PhD project

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

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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 :

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

where $c^{\dagger}_{i,\sigma}$ and $c_{i,\sigma}$ describes respectively the creation and annihilation operator at site i with spin σ = ±1/2 and $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$ 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), μ corresponds to the chemical potential, U is the local Coulomb interaction and the on-site potentials ε_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 :

[1] P. W. Anderson, *Physical Review* **109**, 1492 (1958).
[2] E. Abrahams, *50 Years of Anderson Localization* (World Scientific, 2010).
[3] F. Pietracaprina, V. Ros, and A. Scardicchio, *Physical Review B* **93**, 054201 (2016)
[4] G. Parisi, S. Pascazio, F. Pietracaprina, V. Ros, and A. Scardicchio, *Journal of Physics A: Mathematical and Theoretical* **53**, 014003 (2019).
[5] V. Dobrosavljevic and G. Aeppli, *Metal-insulator transitions* in proc. of 2d Quantum Metamaterials: 2018 Nist Workshop (World Scientific, 2019).
[6] N.F. Mott and R. Peierls, *Proceeding of the Physical Society* **49**, 72 (1937)
[7] N. F. Mott, *Proceedings of the Physical Society.* Section A, **62**, 416 (1949).
[8] J. Hubbard, *Proceedings of the Royal Society London*, Section A **276**, 238 (1963).
[9] J. Hubbard *Proceedings of the Royal Society London*, Section A **277**, 237 (1964).
[10] J. Kanamori, *Progress of Theoretical Physics* **30**, 275 (1963).
[11] M. C. Gutzwiller, *Physical Review Letters* **10**, 159 (1963).
[12] W. Metzner and D. Vollhardt, *Physical Review Letters* **62**, 324 (1989).
[13] A. Georges and G. Kotliar, *Physical Review B* **45**, 6479 (1992).
[14] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Review of Modern Physics* **68**, 13 (1996)
[15] K. Held*, Advances in Physics* **56**, 829 (2007)
[16] V. Dobrosavljevic, N. Trivedi & J. M. Valles Jr., *Conductor-Insulator Quantum Phase Transitions*, (2012).
[17] M. Imada, A. Fujimori & Y. Tokura, *Review of Modern Physics* **70**, 1039 (1998).
[18] F. Qi, et al., *Physical Review B* **86**, 125105 (2012)

Keywords :

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

Profile and skills required :

- Master degree in theoretical physics or condensed matter physics.
- A good knowledge of basic concepts in many-body quantum physics (Green's function formalism) or in statistical physics (Anderson localization) would be greatly appreciated.
- 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 :

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How to apply :

Applications should be submitted to Cyril MARTINS (cyril.martins@irsamc.ups-tlse.fr). They must include a CV highlighting the skills required for the research project and a description of the Master's internship. Contact details of the M2 internship supervisor should be provided.