Master 2: International Centre for Fundamental Physics

INTERNSHIP PROPOSAL

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Internship location: Ecole Polytechnique and Collège de France
Thesis possibility after internship: YES
Funding: NO (need to apply to a scholarship)

Ordered multipolar moments in correlated insulators

Strongly correlated electrons are at the origin of many important phenomena in condensed matter systems, like, for example, unconventional superconductivity, local-moment magnetism, and colossal magnetoresistance. This project is focused on a particular kind of strongly correlated materials: correlated insulators of heavy elements exhibiting unusual low-temperature ordered phases. Their (Mott) insulating behavior due to narrow bandwidths and strong onsite Coulomb repulsions of their partially filled *d* or *f* bands. Moreover, the large spin-orbit coupling in heavy (4*d* or 5*d*) transition-metal, lanthanide and actinide ions entangles their orbital and spin moments. In result, at low temperature such materials may host unusual phases due to ordering of high-rank ionic moments of the charge or magnetic density, i.e., multipole moments. While conventional magnetic orders are readily detected by magnetization measurements or neutron diffraction, multipolar orders are hard to resolve experimentally. Multipolar moments can be coupled by different types of intersite interactions - purely electronic exchange (like superexchange), coupling through the lattice (electron-lattice interaction and Jahn-Teller effect) and classical electrostatics. The rich physics of multipolar orders was first revealed in *f*-electron systems [1], more recently multipolar orders in heavy transition metal compounds excited a lot of interest [2,3]. Multiple competing order parameters and coupling mechanisms render their theoretical description challenging; predictive material-specific approaches are still lacking at present.

This project will build up on previous work [4-7] in this domain carried out by the CPHT "Correlated Materials" group and its international collaborators. It is based on first-principles methodology to evaluate superexchange interactions between multipolar moments [4]. Other type of interaction, both exchange and electron-lattice type, are planned to be evaluated for spin-orbit Mott insulators in an ab initio way. Effective many-body quantum Hamiltonians describing their low-energy physics are subsequently to be solved to obtain low-temperature ordered phases and their experimentally measurable response functions. Hence, this project aims at advancing both (1) first-principles approaches for constructing low-energy quantum Hamiltonians and (2) quantum approaches for solving these Hamiltonians. In particular, the Master project will be focused on implementing a general approach for solving low-energy Hamiltonians within a mean-field approximation. The resulting software package will be able to treat both exchange and electron-lattice coupling on the equal footing.

[1] P. Santini et al. Rev. Mod. Phys. **81**, 807 (2009).
[2] W.Witczak-Krempa et al. Annu. Rev. Condens. Matter Phys. **5**, 57 (2014).
[3] T. Takayama et al. J. Phys. Soc. Jpn. **90**, 062001 (2021).
[4] L. V. Pourovskii. Phys. Rev. B 94, 115117 (2016).
[5] L.V. Pourovskii and S. Khmelevskyi. Phys. Rev. B **99**, 094439 (2019).
[6] L. V. Pourovskii and S. Khmelevskyi. PNAS **118**, e2025317118 (2021).
[7] L. V. Pourovskii, D. Fiore Mosca, C. Franchini, Phys. Rev. Lett. **127**, 237201 (2021).

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES Soft Matter and Biological Physics: NO
Quantum Physics: YES Theoretical Physics: YES