Study of two correlated electrons confined by harmonic potentials

K. V. Rodriguez*, D. M. Mitnik§ and G. Gasaneo*

* Departamento de Física, Universidad Nacional del Sur and CONICET, 8000 Bahía Blanca, Buenos Aires, Argentina
§Instituto de Astronomía y Física del Espacio, CONICET and Universidad Nacional de Buenos Aires, C C 67, Suc. 28, (C1428EGA), Buenos Aires, Argentina.

Synopsis We extend the Angular Correlated Configuration Interaction method to two confined correlated electrons confined by harmonic potentials.

Studies of quantum objects confined by different forms of external potentials have attracted the attention of both physicist and quantum chemists since the early days of quantum mechanics [1,2].

In this report, we study the ground state of two electrons where each particle is confined by an harmonic-oscillator potential,

$$V(r_{i3}) = \frac{1}{2}\omega_{i3}^2 r_{i3}^2 \qquad (1)$$

with ω the frequency and $i=1,2;$ and with a Coulomb interaction between them.

In relative coordinates, the Hamiltonian of this two-particle system can be associated with a three-body one. So, to study the structure of the confined, correlated two electrons, we propose the use of a generalization of the Angular Correlated Configuration Interaction (ACCI) method presented in [3].

The ACCI was originally introduced to deal with Coulomb potentials but it is not restricted to them. Its extension to general systems is one of the aims of this communication.

Within the ACCI approach the solution of the Schrödinger equation is written as a linear combination of correlated basis functions. The key of the approach is that the basis functions exactly solve the diagonal part of the kinetic energy as well as all the interactions involved.

The trial wave functions are constructed using the angularly correlated basis proposed in [4,5] and following the methodology proposed in [3,6], where each term of the basis is multiplied by a power series on the interparticle coordinates (r_{13}, r_{23}, r_{12}).

The trial wave functions read

$$\Psi_{C3-N} = \sum_{n_1 n_2 n_3} \varphi_{n_1}(r_{13})\varphi_{n_2}(r_{23})\chi_{C3}(n_3, r_{12}) \times \sum_{i,j,k\neq 1} c_{ijk}^{n_1 n_2 n_3} r_{13}^i r_{23}^j r_{12}^k \qquad (2)$$

where $\varphi_{n_i}(r_{i3})$ are $l=0$ harmonic-oscillator functions and $\chi_{C3}(n_3, r_{12}) = {}_1F_1(-n_3, 2, -r_{12}/n_3)$ is the angular correlation factor [4,5]. The functions Ψ_{C3-N} involve N linear parameters $c_{ijk}^{n_1 n_2 n_3}$ which are obtained by solving a generalized eigenvalue problem.

By increasing the number of configurations included (n_1, n_2 and n_3) and the number of linear parameters c, the energy convergence can be systematically improved.

Another aim of this communication is to present the mean energies <E> and its behavior as a function of the frequencies, ω_{i3}.

References

[1] Fock V 1928 Z Phys. **47** 446-8.
[2] Darwin C G 1930 Proc. Camb. Phil. Soc.27 86-90.
[3] K V Rodriguez et al J. Phys. B 40 3923
[4] G Gasaneo and L U Ancarani 2008 *Phys. Rev. A* 77 012705
[5] L U Ancarani and G Gasaneo 2007 *Phys. Rev. A* 75 032706
[6] K V Rodriguez and G Gasaneo 2005 *J. Phys. B* 38 L259

E-mail: kkrodri@gmail.com
E-mail: dmitnik@df.uba.ar

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
Published under licence by IOP Publishing Ltd