Aufbau Principle and Singlet-Triplet Gap in Spherical Hooke Atoms

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Abstract

Singlet and triplet spin state energies for three-dimensionalHooke atoms, i .e. electrons in a quadratic confinement, with even number of electrons (2, 4, 6, 8, 10) is discussed using Full-CI and CASSCF type wavefunctions with a variety of basis sets and considering perturbative corrections up to second order. The effect of the screening of the electron-electron interaction is also discussed by using a Yukawa-type potential with different values of the Yukawa screening parameter (λee =0.2, 0.4, 0.6, 0.8, 1.0). Our results show that the singlet state is the ground state for 2 and 8 electron Hooke atoms, whereas the triplet is the ground spin state for 4, 6 and 10 electron systems. This suggests the following Auf bau structure 1s $<$ 1p $<$ 1d with singlet ground spin states for systems in which the generation of the triplet implies an inter-shell one electron promotion, and triplet ground states in cases when there is a partial filling of electrons of a given shell. It is also observed that the screening of electronelectron interactions has a sizable quantitative effect on the relative energies of both spin states, specially in the case of 2 and 8 electron systems, favouring the singlet state over the triplet. However, the screening of the electron-electron interaction does not provoke a change in the nature of the ground spin state of these systems. By analyzing the different components of the energy, we have gained a deeper understanding of the effects of the kinetic, confinement and electron-electron interaction components of the energy.

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