GW density matrix with ABINIT

Fabien Bruneval[1] and Marc Torrent[2]

[1] Service de Recherches de Métallurgie Physique, CEA, DEN, Université Paris-Saclay, F-91191 Gif-sur-Yvette
[2] CEA, DAM, DIF. F-91297 Arpajon cedex

The *GW* approximation is a succesful approximation to the many-body self-energy that is generally used to produce band structures and band gaps of semiconductors. It has been shown to be extremely successful in do so during the last 30 years [1].

However, the *GW* approximation can give access to other physical quantities and, most noticeably, to the density matrix. The density matrix allows one to directly calculate the expectation value of any local and non-local operator, such as the kinetic energy, the electron density, the electrostatic potential, the exchange energy, etc.

We have recently derived a simple perturbative expression [2] for the GW density matrix and we have tested it for molecular systems in the Gaussian basis code MOLGW [3]. The first results are very promising.

In this contribution we present our strategy how to generalize the expression to periodic systems and how to implement it in ABINIT.

References

[1] M. Hybertsen and S.G. Louie, Phys. Rev. B **34**, 5390 (1986).

[2] F. Bruneval, Phys. Rev. B **99**, 041118(R) (2019).

[3] F. Bruneval *et al.*, Comput. Phys. Commun. **208**, 149 (2016).