Ab Initio Total Energies from Many−Body Perturbation Theory

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

Progress has become slow in constructing ever better approximations to the exact Kohn−Sham energy functional of density−functional theory that are applicable in a wide range of situations. In my view this reflects the extreme complexity of the exact functional, including, for example, its ultra−non−local dependence on the electron density in certain situations.

These non−analyticities in the exchange−correlation energy functional 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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