Theory of electronic excitations: beyond the state-of-the-art

This thesis is part of a research line that has the scope to build a new theoretical approach for describing electronic excitations. The general aim is to understand and predict spectroscopic properties of a wide range of materials, including the so-called « strongly correlated » ones: for these materials, the effects of the Coulomb interaction between electrons are particularly strong, and perturbative approaches may fail to describe excitations, even qualitatively. The PhD student will combine mathematical tools and physical intuition in order to progress along some promising lines of development, in the framework of Green's functions theory. In particular, a non-perturbative approach for the calculation of many-body Green's functions has been proposed by us recently [1,2], and the PhD student will work on bringing this approach from the stage of modelling to the description of realistic systems. Combining analytical work and computer coding, he/she will test and improve the approach. According to the results, an ambitious application will be chosen, of technological and/or fundamental interest for experimentalists; such an application might for example be the calculation of electronic excitations in a nanostructure made of a transition metal oxide.

[1] Lani, Giovanna; Romaniello, Pina; Reining, Lucia, *« Approximations for many-body Green's functions: insights from the fundamental equations »*, New J. Phys. **14**, 013056 (2012)
[2] Guzzo, Matteo; Lani, Giovanna; Sottile, Francesco; Romaniello, Pina; Gatti, Matteo; Kas, J.J.; Rehr, J.J.; Silly, M.G.; Sirotti, F.; Reining, Lucia, *« Valence Electron Photoemission Spectrum of Semiconductors: Ab Initio Description of Multiple Satellites »*, Phys. Rev. Lett. **107**, 166401 (2011)

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