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RPA Correlation Energy in ACFD Formalism with Thomas-Fermi-von Weizsäcker Approximation VIET HUY NGUYEN, STEFANO DE GIRONCOLI, Intl School for Adv Studies (SISSA), Trieste Italy — It is well known that LDA or GGAs approximations in DFT do not describe correctly systems where long range correlations are important. In the Adiabatic Connection Fluctuation-Dissipation (ACFD) formalism correlation energy can be computed accurately from Kohn-Sham and interacting linear response functions. Although computationally very demanding, this formalism has shown to describe correctly systems where standart DFT fails qualitatively by combining RPA xc-kernel with short-range local-density corrections (RPA+). On the other hand, Thomas-Fermi-von Weizsäcker approximate kinetic response function can capture reasonably well asymptotic long range interactions via van der Waals coefficients, and has the computationally desirable feature that it only involves a single auxiliary wavefunction regardless of the number of electrons in the system. Here, we show how to use this approach to calculate approximate RPA correlation energies. Numerical results for atoms show that this approach gives approximate RPA correlation energies closer to the experimental values than those obtained by full RPA and, when combined with a short-range local-density correction, it gives results at least as good as those of full RPA+. The possibility is therefore open to address large systems where correlations need to be treated beyond LDA and GGAs.

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