

Some theoretical and practical aspects of RPA in the context of many-body perturbation theory

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The knowledge of the electronic response function of a material to a perturbation allows one to derive spectra such as absorption or electron energy loss, and to describe correlation effects such as the screening of the hole left by the photoelectron in a photoemission experiment. In the framework of “theoretical spectroscopy”, we are interested in both situations. The Random Phase Approximation (RPA) being the most often used approximation in this context, it is of particular interest to analyze and understand its performance.

More specifically, I will discuss the RPA in the framework of the GW approximation, i.e. when it is used in order to calculate the dynamical screening of the effective Coulomb interaction W needed to build a self-energy. I will touch upon the following questions:

- Computational: where are the main bottlenecks, and can we do better?
- Performance: how far can we go with the RPA, when does it *really* fail?
- Principle: which problems are *not* the fault of RPA, but of the nature of the response function itself?

Some results are contained in [1,2].

[1] M. Gatti et al., Phys. Rev. Lett. **99**, 266402 (2007).

[2] P. Romaniello, S. Guyot, and L. Reining, J. Chem. Phys. **131**, 154111 (2009).