitation of the organizer A. Bianconi I gave a talk entitled *Two-channel Stoner mechanism for ferromagnetic/antiferromagnetic phase transitions in metallic magnets*
   `https://www.superstripes.net/superstripes-2019/invited-speakers`

3. 17/09/2019 "45. Zjazd Fizyków Polskich", Kraków, Poland. At the invitation of the organizer prof. J. Spałek I gave a talk entitled *Correlated fermions out-of-equilibrium*
`http://www.45zfp.uj.edu.pl/#/program/ksiazka-streszczen`

4. 18/09/2018 "From Spins to Cooper Pairs: Fundamental Aspects of Superconductivity", Zakopane, Poland. At the invitation of the organizer prof. J. Spałka I gave a talk entitled *Mechanisms of phase transitions between ferro- and antiferro- magnetic orderings in itinerant d and f electron materials*
`http://th-www.if.uj.edu.pl/ztms/eng/conference2018/speakers.php`

5. 8/06/2017 "Superstripes 2017", Ischia, Italy. At the invitation of the organizer A. Bianconi I gave a talk entitled *Topological Kondo semi-metals*
`https://www.superstripes.net/superstripes-2017/confirmed-invited-speakers?start=2`

7.3.2 Talks

1. 12/12/2019 "Recent Developments in the Theory of Topological Systems", Institute of Physics UMCS, Lublin, Poland. At the conference I gave a talk entitled *Electrical control of entanglement for spin 3/2*

2. 5/09/2018 "New Generations in Strongly Correlated Electron Systems 2018", San Sebastian, Spain .At the conference I gave a talk entitled *Efficient variational approach to strongly correlated fermions at and far from equilibrium*

3. 2/10/2017 "FisMat 2017 Conference", Trieste, Italy. At the conference organized at International Center of Theoretical Physics I gave a talk entitled *Variational Schrieffer-Wolff transformation: Mott physics at and far from equilibrium*

4. 12/07/2016 "Condensed Matter in the City", London, Great Britain. At the conference organized by Royal Holloway University of London gave a talk entitled *Correlation driven failed topological Kondo insulators*

5. 29/09/2016 "New Generations in Strongly Correlated Electron Systems 2016", Trieste, Italy. At the conference I gave a talk entitled *Many-body breakdown of the indirect gap in topological Kondo insulators*

6. 7/07/2015 "20th International Conference on Magnetism", Barcelona, Spain. At the conference I gave a talk entitled *Classical and quantum criticalities in the itinerant ferromagnet UGe_2: A microscopic interpretation*

7. 25/09/2014 "From Spins to Cooper Pairs: New Physics of the Spins", Zakopane, Poland. At the conference I gave a talk entitled *Microscopic model for ferromagnetism in UGe_2*

8. 23/11/2013 "Katowicko-Krakowskie Seminarium z Fizyki Ciała Stałego", Kraków, Poland. At the conference I gave a talk entitled *Andreev processes in graphene*

9. 12/10/2013 "XVI National Conference on Superconductivity", Zakopane, Poland. At the conference I gave a talk entitled *Seebeck effect in the graphene-superconductor junction*

10. 6/10/2011 "XVI Training Course in the Physics of Strongly Correlated Systems", Vietri sul Mare, Italy. On the workshop I gave a talk entitled *Magnetization of liquid helium 3 within SGA approach to Hubbard model: Comparison with experiment*

7.3.3 Posters

1. 10/2013 "XVI National Conference on Superconductivity", Zakopane, Poland. Poster entitled *Diagrammatic expansion for the Gutzwiller wave function*

2. 09/2013 "Autumn School on Correlated Electrons: Emergent Phenomena in Correlated Matter", Jülich, Germany. Poster entitled *Diagrammatic expansion for the Gutzwiller wave function*

3. 09/2012 "Autumn School on Correlated Electrons: from Models to Materials", Jülich, Germany. Poster entitled *Thermoelectric effect in the normal conductor-superconductor junction: A BTK approach*

4. 10/2011 "XVI Training Course in the Physics of Strongly Correlated Systems", Vietri sul Mare, Italy. Poster entitled *Magnetic an thermodynamic properties of SGA mean-field approach to Hubbard model: Application to liquid helium 3*

7.3.4 Seminars

1. 26/04/2021 Ames Laboratory, USA; inviting : prof. P. Canfield; title: *Antiferromagnetic component due to orbital selective ferromagnetism in* $La_5Co_2Ge_3$ - online seminar

2. 19/10/2018 Institute of Physics, University of Warsaw, Warszawa, Poland; inviting: prof. P. Jakubczyk; title: *Numerically efficient variational methods to strongly correlated fermion systems at and out of equilibrium*

3. 21/05/2018 Institute of Physics, Jagiellonian University, Kraków, Poland; inviting: prof. J. Spałek; title: *Efficient variational approach to strongly correlated fermions at and far from equilibrium*

4. 10/01/2018 Institute of Physics, Polish Academy of Sciences, Warszawa, Poland; inviting: prof. A. Wiśniewski; title: *Theoretical understanding of itinerant ferromagnetism in d and f electron compounds.*

5. 14/12/2017 Institute of Physics, Polish Academy of Sciences, Warszawa, Poland; inviting: prof. Ł. Cywiński; title: *Efficient variational approach to strongly correlated fermions at and far from equilibrium*

6. 10/02/2017 International School for Advanced Studies (SISSA), Trieste, Italy; title: *Gutzwiller wave function based methods*

7. 28/11/2014 Institute of Science and Technology Austria; inviting: dr. J. Kaczmarczyk; title: *Magnetism of the heavy fermion compound* UGe_2 *described on the basis of the Anderson lattice model*

8. 14/10/2014 Institute of Physics, Maria Curie Skłodowska University; inviting: prof. T. Domański; title: *Microscopic mechanism for ferromagnetism in* UGe_2

9. 8/01/2014 Institute of Physics, Wrocław University of Science and Technology; inviting: prof. P. Machnikowski; *Andreev processes in the graphene based superconducting hybrid structures.*

10. 14/03/2013 Institute of Physics, University of Warsaw; inviting: prof. J. Majewski; title: *Andreev processes in graphene-superconductor hybrid structures*

(signature of the applicant)