Basis sets for calculations of "confined" systems

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The static dipole polarizabilities of two-electron systems confined by a spherical harmonic-oscillator potential have been calculated by the Coupled Cluster (CCSD) method. The combined effect of the confining potential ω and the central electrostatic field on the polarizabilities of the quantum dot (QD), and the confined systems, H^-, He, and Li^+, respectively, have been investigated. The polarizabilities of the quantum dot can be calculated analytically. The analytical values are perfectly reproduced by the numerical calculations. The work is also oriented on the study of properties and applicability of standard and empirical basis sets in calculation of simple model two-electron systems surrounded by the confining potential. The scheme of basis set construction for two-electron quantum dot is based on the optimization of the initial smallest and largest Gaussian basis function exponents which minimize the CCSD energy. It uses even-tempered technique to obtain a basis set of requested size. Possibilities of usage of such basis sets on many electron quantum dots including the relationship between optimal exponents and number of confined electrons are also discussed.