

# Ab Initio Total Energies from Many-Body Perturbation Theory

Pablo García-González, Paula Sánchez-Friera, Rex Godby  
*Department of Physics, University of York, York YO10 5DD, United Kingdom*

The exact Kohn-Sham exchange-correlation energy functional of density-functional theory is known to have certain pathological aspects that are not amenable to efficient approximation, limiting the accuracy of Kohn-Sham DFT for complex systems. These aspects of the functional include an ultra-non-local dependence on the electron density in certain situations.

These non-analyticities may be circumvented by reformulating the total energy using Green's-function many-body perturbation theory, starting from a Kohn-Sham non-interacting system as the "zeroth-order" approximation, as a practical alternative to DFT. A real-space-imaginary-time representation [1–3] offers an efficient framework for implementing a fully self-consistent GW approximation, which is a conserving approximation. We show very promising results for total energies of homogeneous and inhomogeneous systems within such an approximation [4]. We shall also demonstrate promising results using an related, very inexpensive, approach [5] which uses a very simple model self-energy within the framework of generalised Kohn-Sham theory, and costs barely more than a LDA calculation.

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