Working equation of LR-TD-DFT First-order polarization propagator approximation

Jacob Pedersen[1] and Kurt Mikkelsen[1]

[1]University of Copenhagen

April 12, 2021

Abstract

We present the derivation of a new response method termed rst order po- larization propagator approximation. The electronic structure is given by a density functional representation. We provide a detailed derivation of the method along with explicit expressions for the relevant integrals and matrix elements.

Hosted file

`workingequations (1).pdf` available at https://authorea.com/users/407388/articles/517706-working-equation-of-lr-td-dft-first-order-polarization-propagator-approximation