Spectral Properties of Confined Systems

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Advances in semiconductor technology during the last two decades has allowed to create very small spatial structures, so called quantum dots and wires, for which the quantum structure is resolvable. Quantum dots, also known as artifitial atoms, may be modelled by confining electrons into an external potential. Similarly, foreign atoms and molecules embedded into liquid helium and helium droplets, into fullerenes and into zeolites may be modelled by confining atoms and molecules into an appropriate external potential. A review about theoretical studies of spatially confined quantum systems has been given by Jaskólski [1]. A rather complete list of recent studies of spatially confined atoms has been published by Connerade [2]. Most of these studies are concerned with one-electron systems or with many-electron atoms described at the Hartree-Fock level. In the majority of the studies an infinite rectangular potential well or wells for which the potential is infinite outside of a certain range have been used. Very little is known about the influence of the electron correlation and the form of the confinement on the properties of confined system.

In this work we apply standard quantum-chemical models like the Hartree-Fock (HF), the couple cluster (CC) and the configuration interaction (CI) method to study the effects of the spatial confinement of atoms. The confinement is modeled by an external one-particle potential. The calculations are performed using, among others, the OpenMol Program [3]. In particular, we analyze the dependence of the nuclear charge and of the electron interaction on the position of the energy levels when the atom is subject to various external potentials [4]. We also study the transition from the *weak confinement* regime, when the specific properties of an atom are only slightly changed by the confinement to the *strong confinement regime*, when the confining potential dominates and the atom looses its specificity becoming nearly a quantum dot.

References

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