Master 2: ***International Centre for Fundamental Physics***

INTERNSHIP PROPOSAL

Laboratory name: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
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Internship location: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Campus Jussieu, Paris
Thesis possibility after internship: YES
Funding: NO

Investigating the Mott metal insulator transition with the self-consistent random phase approximation

A correct description of interacting electrons can in principle be achieved through the many-electron wave function obtained by solving the Schrödinger equation. However, for computational studies on real materials such an approach is often impractical and far too demanding. In diagrammatic many-body perturbation theory the relevant observables are calculated from the Green's function, a simpler quantity for which different levels of approximations can be built systematically. The drawback is that it remains challenging to incorporate effects of strong electronic correlation, crucial for studying phenomena mainly driven by the electron-electron interaction, such as the Mott metal-insulator transition and certain mechanisms for high-temperature superconductivity.

In this project we will evaluate the performance of new approximations based on the Green's function, starting from the so-called random phase approximation (RPA). The RPA has shown to combine high accuracy with reasonable computational cost, making it a good starting point for further refinements. We will start by looking at the hydrogen dimer, a simple system where the degree of correlation varies with the interatomic separation. Approximations will be studied self-consistently and compared to exact results. The same techniques will then be applied to study realistic antiferromagnetic insulators, such as NiO, that exhibit a Mott insulator-metal transition at finite pressure.

References: Phys. Rev. B, 98, 045117 (2018), Phys. Rev. B, 103, 075101 (2021)

Techniques/methods in use: Many-body Green's functions, Density Functional Theory, ab-initio codes (Quantum ESPRESSO, VASP)
Applicant skills: Background in solid-state physics. Interest in theory and programming. Skills in Python or Fortran are required.

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