

Two-electron atoms under spherical confinement

S. Bhattacharyya^{*1}, J. K. Saha[†] and T. K. Mukhopadhyay[†]

^{*} Dept. of Physics, APC College, New Barrackpore, Kolkata-700131, India

[†] Dept. of Physics, Narula Institute of Technology, Agarpara, Kolkata-700109, India

Synopsis : The effect of spherical confinement on the ground state of helium-like have been calculated by using correlated Hylleraas basis sets within the variational framework. The thermodynamic pressure on the ions in the ground state due to confinement and the critical values of the confining radii close to fragmentation limit are also estimated.

Spectroscopic study on the behavior of energy levels and other structural properties of quantum systems under various external confinements is gaining momentum continuously in the recent years. The effect of external environment on the spectral properties of the atoms is due to the modification of the Coulomb potential. A variety of physical problems are provided by nature in relation to spatially confined systems such as atoms or molecules in zeolite sieves [1] and fullerenes [2,3], solutes under solvent environment [4] *etc.* Some of the properties of matter under high pressure as observed in Jovian planets [5] can be explained using such concepts of confined systems.

The effect of spherical confinement on the ground state of helium-like ions ($Z = 1-5$) and the first four ($1S^e$) excited states for $Z = 2-5$ have been studied in details by using correlated Hylleraas basis sets within the variational framework. The correlated wave functions used here are consistent with the finite boundary conditions due to spherical confinement. The wave function has been normalized for each confining radius R to take proper account of the reorientation of charge distribution within the spherical cavity. The present methodology enables us to evaluate the finite domain integrals analytically in the Hylleraas basis for which the present basis set becomes highly flexible avoiding linear dependency for larger dimensions.

Within a sphere of radius R , the confining potential imposes a thermodynamic pressure on the ion inside due to finite boundaries. The pressure experienced by an atom inside the cavity can be obtained from the first law of thermodynamics under an adiabatic approximation.

For almost every system at each radius of confinement, the present energy values are lowest yet obtained. It is observed that for low values of confinement radius, the generated pressure tends to be very high which pushes the system towards instability. The pressure corresponding to the critical radius

can be evaluated to show the nature of the pressure required for destabilizing each system.

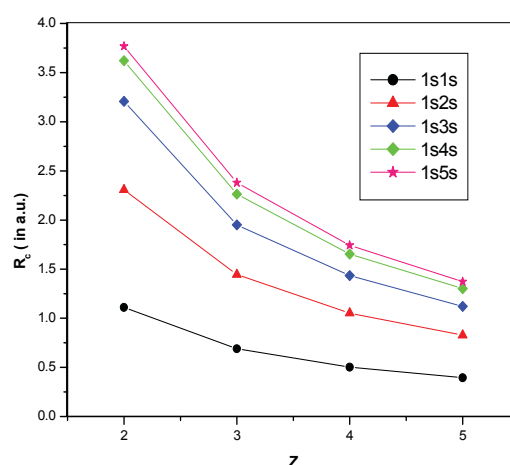


Figure 1. Variation of critical radius (R_c) of the impenetrable spherical cavity for bound $1sns$ ($n=1-5$) ($1S^e$) states with Z .

The present results for energy values and the thermodynamic pressure for the confined ions as well as corresponding confining radii close to fragmentation limit can be set as benchmark for the future references. The methodology employed in this work can be extended to study the effect of other potentials confining the ions in a finite cavity.

References

- [1] P A Jacobs 1997 *Carboniogenic Activity of Zeolites* (Amsterdam: Elsevier)
- [2] J P Connerade, V K Dolmatov, S T Mansion 1999 *J. Phys B* **32** L395
- [3] J A Ludlow, T G Lee and M S Pindzola 2010 *J. Phys. B* **43** 235202
- [4] S Canuto (Ed.) 2008 *Solvation Effects on Molecules and Biomolecules, Computational methods and Applications* (Springer)
- [5] T Guillot 1999 *Planet Space Sci.* **47** 1183

¹ E-mail: sukhamoy.b@gmail.com

