Gaussian basis set approach to one-loop self-energy

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The accurate computation of QED corrections to the energy levels of molecules, to all-orders in the external Coulomb potential, presents a significant challenge. The use of Gaussian basis sets is an essential ingredient in extending such calculations to polyatomic molecular systems. At the one-loop level, the corrections to the electron-nucleus interaction are vacuum polarization and the electron self-energy. The leading-order (in $Z\alpha$) vacuum polarization correction can be included in molecular computations as an effective local potential (Uehling potential) [1]. The computation of the complete many-potential vacuum polarization density was carried out recently in a Gaussian basis set [2]. The evaluation of the self-energy correction on the other hand is more involved. In this contribution, I present a method that combines the rigorous bound-state QED approach, the many-potential expansion, with a Gaussian basis set expansion to obtain accurate values for the one-loop self-energy correction in a hydrogen-like atom [3].

References

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