Green's function methods from first principles: GW, dynamical mean field theory and beyond

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Keywords: Electronic structure; electronic correlations; metal-insulator transition; Green's function; Dynamical Mean-Field Theory (DMFT); Hedin's equations and GW; constrained Random-Phase Approximation (cRPA) Transition metal oxide; f-electron systems; iron-based pnictides and chalcogenides; cuprates; iridates

Materials with partially filled d- or f- electron shells generally have a wide range of properties (magnetism, superconductivity, optics, or more exotic ones like thermo-electricity, magneto-resistance) relevant for technological applications, and yet most of these quantum phenomena remain important theoretical challenges to understand. Indeed, due to the moderated or strong electronic correlations at stake in these compounds, electrons exhibit both itinerant and localized characters and one-particle picture is no longer enough to achieve a good description of the electronic structure.

Important progress in the understanding of these compounds has been made with the application of Hedin's equations (within his most famous approximation called “GW”) [1] or the dynamical mean field theory (DMFT) [2] to the electronic structure problem. Green's function based methods are indeed able to treat the electron-electron interaction within systematic and controlled approximations, can include the effect of temperature and access excited state properties via the spectral function.

Today, methodological progresses, together with the release of open-source codes such as Triqs [3], and the improvement of the existing ones may open a new era in the field, where combining GW and DMFT into the GW+DMFT [4] method could not only overcome important limitations of each side but also become the golden standard of *ab initio* Green's function methods.

The scope of the present minicolloquium is (i) to present new methodological developments in both GW and DMFT and recent calculations combining both GW and DMFT approaches, and (ii) to illustrate cutting-edge applications to compounds such as iron-based pnictides and chalcogenides, cuprates, iridates, and f-based materials.

[1] L. Hedin, Phys. Rev. **139**, A796 (1965).
[2] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[3] O. Parcollet, et al., Computer Physics Communications **196**, 398 (2015).
[4] S. Biermann, F. Aryasetiawan, and A. Georges, Phys. Rev. Lett. **90**, 086402 (2003).