

# Study of two electrons in a harmonic anisotropic quantum dot using a configuration interaction approach

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**Synopsis** We have developed a computational code based on the HartreeFock and full interaction configuration approaches which allows the study of  $N$ -electron confined quantum systems with different confining potentials and external conditions. The code employs Cartesian anisotropic Gaussian-type orbitals as the atomic basis set, which enables the use of different exponents for each direction space in order to better exploit the characteristics of the confining potential. As an illustration, we have employed it to study a system consisting of two electrons confined by a three-dimensional harmonic potential for different values of confinement strength, leading to different confinement conditions: an isotropic three-dimensional and an anisotropic oblate (or quasi-two dimensional) quantum dot.

The interest in the study of the physical properties of confined quantum systems has increased with the advances of experimental techniques used in nano/mesoscopic-scale structures. Thus, the study of confined quantum systems gives a feedback in the process of designing and synthesizing new materials, and nano/mesoscopic scale structures. On the other hand, the interest of quantum confined systems is not circumscribed to the study of nanostructures. A diverse set of experiments involving: atoms and molecules under pressure, the embedding of atoms and molecules inside cavities such as zeolite molecular sieves, bubbles formed around foreign objects in the liquid helium or neutral plasma, and atoms in fullerenes are also treated using such models of confined quantum systems. Given the wide range of applications, several techniques have been employed along the last years to study the confining properties of different systems. In order to simulate the confining properties of the systems, different types of confining potential have been used in the literature; one finds the isotropic and anisotropic harmonic profile, the Gaussian and the quartic one among others [1].

We have developed a code based in common chemical-physics techniques which allows us to study arbitrary systems in different confining potentials and external conditions [2], such as an applied magnetic field and/or a laser field. It also allows ermits to work with a set of anisotropic functions with different exponents for each space direction, as well as to calculate electronic properties (such as energy, electronic density...) of  $N$ -electrons systems within the Hartree-Fock (HF)

and Full Interaction Configuration (FCI) approaches.

As a first application we have studied the energy spectrum of two electrons confined by a three-dimensional (3D) harmonic potential for different values of confinement strength. The confinement strength is characterized by the frequency of the harmonic-oscillator potential. We have considered the isotropic case, where  $\omega_x = \omega_y = \omega_z$ , and an anisotropic one [3]. Additionally, we plan to study the energy spectrum of two electrons confined by a 3D anisotropic harmonic potential in the presence of a magnetic field. We have used as a basis set the *cartesian anisotropic Gaussian-type orbitals* (c-aniGTO). From this choice we discuss how to establish their exponents. We have observed that an efficient manner of proceeding was to take more than one function for each atomic orbital, i.e. instead of using only one function of the type  $s$ ,  $p$ ,  $d$  and *etc*, we have used two of each type with different exponents.

## References

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