PhD Report - Third Year

Student: Francesco Foggetti

Cycle: XXXIII

Tutor(s): Dr. Sergey Artyukhin, Prof. Alberto Diaspro

Year: 2019/2020

Contacts: francesco.foggetti@iit.it

1 Research activity

In the third year of my PhD I worked to complete the ongoing projects while also starting new projects. A paper that I begun working on in the second year has been completed and published. I also stayed at Maxim Mostovoy's group in Groningen for a period to work on anisotropic exchange interactions.

1.1 Magnetic monopoles and toroidal moments in $LuFeO_3$ and related compounds

This is a second year project that has been completed and published in the first months of this year. Detailed description is given in last year report.

1.2 Distortion induced polarization in metal-organic-perovskites

This project has been started in the previous year, and includes phenomenological and numerical simulations. I have completed the first part and the collaborators responsible for the numerical part encountered difficulties. The paper has been written and it went through minor corrections during the course of this year and it is close to completion. The project has been properly described in the last year report.

1.3 Soft magnon contributions to dielectric constant in spiral spin structures

This project started at the end of the second year and the paper is now about to be submitted.

The main focus of this project is to analyze how non-uniform spin order affects dielectric properties of materials. The analysis is focused on materials that exhibit a spiral spin order (e.g. $TbMnO_3$ and $MnWO_4$). A microscopic model describing coupled ferroelectricity and spins allowed us to compute electric and magnetic susceptibilities as well as magnetoelectric (ME) response. ME coupling due to Dzyaloshinkij-Moriya interaction and the spiral contained in the *ab* plane, result in a number of symmetry costraints on the suscepitibility tensors (either magnetic, electric or ME).

I identified an important response from chiral domain walls (DW) that are regions that separate two domains with opposite spin rotation sense. The presence of the wall turns individual sharp magnon bands into a set of broader features, introduces soft domain wall-localized excitations that couple with those in the bulk, giving new opportunities for technological applications (i.e. dielectric properties, spintronics, ME manipulation of electric properties).

1.4 Microscopic description of exchange interactions in CrI_3

I started this project in collaboration with Maxim Mostovoy's group during my research stay in Groningen. The project is underway and I am currently working on it together with a PhD student of Prof. Mostovoy's group. Promising preliminary results have already been obtained.

This project is a theoretical analysis of microscopic mechanisms that take place in 2D magnetic materials with strong spin-orbit coupling on the ligands. Chromium trialides are in fact a very interesting class of materials that have been reported to have ferromagnetic order in 2D crystals. In this project we consider CrI_3, an interesting Chromium trihalide that may also host unconventional behaviour due to the high spin orbit coupling on iodine atoms. The primary focus is on Kitaev-like interactions, that may lead to spin liquid states and other non-trivial magnetic orders.

In this work we describe CrI_3 within the Hubbard model and use perturbation theory to compute the energy correction due to hopping of electrons from metal to halide sites. Ligand field theory is used to describe all possible channels that contribute to the perturbed state, and spin-orbit coupling correction is then added.

First results give the exchange constants between Cr spins in terms of Kanamori parameters. Ising-like exchange interaction between spin components along the z direction is obtained. A symmetry analysis of the material shows that different kinds of interactions (i.e. compass and Kitaev terms) are still possible and we are currently looking for channels in the perturbation expansion that may contribute to these particular interactions.

1.5 Skyrmion signatures in the ultrafast time domain: coherent and incoherentphoto-excited spin dynamics of Néel-type skyrmion host GaV_4S_8

In this project I work to interpret the results from time-resolved magneto-optical Kerr effect experiment on a single crystal of GaV_4S_8. The material is a multiferroic semiconductor. The phase diagram in the temperature-magnetic field plane consists of ferromagnetic, cycloidal and skyrmionic phases. The experiment studied the magnetization response to a laser pulse within different magnetic phases. My work in this project is to understand the different relaxation dynamics after the photoexcitation. One important effect of the photoexcitation is to modify the ratio between exchange interactions and anisotropy, thus exciting the modes that transform the equilibrium magnetic texture to that required by the new ratio. I simulated the experiment and studied the excitations and their influence on the magnetization oscillations. Interesting results have already been obtained, and the manuscript is being submitted.

1.6 Scattering features and non reciprocal magnons in Ni_3TeO_6

Ni_3TeO_6 is an insulating material with a corundum structure and a G-type antiferromagnetic order. Strong distortions inside the material and closely placed Ni ions coordinated in face-sharing octahedrons result in unusual magnetic interactions. I used microscopic Hamiltonian and linear spin wave theory to rationalize the inelastic neutron scattering data. Simulated spectra are in good agreement with the experimental data.

1.7 The origin of Devil-staircase in $IrTe_2$

$IrTe_2$ is a transition metal dichalcogenide with a layered structure, made of triple triangular Te-Ir-Te layers. In the Ir layers, below 220 K, stripes of Ir dimers emerge in which Ir-Ir bonds shrink by about 20%. At lower temperatures, a multitude of dimerized phases with different dimer arrangements is seen. The nature of the dimerization has not been understood for a decade. My work explains how the Devil-staircase-like phase diagram emerges from the competition between energy gain on dimerization and entropy.

2 Other Information and activities

Visiting Maxim Mostovoy's group in Groningen (Jan 22nd - Feb 21st)

Conferences: Talks at APS (March, Denver) and DPG (March, Dresden) were accepted but conferences were canceled due to COVID19 emergency

Seminar: 18/10/19 "Single-Exciton Gain and Stimulated Emission Across the Infrared Optical Telecom Band from Robust Heavily-doped PbS Colloidal Quantum Dots"

Publications: F. Foggetti, S. W. Cheong, S. Artyukhin, Magnetic monopoles and toroidal moments in $LuFeO_3$ and related compounds, Phys. Rev. B 100, 180408(R) doi 0.1103/PhysRevB.100.180408