

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Post-GW energies from an extended Bethe-Salpeter scheme

EMANUELE MAGGIO, Univ of Vienna, GEORG KRESSE, University of Vienna
— Hedin’s breakthrough in many-body physics is a computationally manageable scheme to implicitly account for many-body effects thanks to the introduction of a self-energy, whose expression is known but in practice approximated by truncation at some order in the inter-particle interaction.

Hedin’s scheme allows the computation of quasi-particle addition and removal energies. The introduction of an added particle (or hole) to the system will trigger the formation of higher order neutral excitations (particle/hole pairs formation). The widespread GW approximation only partially accounts for these effects by replacing the bare interparticle interaction with a dressed one. Other effects are contained in the vertex function and are typically disregarded.

In the present work, we move beyond the GW level by including vertex effects in the self-energy. This is implemented by expressing the self-energy in terms of the reducible two-particle scattering amplitude. The latter is related to the kernel of the Bethe-Salpeter equation and to the corresponding polarisation propagator. The proposed implementation allows us to evaluate the quality of quasi-particle spectra for a range of realistic solids and molecular systems.

Emanuele Maggio
University of Vienna

Date submitted: 28 Jan 2016

Electronic form version 1.4