PhD Report - Second Year

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Cycle: XXXIII

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Year: 2018/2019

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1 Research activity

While the first year was dedicated mostly to courses and learning new tools, in the second year I focused on research projects while keeping on learning through schools, courses and other activities.

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

The main project I worked on during the year is related to the study of magnetic excitations and magnetic structure of hexagonal $LuFeO_3$. The whole class of hexagonal manganites and ferrites exhibits interesting features due to magnetic frustration (competing exchange interaction). Materials in this class host magnetic ions inside corner-sharing bipyramids, forming triangular layers, interspaced with layers of rare earth ions. Due to size mismatch between the bipyramids and rare earth ions, the former tilt towards the common center, thus giving rise to a tripling of the unit cell volume (trimerization).

In my work I show how magnetic monopoles and toroidal moments arise in the trimerized triangular lattice. Fig. 1 illustrates how non-zero contributions from these magnetic orders arise due to trimerization.

The possible magnetic orders in this class of materials were analyzed by simulating the spin structure of $LuFeO_3$ through a generalized Heisenberg Hamiltonian and by computing the magnetic susceptibility of the system. The susceptibility determines the magnon spectrum that characterizes all the spin excitations (magnons) induced in an inelastic neutron scattering (INS) experiment. Model parameters are tuned to reproduce experimental results. Different INS signals are obtained for various magnetic phases of the material, thus allowing for

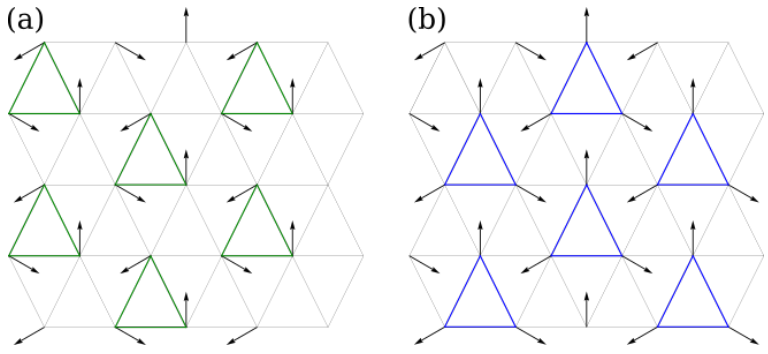

Figure 1: 2D triangular lattice with trimerization. Triangles in the lattice have shorter bonds due to trimerization so that the contributions from different triangles from toroidal moments (a) or magnetic monopoles (b) are not compensated from the rest of the lattice

the possibility to discriminate between monopolar and toroidal orders. In particular, non-reciprocal magnon propagation is predicted for toroidal ordering and is corroborated by the symmetry analysis.

We hope the work motivates experimental verification of the results, and opens the path to new spintronic devices with unidirectional magnon transmission. The paper was resubmitted after a minor revision.

1.2 Soft magnon contributions to dielectric constant in spiral spin structures

Within the second project currently underway I'm exploring a link between magnetic excitations and dielectric properties of materials. The premise to this work is that magnetic frustration (competing magnetic interactions) often results in interesting magnetic and dielectric properties not possessed by traditional magnetic materials. An interesting spin system that is also non computationally too expensive to analyze is the quasi-one dimensional spin spiral. Such a minimalist model does provide an insight on the role of chiral domain walls (DWs) in dielectric properties of spiral multiferroics such as $TbMnO_3$ and $MnWO_4$. By using analytical tools developed in my previous work I have computed magnetic excitations of the spin spiral structure, related to topological defects (chiral domain walls), at which the spin rotation axis is reversed. The analysis underway aims to understand the link between soft domain wall-localized magnons, domain wall dynamics and giant low-frequency dielectric constant, observed in $TbMnO_3$. If such a connection between magnons and dielectric properties exists we could be able to describe a new mechanism to magnetically manipulate electrical properties in materials that possess the described spiral spin configuration.

1.3 Distortion induced polarization in metal-organic-perovskites

The project is related to hybrid organic-inorganic perovskites, a promising subclass of perovskites in which organic molecules substitute inorganic ions in the usual ABO_3 structure, often leading to cheaper materials with superior performance or new functionalities. In this work the hybrid perovskite $(DMA)Fe(COOH)_3$, with dimethylammonium (DMA) being $NH_2(CH_3)_2$, is analyzed. Here a spontaneous electric polarization is observed, although its origin is debated. I explain the presence of electric polarization through Landau theory of symmetry breaking. In its high temperature phase, the material is characterized by the absence of polarization while the orientations of DMA molecules are disordered. At a lower temperature the systems undergoes a phase transition, where DMA molecules order in a toroidal pattern, and at the same time the polarization appears. By analyzing the distortions between the high and low temperature structures, I identified the the order parameters of the transition, and built a Landau-type model using the combinations of order parameters, invariant under the operations of the parent group. These invariants describe the energetics of structural modes governing the transition, and their interactions. A phase diagram of the theory is explored, and an improper ferroelectric phase, where the polarization is induced through an unharmonic interaction with the structural modulation, is found. While the phenomenological part has been completed, collaborators are working on the estimate of the model parameters of the realistic material from first-principles calculations.

2 Attended Classes

- Sistemi Mesoscopici e Nanodispositivi (Maura Sassetti, Dario Ferraro - 46 hours)

3 Other Activities

3.1 Schools

- **8th MaNEP Winter School - Symmetry and Topology: New twists in condensed matter** (Jan 13th - 18th, 2019, Saas-Fee, Switzerland)
- **TRR 80 Summer School - Functionality of Correlated Materials** (June 24 -28, Frauenchiemsee, Germany), poster presentation, lecture tutoring
- **Advanced Electronic Structure Methods in Condensed Matter Physics** (July 8th - 10th, 2019, EPFL, Lausanne, Switzerland), poster presentation

3.2 Conferences and Workshop

- **DPG Spring Meeting** (March 31 – April 5, 2019, Regensburg, Germany), oral presentation
- **2019 ETSF Young Researchers Meeting** (June 03 - 07, 2019, San Sebastián, Spain), poster presentation.

3.3 Seminars Attended

18/02/19 **A new concept of quantum measurement in Transmission Rlectron Microscopy that changes the Paradigm in both TEM Material Science and Cryomicroscopy**
Dr. Vincenzo Grillo, CNR-Nano MODENA

04/03/19 **Novel plasmonic and photonic nanomaterials for optoelectronic and bio applications**
Dr. Gleb Tselikov, Laboratory Lp3- CNRS, France

22/05/19 **Spin-orbit Mott insulators: from Kitaev model to Higgs mode**
Prof. Giniyat Khaliullin, Max Planck Institute for Solid State Research

19/06/19 **Electric-magneto optical Kerr effect in hybrid organic-inorganic perovskites**
Dr. Alessandro Stroppa, CNR-SPIN c/o Dip.to di Scienze Fisiche e Chimiche - Università degli Studi dell'Aquila

10/09/19 **Metal-Insulator-Metal Plasmonic Colour Filters for Multispectral Imaging Applications**
Nadia Pinton, Department of Engineering Science, University of Oxford, and School of Engineering Science, University of Glasgow

11/09/19 **Unravelling the origin of double peak emission of hybrid perovskites**
Dr Fabian Panzer, University of Bayreuth

4 Publications

- Magnetic monopoles and toroidal moments in $LuFeO_3$ and related compounds - **submitted**