How accurate is RI-RPA? Quality of resolution-of-the-identity methods for RPA correlation energies

Henk Eshuis, Julian Yarkony and Filipp Furche
Department of Chemistry, University of California,
1102 Natural Sciences II, Irvine, CA 92697-2025, USA

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Recently the random phase approximation (RPA) has seen renewed interest as a way of computing molecular correlation energies in a Kohn-Sham context. The RPA has the attractive feature of describing long-range interactions correctly [1], thus addressing a long-standing problem in density functional theory. Additionally it has been shown recently that the RPA can be cast in a computationally attractive form, making it a promising method for larger molecules (30-100 atoms) [2]. The off-diagonal parts of the orbital rotation Hessian matrices are rank-deficient and can be therefore be represented accurately in a relatively small auxiliary basis set using resolution-of-the-identity (RI) methods, in the same vein as in RI-MP2 [3, 4]. In this work we study the accuracy of RI-RPA correlation energies for several testcases. I will show that the error due to RI is small and comparable to the error of RI-MP2. I will discuss why RI-RPA can make RPA calculations more efficient.

References

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