Dielectric matrix formulation of correlation energies within the Random Phase Approximation: Inclusion of screened exchange effects

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Starting from the general expression of the ground state correlation energy in the adiabatic connection fluctuation dissipation theorem (ACFDT) framework, it is shown that the dielectric matrix formulation, which is usually applied to calculate the random phase approximation (RPA) correlation energy, can also be used for alternative RPA expressions including exchange effects. Within this framework we derive equations for the correlation energy within the second order screened exchange (SOSEX), an approximate time-dependent Hartree-Fock (TDHF), and second order Moller-Plesset (MP2) levels of theory. The accuracy of these approaches can be further improved by introducing the effect of the screening to obtain an approximate formulation of the Bethe-Salpeter equation for correlation energies. The proposed formalism is particularly suitable for implementation in periodic boundary condition plane-wave codes, in particular by using a compact basis set to represent dielectric matrices [1,2]. To demonstrate the accuracy of these approaches the binding curves of several diatomic molecules will be shown. [1] Y. Ping, D. Rocca, and G. Galli, Chem. Soc. Rev., 42, 2437 (2013) [2] D. Rocca, J. Chem. Phys. 140, 18A501 (2014)