Understanding and quantifying electron correlation

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Abstract

A deep understanding of electron correlation is crucial for the development of electronic structure methods, including natural orbital functional theory and new density functional approximations. When studying electron correlation it is useful to distinguish between two correlation types, dynamic electron correlation and static (or non-dynamic) electron correlation. In this work we present new means to quantify some of these electron correlation signatures using natural orbitals and their occupancies. In particular, we present two simple expressions to account for dynamic electron correlation employing natural orbitals and their occupancies. These expressions might prove useful to define more robust approximated functionals within density functional theory or natural orbital functional theory.

References

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