Cargese School "COR.S.O":

New physics due to **S**pin-**O**rbit coupling in **COR**related electron systems

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1. Scientific context and challenges

In correlated quantum materials (e.g. transition-metal oxides, organic salts, manganites, high-temperature superconductors) the strong many-body electronic correlation has given birth in the last decades to new exotic phenomena (e.g. new magnetic phases, quantum criticality, colossal magneto-resistance, high superconducting critical temperatures). The hallmark of the strong correlation is the presence of unusual insulating properties (referred as "Mott physics") which cannot be understood within the framework of the standard band-theory of solids. In order to explore the effects of strong correlations, in the last decades new sophisticated experimental (ARPES, STM) and theoretical tools (like for example dynamical mean field theory) have been developed. This has advanced both our understanding of quantum materials and at the same time has produced new the state-of-the-art research techniques.

In the last few years the spin-orbit (SO) interaction has been shown to stabilize new exotic states of matter. This has triggered a burst of research activity in the area of the so called "topological insulators", which are the most striking example of this new physics. These systems are insulating in the bulk, but have interesting metallic "edge states" on their surface [1] originating from the combined effect of strong spin-orbit interaction and the electronic band structure. These edge states display remarkable properties, such as spin-current polarization, and their existence is intimately related to the insulating gap in the bulk, which makes them very stable to external perturbations. Hence the creation and manipulation of topological matter already promises to open up new paths for potential future technological developments.

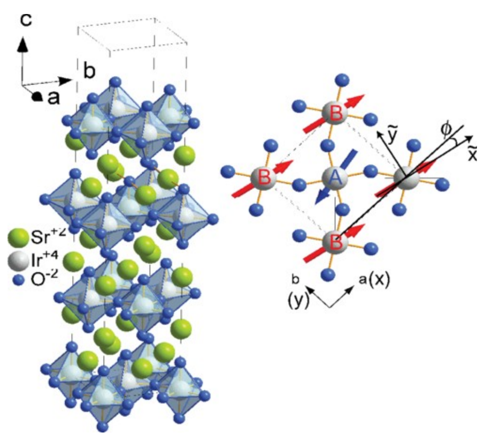

Fig. 1. Crystal and magnetic structure of the spin-orbit Mott insulator Sr_2IrO_4 with corner-sharing IrO_6 octahedra *(*figure taken from reference [2]*)*.

An interesting question that has emerged from the two scenarios above focuses on the possible interplay between the strong electronic correlation and the spin-orbit interaction. It is not generally known yet how the spin-orbit interaction may modify the properties of a correlated material and vice versa, and what kind of quantum phases may then emerge from the marriage or competition.

Several experimental and theoretical groups, coming from both the strongly-correlated and the topological-matter community, have recently addressed this question in different quantum materials with successful outcomes. At the current research stage, it has been possible to show that new paths towards new exotic quantum phenomena can indeed be traced at the intersection of the strongly-correlated and topological fields.

Iridium-oxide materials have in particular caught a lot of attention because, presenting at the same time narrow 5*d* bands (typically strongly correlated) and heavy iridium atoms (the spin-orbit interaction scales as the fourth power of the atomic number), which make them an ideal playground to test the interplay between strongly correlated and spin-orbit physics. The archetype material is Sr_2IrO_4, which has been already widely studied and which gives us a first clear example of a physical system whose ground state properties can be explained only by taking into account both SO and electronic correlations (as we will explain more in detail in the following section). Many other interesting quantum phenomena are expected to arise from the competition between SO and electronic correlations in the large family of iridium oxides, including phases with non-trivial topological properties and exotic surface states (akin to the topological insulator edge states) and quantum spin liquids or unconventional magnetically ordered states. Materials realizing a wide range of magnetic lattices of iridium ions have been synthesized, including geometrically-frustrated pyrochlore and hyperkagome, as well as lattices with local three-fold coordination such as honeycomb or hyperhoneycomb with the potential to realize frustration from bond-dependent anisotropic interactions (so called “Kiteav” spin models).

In addition to the iridium oxides, interesting SO effects have also been recently detected at the interface, or even at the surface, of other oxide-based materials, such as Ti_2O_3. Here we have another playground where SO interaction can meet electronic correlated states, and the wide tunability of these oxide heterostructures allows for the possible experimental realization of many new interesting electronic phases.

This rising field of research has generated over the last years many novel ideas [1] to explain new experimental results [3] that do not fit into the well-established paradigms of known behavior for strongly correlated materials. New doors have been constantly opening, with new theoretical ideas flourishing [4] and new experimental efforts taken to try to search for new phase [5].

We therefore think that now is an ideal time to promote a school in this subject, where many of the key recent results in the field could be presented and discussed and emerging new research paths could be highlighted to our young generation of scientists. This would be most beneficial for the community, helping the interchanging of ideas, promoting new projects and collaborations between different players of this fast growing field, helping the mutual interaction between theorists and experimentalists, coming from either the strongly correlated or the topological matter communities.

2. Topics

Spin-orbit Mott insulators – Mott insulators are the byproduct of the strong electron correlation. Many of them are based on 3d transition metals (V_2O_3, cuprates, etc.) with narrow, half-filled bands. This situation favors insulating states via the Mott electron localization mechanism. In iridium oxides (iridates) 5d orbitals are more extended spatially than the 3d ones leading to a strong reduction in the Coulomb repulsion. Furthermore taking into account the splitting of bands due to crystal field effects leads to the highest occupied electron band being far away from half-filling. Therefore taking into account both of the above effects one would expect the Mott states to be less favorable in the iridates. However, it turns out that many iridates are in fact insulators, and the currently accepted physical picture is that they realize a new form of insulator, so called *spin-orbit Mott insulator* [3], where the spin-orbit interaction is essential in splitting the electron bands and opening up an insulating gap. The layered perovskite Sr_2IrO_4 is certainly the most studied case and is becoming a reference example. There are then many questions that remain open about the properties of a SO-Mott insulator including its full spectrum of magnetic/electronic excitations which include magnons, spin-orbital excitons and interband transitions. Another key issue is the effect of charge doping. In many Mott insulators doping has been shown to bring about new exotic phases, such as high-temperature superconductivity in the layered cuprates. Theoretical ideas [4] have already been put forward that high-temperature superconductivity of a different kind to the one in the cuprates could occur in doped spin-orbit Mott insulators, such as Sr_2IrO_4. Experimentally there are only few reports [6] so far on successful doping of Sr_2IrO_4 or Ba_2IrO_4. While these two materials apparently only differ in a local tilt of the IrO_6 octahedra, it is only the Ba one that becomes metallic under pressure. Therefore the understanding of how to dope iridates and what happens in this case to SO Mott insulators is currently one of the priority challenges in the field.

Topological Kondo Insulators – Kondo insulators are a particularly simple type of a heavy fermion material where highly renormalized f-electrons, hybridized with conduction electrons, form a completely filled band of quasiparticles with excitation gaps in the millivolt range. While these materials are strongly interacting electron systems, their excitations and their ground-states can be regarded as adiabatically connected to non-interacting band-insulators. It has been recently shown that most (time-reversal invariant) band-insulators can be classified by the topological structure of their ground-state wavefunctions [7]. One of the dramatic consequences of this discovery is the existence of a new class of “topological” band-insulators in which strong SO coupling leads to a ground-state that is topologically non-trivial, giving rise to gapless surface excitations. It has been recently proposed [8] that that the "old" heavy fermion materials, longtime studied in the context of quantum criticality, represent indeed strong candidates to host new SO-driven topological phases, where the strong correlation may stabilize "heavy" Dirac quasiparticles.

Novel magnetic phases and quantum spin liquids – Complex magnetic behavior can arise when the combined effect of the strong SO interaction and crystal field effects stabilize spin-orbit entangled magnetic moments, such as J_{eff}=1/2 for Ir^{4+} ions located in the centre of IrO_6 octahedra (see Fig. 1). Such spin-orbit moments are proposed theoretically to interact via strongly-anisotropic exchange interactions where the anisotropy axis depends on the bond orientation; on certain lattices this could lead to strong frustration effects that can stabilize novel forms of cooperative magnetism, such as the Kitaev model on the honeycomb lattice proposed to have a quantum spin liquid ground state with novel excitations (Majorana fermions and fluxes)[8,9]. Much research has been devoted to exploring experimentally the honeycomb iridate Na_2IrO_3 and the various polytypes of Li_2IrO_3 with planar and three-dimensional generalizations of the honeycomb lattice as potential realizations of Kitaev physics [11]. Also the Na/Ir ordered spinel $Na_4Ir_3O_8$ has been much explored as a candidate spin liquid on a unique hyperkagome 3D frustrated lattice [12]. Its spin-liquid properties were revealed by macroscopic measurements. Recent theoretical developments strongly suggest the need to go beyond the Heisenberg model and include anisotropic interactions due to the presence of the SO coupling and possibly also multi-spin interactions due to the proximity to a metal insulator transition, both of which may stabilize spin liquid phases. The recent discovery of $Na_3Ir_3O_8$ [13], a hole doped version of the hyperkagome found to be semi-metallic, further strengthens the importance of this question.

New topological phases – Since the discovery of graphene in 2005, the study of Dirac fermions has led to many novel research areas such as topological insulators and Weyl semi-metals (the 3D version of graphene). Both of those novel electronic phases need strong SO coupling for their stability and ever since their theoretical prediction there has been an open question whether those phases could be realized in correlated quantum materials. Among iridates for example, the multilayer Sr_2IrRhO_6 was proposed to be a candidate topological insulator [14] and iridate pyrochlores were predicted to potentially realize Weyl semi-metals [15]. There is a growing interest within the community of strongly correlated materials to look for correlation-driven mechanisms that in conjunction with a topologically relevant interaction, like the SO interaction, could stabilize new topological non- trivial phases, akin to topological insulators and Weyl semi-metals in uncorrelated matter. For instance, the already mentioned Sr_2IrO_4 could have such non-trivial topological properties already [1], realizing a topological Mott insulator with gapless *spin-only* excitations on the surface.

Oxide heterostructures- Besides providing rich and interesting quantum phenomena for fundamental studies, transition-metal oxides are nowadays considered as candidates to be building blocks of functional materials for "oxitronics" (oxide-based electronics). By controlling an external parameter, such as doping, temperature or pressure, or even by modulating size and geometry, these materials display a great variety of magnetic (paramagnetic, ferro- and antiferro-magnetic) and electronic (metallic or insulating) phases [16]. Akin to silicon for conventional electronics, strontium titanate ($SrTiO_3$) is becoming more and more the reference playground material for oxitronics. At the two-dimensional interfaces formed on the surface or in heterostructures, this material displays exotic phenomena, such as metal-insulator transition, superconductivity, and/or giant magneto-resistance. More recently ARPES experiments [17] have shown the presence of important Rashba spin-orbit coupling, which could potentially explain the large splitting observed in the 5d bands. Clearly an important question is whether non-trivial topological phases could be engineered in oxide heterostructures/surfaces, as this could open up potentially new practical applications.

3. Provisional program

Structure of the school:

We propose to have 6 main lecturers to give 2-3 one-hour lectures each. The lectures will be associated with one-hour talks on more specific topics given by the invited speakers. We are right now in the process of contacting the main lectures in order to establish the principal structure of our program. In a second step we will also contact speakers. We have already invited the lecturers below, some have already confirmed their participation to the school, and others have given indication they plan to confirm soon.

Invited Lecturers

1) Silke Biermann (Ecole Polytechnique Paris), lecturer (**theory**)
Silke.Biermann@cpht.polytechnique.fr
Spin-orbit in the iridates within DFT + DMFT

2) Yong Baek Kim (University of Toronto), lecturer (**theory)**
ybkim@physics.utoronto.ca
Theoretical background and overview of novel electronic phases stabilized by the spin-orbit interaction

3) Zahid Hasan (Princeton University) (**experiments**)
mzhasan@Princeton.EDU
1. Topological phases in correlated materials and spin-orbit effects at interfaces/in heterostructures.
2. Topological Superconductivity & topological Weyl phases
3. Mott physics in the presence of strong spin-orbit interaction, Iridates and related systems

4) Hidenori Takagi* (MPI Stuttgart-University of Tokyo), lecturer (**experiments**)
h.takagi@fkf.mpg.de
Synthesis and physical properties of novel iridates and 3D Dirac materials

5) Des McMorrow (LCN London), lecturer (**experiments**)
d.mcmorrow@ucl.ac.uk
Experimental studies of novel order and dynamics stabilized by the spin-orbit interaction in 5d materials

6) Andrea Caviglia lecturer (**experiments**)
A.Caviglia@tudelft.nl
Spin-orbit-coupling phenomena in oxide interfaces

Invites Speakers

7) Krjstian Haule (Rutgers University) (**theory**)
haule@physics.rutgers.edu
Electronic structure calculations iridium pyrochlores and Ruddlessen Poppers iridates and IrTe2

8) Hae Young Kee (University of Toronto), speaker **(theory)**
hykee@physics.utoronto.ca
Topological phases and correlation effects

9) B.J. (Bumjoon) Kim (MPI Stuttgart), speaker (**experiments**)
bj.kim@fkf.mpg.de
Emergent magnetism and superconductivity in strongly spin-orbit coupled oxides

10) Piers Coleman (Rutgers), speaker (**theory**)
coleman@physics.rutgers.edu
Topological Kondo insulators

11) Andres Santander-Syro (Université Paris Sud) (**experiments**)
andres.santander-syro@u-psud.fr
Giant spin splitting of the two-dimensional electron gas at the surface of $SrTiO_3$

**to be confirmed*

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