## 2-year postdoctoral position

**Title :**   **Metal-insulator transitions in correlated systems with disorder**

**Supervisor :**   Cyril MARTINS

☎ :   05 61 55 60 45

**Email** :   cyril.martins@irsamc.ups-tlse.fr

**Laboratory :**   Laboratoire de Chimie et Physique Quantiques (LCPQ)
Université Toulouse III – Paul Sabatier, Toulouse, France

**Starting date :** October 1st, 2024

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**Project description :**

In 1958, P. W. Anderson argued that sufficiently strong randomness in the ionic potential of a crystal may induce the absence of diffusion of the charge carriers and lead to a sharp metal-insulator transition [1]. Since then, this mechanism dubbed "*Anderson localization*" has been a hot topic in condensed matter physics [2] and many statistical methods (such as the Forward Approximation (FA) [3,4]) have been developed to capture and study the Anderson transition. Recently, some studies have shed some light on the many-body localization problem at high energy in one dimension (d = 1) but the problem of interacting electrons in the presence of disorder remains a largely open problem for d > 1 [5].

Conversely, Mott physics, where Coulomb repulsion between electrons may induce an insulating state, has been firmly established, but only in periodic ionic potentials [6,7]. Key insights into the Mott metal-insulator transition came from key lattice models [8-11], and the advent of Dynamical Mean-Field Theory (DMFT), a formalism introduced in the 1990s which can be understood as a quantum many-body extension of classical mean-field approaches [12-14]. Since then, realistic DMFT calculations – when combined with density functional theory – have even emerged as a reliable and quantitative tool for correlated materials [15] but the conventional DMFT framework falls short in capturing Anderson localization and the metal-insulator transition amid interactions and disorder still remains a profound challenge [16].

And yet, any sample of a material contains impurities, vacancies, and other imperfections. What is more, most interesting phenomena in strongly correlated materials, e.g., superconductivity, various metal-insulator transitions, magnetoresistance or large thermoelectric effects, arise under chemical doping which, besides charge carriers, also introduces disorder [17].

In this project, we will devise and implement new methodologies to account for effects of disorder in strongly correlated materials by developing a new approach that combines the DMFT many-body technique with the forward approximation (FA). We will focus on the simplest model that account for the interplay between local Coulomb interaction and on-site disorder, the Anderson-Hubbard model :

$$H = \sum_{\langle ij \rangle} \sum_{\sigma} \left( -t + (\mu - \varepsilon_i)\delta_{ij} \right) c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow},$$

where $c_{i,\sigma}^{\dagger}$ and $c_{i,\sigma}$ describes respectively the creation and annihilation operator at site i with spin $\sigma = \pm 1/2$ and $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$ is the number operator at each site. In this model, $t$ is the hopping amplitude between a site i and its nearest neighbors (indexed by j), $\mu$ corresponds to the chemical potential, $U$ is the local Coulomb interaction and the on-site potentials $\varepsilon_i$ at each site i are considered as independent random variables uniformly distributed in the interval $[-W/2, W/2]$.

We will first investigate the metal-insulator phase-diagram of this Anderson-Hubbard model on a finite Cayley tree and then on several lattices in dimension d=2 and 3. Ultimately, we will apply this new approach to first-principles Hamiltonians and perform realistic calculations for correlated materials with disorder. One possible application would be to explain the metal-insulator transition in Ru/Rh-doped $Sr_2IrO_4$ as a function of doping [18].

## References :

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## Keywords :

Metal-insulator transition, Anderson localization, disordered systems, strongly correlated materials, Hubbard model, dynamical mean-field theory (DMFT).

## Profile and skills required :

- A PhD in physics (theoretical physics or condensed matter physics).
- A good background in many-body quantum physics (Green's function formalism, DMFT) or in statistical physics (Anderson localization).
- Skills in at least one programming language among Fortran, Python and or C/C++ ; some experience of working in a UNIX/Linux environment and of using supercomputers would be appreciated.
- Excellent communication skills in English.

## Funding :

## How to apply :

Applications should be submitted to Cyril MARTINS (cyril.martins@irsamc.ups-tlse.fr). They must include a curriculum vitae (including names of potential referees), a list of publication and a short statement of you research interest and how they relate to the project.