

Few electron systems confined in gaussian potential wells and connection to Hooke atoms

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Abstract

In this work, we have computed and implemented one-body integrals concerning gaussian confinement potentials over gaussian basis functions. Then, we have set an equivalence between gaussian and Hooke atoms and we have observed that, according to singlet and triplet state energies, both systems are equivalent for large confinement depth for a series of even number of electrons $n = 2, 4, 6, 8$ and 10 . Unlike with harmonic potentials, gaussian confinement potentials are dissociative for small enough depth parameter; this feature is crucial in order to model phenomena such as ionization. In this case, in addition to corresponding Taylor series expansions, the first diagonal and sub-diagonal Padé approximant were also obtained, useful to compute the upper and lower limits for the dissociation depth. Hence, this method introduces new advantages compared to others.

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