THE SELF INTERACTION CORRECTION REVISITED

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The Self Interaction Correction (SIC) is a long standing problem in Density Functional Theory (DFT). It causes several major difficulties especially with the universally used simple and efficient Local Density Approximation (LDA). The standard SIC approaches lead to the introduction of orbital dependent functional which exhibit several formal and technical problems. The Optimized Effectove Potential (OEP) methods allow to deal with such difficulties but in an approximate manner. The fully time dependent cases remain especially problematic, which leads to significant difficulties for the treatment of ionization "on the fly".

We discuss an extension of time-dependent DFT including SIC. A strictly variational formulation is given taking care of the necessary constraints. A manageable and transparent propagation scheme using two sets of wavefunctions is proposed and applied to laser excitation with subsequent ionization of a dimer molecule.

We also propose a simplification of the Optimized Effective Potential (OEP) applied to the Self Interaction Correction (SIC) scheme of Density Functional Theory (DFT). The new scheme acceptably fulfills several key formal properties and turns out to be both simple and accurate. We show examples of applications on model molecules in terms of observables known to be especially sensitive to details of the SIC-OEP approach. This latter approach might be applicable to low energy phenomena.