EXMAG Report Summary
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Periodic Reporting for period 2 - EXMAG (Excitonic Magnetism in Strongly Correlated Materials)

Reporting period: 2016-09-01 to 2018-02-28

Summary of the context and overall objectives of the project

Spontaneous symmetry breaking leading to states of matter with long-range order is one of the central topics in condensed matter physics. Common types of order, such as ferro- and anti-ferromagnetic, are characterized by spin or charge densities modulated on inter-atomic scale, therefore well studied thanks to various scattering experiments. Order parameters that are not of this type are much more difficult to detect, giving rise to names such as hidden order or electronic nematicity. Their impact on transport or thermodynamic properties may, nevertheless, be substantial. In the EXMAG project we will investigate excitonic condensation in systems with strongly correlated electrons as a new mechanism leading to unconventional ordered states. The objective of the project is to characterize the physical properties of various excitonic phases and to find their realization in real materials. We will focus on intermediate coupling strength and doped systems where the interaction between the excitonic order and the charge carriers is expected to lead to new physics. In particular, we want to explore the potential of the excitonic order to induce instabilities, e.g. magnetic or superconducting, that are not present in the normal phase. We will also address the possibility of topologically non-trivial quasi-particle band-structures in the excitonic phase. Our main tool will be numerical simulations based on the dynamical mean-field theory and ab initio band-structure methods. We will pursue two main lines of research: investigation of simple models allowing access to many physical observables and studies of real materials capturing the chemical complexities at the cost of more severe approximations. Ultimately, we want to understand in detail the properties of the excitonic magnets and their potential functionalities, and to identify the main control parameters and promising materials.

Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far

We have performed extensive dynamical mean-field calculations on the two-ban Hubbard model in the parameter regime where excitonic condensation is found. We found several different excitonic phases, characterized their relationship to model parameters and developed simplified theoretical description that explains the numerical data. The most interesting results is the observation of time-reversal invariant excitonic phase with broken spin-rotation symmetry, which can be described as a state with dynamically generated spin-orbit coupling. Besides systematic model studies, we have performed model calculations tailored to explain several aspects of the physics of perovskite cobaltites.

We have performed several first-principles (density functional) calculations of cobaltite materials that lead to solutions with excitonic order. This lead us to predict existence of mobile spinful excitons in LaCoO3. Recently, this prediction was confirmed
by resonant inelastic x-ray scattering experiments in a joint work with several experimental groups. This observation, in our opinion, opens are new framework for description of this classic material.

Finally, we have worked on proposing experimental techniques for detection of excitonic condensates. We have developed a new numerical tool to calculation of core-level spectroscopies and demonstrated its capabilities by systematic comparison to available experimental data. While motivated by excitonic physics the tool has a broad range of applications. The very good quantitative agreement with high-resolution experimental data allowed us to demonstrate the sensitivity of core-level photoemission spectra to the long-range order or details of crystal structure. This opens new possibilities for these experiments, which primarily serve as local probes.

**Progress beyond the state of the art and expected potential impact (including the socio-economic impact and the wider societal implications of the project so far)**

Answering the key questions of perovskite cobaltites. In collaboration with experimentalists we will improve our observation of dispersive excitations in LaCoO3, in particular the low-energy ones that are inaccessible with the present experiment due to momentum-transfer restrictions. We have initiated studies on layered LaSrCoO4 and will provide theoretical support for interpretation of experiments. We are developing theory of angular and polarization dependence of x-ray scattering, which can be used to unambiguously identify the excitonic condensates, i.e. is sensitive to coherence between different atomic multiplets.

We will investigate the dynamical susceptibilities of the two-band Hubbard model in the normal as well as excitonic states. We plan to used the excitonic condensation as a model of a continuous phase transitions to investigate general aspects of spontaneous symmetry breaking and dynamical mean-field approximation, e.g. we want to address the question of description of Goldstone and amplitude (Higgs) modes in dynamical mean-field theory.

We will proceed with the search for excitonic magnets using density functional theory, in particular we plan to spend some time with ruthenates, which appear promising still controversial candidates.

We will further develop the tools for calculation of various core-level spectra, perform comparative studies to verify their performance and apply them to potential excitonic magnets.

We will proceed with investigation of Hubbard type models exhibiting excitonic condensation. We will focus on competition with other ordered phases, their possible coexistence and role of the lattice geometry.

**Related information**