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

INTERNSHIP PROPOSAL

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Internship location: CPHT, Ecole Polytechnique

Thesis possibility after internship: YES
Funding already obtained for a PhD: NO, will be requested via the doctoral school.

Impact of Dynamically Screened Coulomb Interaction in Correlated Electronic Systems

Materials with strong electronic Coulomb correlations are one of the most interesting subjects in modern condensed matter physics. Many of these systems are characterised by strong collective electronic fluctuations, such as plasmons, magnons, Cooper pairs, etc., that can be observed, for instance, in scattering experiments. These collective fluctuations strongly influence different electronic, magnetic, optical, and transport properties of the system.

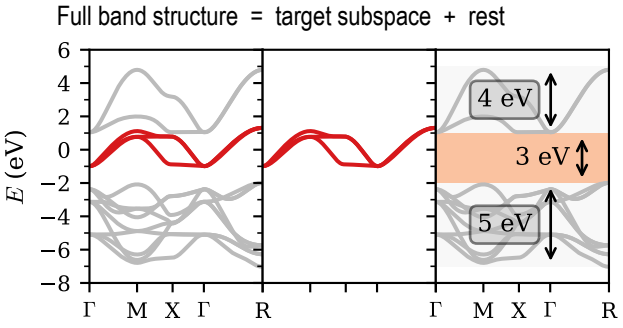

Figure 1: Downfolding of the full electronic band structure to a correlated ("red") subspace [*Phys. Rev. B* **104**, 045134 (2021)].

The theoretical description of strongly correlated materials is challenging. A "simple" analytical or perturbative treatment of such systems is not possible due to large electron-electron correlations. An accurate theoretical solution of the problem can be performed only via a complex multi-step procedure that involves a combination of advanced theoretical methods. A theoretical analysis of correlated electronic systems usually starts with calculating ground state properties on the basis of Density Functional Theory (DFT) [*Rev. Mod. Phys.* **87**, 897 (2015)]. This procedure allows one to construct realistic interacting electronic models that are further solved by quantum many-body techniques in order to account for the effect of electronic interactions in a more accurate way beyond DFT.

However, advanced many-body calculations are numerically demanding and cannot feasibly be applied to the entire electronic band structure obtained through DFT. Therefore, the many-body solution is typically computed only within a low-energy subspace of correlated orbitals near the Fermi energy. This requires downfolding the initial band structure to a target subspace of orbitals, as illustrated in Figure 1. The downfolding process specifically includes calculating the screened electronic interaction within the correlated subspace, induced by the background (or "rest") orbitals, using the constrained Random Phase Approximation (cRPA) [*Phys. Rev. B* **70**, 195104 (2004)]. Generally, the renormalized interaction from cRPA calculations is dynamic (frequency-dependent). However, due to the lack of appropriate methods for handling frequency-dependent interactions, only the static component of the interaction is employed in most many-body calculations.

The current project aims to investigate the impact of dynamical Coulomb interaction on the electronic properties of correlated systems, utilizing the recently developed D-TRILEX approach [*Phys. Rev. B* **100**, 205115 (2019); *Phys. Rev. B* **103**, 245123 (2021); *SciPost Phys.* **13**, 036 (2022)].

Methods: Quantum Monte Carlo, Exact diagonalisation, Feynman diagrams, Green's functions.

Profile and skills: Good knowledge in general solid-state physics, solid notions in quantum many-body theory, experience in numerical calculations (Python/C++) is an advantage.

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