Linear scaling reduction scheme based on pair-MP2 for periodic systems

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Contributions to the correlation energy at MP2 level are examined for a finite ring of hydrogen atoms. While it is true, that the most prominent terms are arising from doubly occupied pairs opposite in the reciprocal space, those pair terms alone are not sufficient to capture a fraction of MP2 that would be size extensive and not vanish at the thermodynamic limit. A physically motivated transformation of the mean field solution naturally separates the MP2 contributions into groups of very similar magnitudes. It is therefore possible to evaluate the mean value for each group and analytically integrate over groups of increasing size. The resulting approximation of MP2 is size extensive, has upper and lower bound on the error, and scales linearly from the number of basis functions. The method is thoroughly benchmarked against MP2 and CCSD with STO-6G and cc-pVDZ for closed shell hydrogen rings[1,2].

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References

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