RPA and the Adiabatic Connection

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We have recently implemented a scheme for the accurate calculation of the adiabatic connection (AC) in density functional theory (DFT) using coupled-cluster techniques [1, 2]. We will discuss how, by utilizing the re-formulation of the random-phase approximation (RPA) correlation energy in terms of a so called ring-coupled-cluster-doubles approach [3, 4, 5], the AC for both the full RPA correlation energy and the 'direct' RPA (dRPA) correlation energy may be calculated using the same scheme. The direct RPA correlation energy being of particular relevance in DFT [6]. These results will be used to shed light on the performance of (d)RPA and give a comparison with CCD, CCSD and CCSD(T) methods. The role of the reference orbitals will be discussed in the context of the AC along with prospects for improving the accuracy of the RPA. In particular, we will examine some recent results [7] for generalized range-dependent ACs [8] and discuss their relevance to the range-separated techniques employed as a first step towards using dRPA in conjunction with density functional approximations with improved accuracy [9, 10].

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