The energy correction due to a finite size nucleus of the hydrogen atom confined in a penetrable spherical cavity

N. Aquino[a], R.A. Rojas[a] and H.E. Montgomery[b]
[a]*Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa,*
Av. San Rafael Atlixco 186, Col. Vicentina, Iztapalapa, 09340 Ciudad de México.
[b]*Chemistry Program, Centre College, 600 West Walnut Street, Danville, KY 40422.*

Received 17 January 2018; accepted 18 March 2018

We have computed accurate values for the ground state energy of a hydrogen atom confined by a finite spherical barrier of height V_0 as a function of the confinement radius R_c. We consider the nucleus as a sphere with a uniform charge distribution instead of as a point particle. The contribution to the ground state energy due to the finite nuclear size is computed as a function of the confinement radius, R_c, and the height of the barrier, V_0, using time-independent perturbation theory. For an impenetrable cavity with $R_c = 0.5$ au, we found that this energy correction is fifty times higher than the corresponding value for the free hydrogen atom. For a finite value of V_0, we found that the maximum of the energy correction is reached at a value R_{cmax}, which is very close to the position at which the electron density is most compact around the nucleus. This is confirmed though evaluation of the Shannon entropy in configuration space.

Keywords: Confined hydrogen atom; finite nucleus correction; Shannon entropy.

PACS: 67.63.Gh; 67.80.fh

1. Introduction

Eighty years ago, Michels *et al.* [1] used the confined hydrogen atom (CHA) as a model to study the change in the polarizability of a hydrogen atom subjected to high external pressure. In this model, the nucleus of the hydrogen atom was clamped at the center of an impenetrable sphere of radius R_c, while the electron could move within the included volume. In this system, ionization is not possible. The way to account for ionization is to allow the walls to be penetrable. This penetrable model was successfully used by Ley-Koo and Rubinstein [2] to explain the ionization of a hydrogen atom trapped in alpha-quartz [3-4].

Many applications have been developed from these models and they have been generalized to cavities with different geometries. This model has subsequently been applied to a wide range of physical problems [1-13]. Observable properties of the systems such the energy spectrum, transition frequencies and probabilities, polarizability and the behavior of atoms trapped in fullerenes, etc., are changed by spatial confinement. Reviews and books on those topics are available [5]. Recent experimental studies show that the electron capture nuclear decay rate is increased under compression [14-16]. A partial explanation of this effect was given using the model of many-electron atoms confined in an impenetrable spherical cavity [17]. With the advent of technology to construct atomic scale confinements, the study of confined systems has become increasingly relevant.

In most of the works on the properties of atoms and molecules, either free of any confinement or confined in cavities, it is assumed that the nuclei are points with charge and mass but without extent. The inclusion of a nucleus of finite size in the free hydrogen atom is accompanied by a shift in the electron energy [20-26]. The magnitude of this shift is very small compared to the energy of the hydrogen atom with a point nucleus. Until now, no one has studied how this energy shift changes for the hydrogen atom, confined in spherical penetrable cavities, when a nucleus of finite size is considered.

Pyarelal and Bhatnagar [20] proposed a model of the hydrogen atom with an impenetrable nucleus of finite size. In that model, the wave functions must vanish at the surface of the nucleus. The reduction in the volume available for movement of the electron produces an increase in the energy of the electronic states. This problem has an exact solution, but the model is unrealistic.

A more realistic model consists of a spherical nucleus of radius r_0, with an uniform distribution of charge. For hydrogen-like atoms with a small nuclear charge, Z, it is well-known that the Schrödinger equation adequately describes those systems [19]. An exact solution to this problem was found by Ley-Koo *et al.* [19], in which they studied the muonic atoms, free of any confinement, with Z up to 90. In this work, we will adopt the model of a spherical nucleus with an uniform charge distribution, and we will use first-order perturbation theory to calculate the correction to the ground-state energy of the hydrogen atom confined in spherical penetrable and impenetrable cavities, as a function of the radius of confinement R_c.

The objectives of this work are twofold: the former is to establish benchmark values for the energy of the ground state of the hydrogen atom confined in a spherical penetrable cavity, the second is to calculate the energy shift of this system when considering a spherical nucleus of finite volume with an uniform distribution of charge.

The organization of this work is as follows: in Sec. 2, we solve CHA with a point nucleus in a spherical, padded cavity. In Sec. 3 we use first-order perturbation theory to compute the energy correction due to inclusion of a nucleus of finite size. In Sec. 4 we show the results of the calculation of the energy correction due to a finite size nucleus, obtained for both penetrable and impenetrable confinements. Finally, in Sec. 5 we give our conclusions.

2. The CHA in a spherical padded cavity

In this section we give a brief description of the solution of the hydrogen atom confined in a spherical padded cavity. A detailed explanation can be found in Refs. 2, 7 and 9.

In atomic units ($m = e = \hbar = 1$), the Schrödinger equation for a hydrogen atom at the center of a sphere of radius R_c and confined by a constant potential V_0 is

$$-\frac{1}{2}\nabla^2 + V(r)\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi), \tag{1}$$

where the potential is

$$V_c = \begin{cases} -\frac{1}{r}, & 0 \le r \le R_c \\ V_0, & r > R_c \end{cases} . \tag{2}$$

Equation (1) can be solved using separation of variables

$$\psi(r,\theta,\phi) = R(r)Y_{l,m}(\theta,\phi) \tag{3}$$

where $Y_{l,m}(\theta,\phi)$ is a normalized spherical harmonic and $R(r)$ is a radial function composed of $R_i(r)$, the wavefunction inside the sphere and $R_e(r)$, the wavefunction external to the sphere.

The Schrödinger equation for the inner region $0 \le r \le R_c$

$$\left[-\frac{1}{2}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\right) + \frac{l(l+1)}{2r^2} - \frac{1}{r}\right] \times R_i(r) = ER_i(r), \tag{4}$$

whose solution is given by [8-9]:

$$R_i(r) = Ae^{-\rho/2}\rho^l M(-\beta + l + 1, 2l + 2, \rho), \tag{5}$$

where $M(a,b,r)$ is the confluent hypergeometric function [18] and

$$\beta = \frac{1}{\sqrt{-2E}}, \quad \rho = 2r/\beta. \tag{6}$$

The external region, $r > R_c$, is described by the Schrödinger equation

$$\left[-\frac{1}{2}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\right) + \frac{l(l+1)}{2r^2} + V_0\right] \times R_e(r) = ER_e(r), \tag{7}$$

which can be written as

$$\left(\frac{d^2}{dy^2} + \frac{2}{y}\frac{d}{dy} - \frac{l(l+1)}{y^2} - 1\right)R_e(r) = 0, \tag{8}$$

where

$$y = kr, \quad k^2 = 2\mu(V_0 - E)/\hbar^2, \tag{9}$$

and whose solution is given by [2]

$$R_e(y) = By^{-l-1}e^{-y}M(-l, -2l, 2y). \tag{10}$$

Hereafter, we restrict our attention to states with $l = 0$ because these are the only states which have non-zero value of $R_i(r)$ when $r = 0$.

The eigenvalues are determined by the requirement that the total wavefunction must be continuous with continuous first derivatives at $r = R_c$. This is most easily accomplished by matching logarithmic derivatives at R_c, resulting in the equation

$$\frac{d}{dr}[\ln R_i]\big|_{R_c} - \frac{d}{dr}[\ln R_e]\big|_{R_c} = 0. \tag{11}$$

The normalization constants A and B are found from the requirements that

$$R_i\left(\frac{2R_c}{\beta}\right) = R_e(kR_c). \tag{12}$$

and the normalization condition

$$\int_0^{r_0}(R_i)^2r^2dr + \int_{r_0}^{\infty}(R_e)^2r^2dr = 1. \tag{13}$$

As mentioned above, the zeroes of the logarithmic derivative equation are the eigenvalues of the problem. The first zero corresponds to the ground state energy. With this value, we construct the wave function in each region. To find the zeroes of the equation we used Mathematica 9 with the command **FindRoot** with 50-digit precision variables. The eigenvalues obtained through this procedure are shown in Tables I-V as a function of the box radius R_c and the potential height V_0. These results are in complete agreement with previous calculations [2,7,9]. The results are shown with 15 digits after the decimal point.

3. Finite nucleus size correction

The Hamiltonian of the hydrogen atom with a finite nucleus confined by a spherical penetrable wall is given by

$$H = -\frac{\nabla^2}{2} + V_r(r), \tag{14}$$

where

$$V_r(r) = \begin{cases} \frac{1}{2r_0}\left[\left(\frac{r}{r_0}\right)^2 - 3\right], & 0 < r < r_0 \\ -\frac{1}{r}, & r_0 < r < R_c \\ V_0, & R_c < r < \infty \end{cases} , \tag{15}$$

TABLE I. CHA ground state energy $E_{10}^{(1)}$, and first-order correction due to the finite nucleus, $E_{10}^{(1)}(R_c)$, as a function of the confinement radius R_c for $V_0 = 0$. Also shown is the ratio between the energy correction of the confined system, $E_{10}^{(1)}(R_c)$, and the correction of the free hydrogen atom E_{10}. Energies are in hartrees and distances are in bohrs.

R_c	E_{10}	$E_{10}^{(1)}(10^{-10})$	$E_{10}^{(1)}(R_c)/E_{10}^{(1)}$
0.75	-0.002551608753406	0.342781939506244	0.345
0.8	-0.017424391031037	0.808141286815622	0.814
0.9	-0.067406311452319	1.325196851197549	1.335
1.0	-0.125000000000000	1.544741614031751	1.556
1.1	-0.180067083549980	1.621160850903080	1.633
1.2	-0.229179151514072	1.627437259807232	1.639
1.5	-0.338167417956141	1.507712255705773	1.519
2.0	-0.431218889241793	1.287458459987721	1.297
2.5	-0.470393522970229	1.151246460119175	1.160
3.0	-0.487223082818398	1.075285232620169	1.083
3.5	-0.494519692585279	1.034355146835889	1.042
4.0	-0.497674689400819	1.012980250520460	1.020
4.5	-0.499025598864902	1.002187518743767	1.009
5.0	-0.499596671366575	0.996918364180960	1.004

TABLE II. CHA ground state energy $E_{10}^{(1)}$, and first-order correction due to the finite nucleus, $E_{10}^{(1)}(R_c)$, as a function of the confinement radius R_c for $V_0 = 5$. Also shown is the ratio between the energy correction of the confined system, $E_{10}^{(1)}(R_c)$, and the correction of the free hydrogen atom E_{10}. Energies are in hartrees and distances are in bohrs.

R_c	E_{10}	$E_{10}^{(1)}(10^{-10})$	$E_{10}^{(1)}(R_c)/E_{10}^{(1)}$
0.4	4.827691517791768	6.456668836007435	6.506
0.5	3.907609648085746	10.240494963124124	10.319
0.6	2.982382648801240	9.598999388792230	9.672
0.8	1.666642892127310	6.980485974979947	7.034
0.9	1.229573168163173	5.926377707785826	5.972
1.0	0.893377387585463	5.081081669583943	5.120
1.5	0.028688218476904	2.781656875168397	2.803
2.0	-0.273954162644265	1.889596355389960	1.904
2.5	-0.397386813501905	1.473407522212738	1.484
3.0	-0.452163079706601	1.256864293020748	1.266
3.5	-0.477542879189045	1.137865941478808	1.146
4.0	-0.489507801753420	1.071253920964084	1.079
4.5	-0.495153894267392	1.034166451405600	1.042
5.0	-0.497794417047201	1.013927192430064	1.021

The first two terms in Eq. (15) are the usual terms of a free hydrogen atom with a finite size nucleus [6,19,21-23], and r_0 is the radius of the hydrogen atom, a proton. The third term is introduced to confine the hydrogen atom in a spherical cavity of radius R_c.

We define the potential

$$\tilde{V}(r) = \begin{cases} -\frac{1}{r}, & r < r < R_0 \\ 0, & r_0 < r < R_c \end{cases} . \tag{16}$$

Adding and subtracting $\tilde{V}(r)$ to Eq. (14), and grouping terms we obtain the

$$H = -\frac{\nabla^2}{2} + V_c(r) + H'(r). \tag{17}$$

This Hamiltonian can be written in the more familiar form

$$H = H^0 + H' \tag{18}$$

TABLE III. CHA ground state energy $E_{10}^{(1)}$, and first-order correction due to the finite nucleus, $E_{10}^{(1)}(R_c)$, as a function of the confinement radius R_c for $V_0 = 10$. Also shown is the ratio between the energy correction of the confined system, $E_{10}^{(1)}(R_c)$, and the correction of the free hydrogen atom E_{10}. Energies are in hartrees and distances are in bohrs.

R_c	E_{10}	$E_{10}^{(1)}(10^{-10})$	$E_{10}^{(1)}(R_c)/E_{10}^{(1)}$
0.3	9.846148432090808	9.930542047590157	10.007
0.5	5.639829938566619	17.491618217286550	17.626
0.6	4.097374126091258	13.822727567461880	13.929
0.7	2.995752750577570	10.917393851422899	11.001
0.9	1.620350180030345	7.179161687379589	7.234
1.0	1.185777102316168	5.992750426662855	6.038
1.5	0.116618456909048	3.048420555184699	3.071
2.0	-0.240385375166330	1.999717840968987	2.015
2.5	-0.382937517117798	1.527421154803173	1.539
3.0	-0.445545908145495	1.285799849400771	1.295
3.5	-0.474425028203553	1.153976852962736	1.162
4.0	-0.488027526391939	1.080287038138810	1.088
4.5	-0.494454829661503	1.039165583170746	1.047
5.0	-0.497468459482318	1.016626789889568	1.024

TABLE IV. CHA ground state energy $E_{10}^{(1)}$, and first-order correction due to the finite nucleus, $E_{10}^{(1)}(R_c)$, as a function of the confinement radius R_c for $V_0 = \infty$. Also shown is the ratio between the energy correction of the confined system, $E_{10}^{(1)}(R_c)$, and the correction of the free hydrogen atom E_{10}. Energies are in hartrees and distances are in bohrs.

R_c	E_{10}	$E_{10}^{(1)}(10^{-10})$	$E_{10}^{(1)}(R_c)/E_{10}^{(1)}$
0.5	14.747970030350280	54.536609722874516	54.956
0.6	9.527707806146348	33.740936784485875	34.000
0.7	6.469926127251262	22.720335291772468	22.895
0.8	4.543380181009424	16.278628704347120	16.403
0.9	3.262189536240119	12.229690823293298	12.323
1.0	2.373990866103664	9.538267646127938	9.611
1.5	0.437018065247256	3.969102513288022	3.999
2.0	-0.125000000000000	2.355893659642013	2.374
2.5	-0.334910185427921	1.695773616320432	1.708
3.0	-0.423967287733454	1.374211998517624	1.384
3.5	-0.464357128440197	1.202793634385484	1.212
4.0	-0.483265302078022	1.107644656981758	1.116
4.5	-0.492205427798878	1.054376061163177	1.062
5.0	-0.496417006591452	1.024902478009865	1.032

From Eq. (17) we immediately identify the first two terms as the Hamiltonian of a hydrogen atom confined in a penetrable spherical cavity, as analyzed in previous section. We note that for H^0, the unperturbed Hamiltonian, the eigenfunctions ψ_{nlm}^0 and eigenvalues E_{nl}^0 are well-known.

The perturbation is given by [6, 21-23]

$$H' = \begin{cases} \frac{1}{2r_0}\left[\left(\frac{r}{r_0}\right)^2 - 3\right] + \frac{1}{r}, & r < r_0, \\ 0, & r_0 < r < \infty \end{cases} . \quad (19)$$

As mentioned above, we are only interested in states with $l = 0$, because the electron density is non-zero at the origin.

The correction of the energy to first-order is given by

$$E_{n_0}^{(1)} = \langle \psi_{n_{00}} | H' | \psi_{n_{00}} \rangle. \tag{20}$$

A straightforward calculation gives the following expression. The eigenfunctions $\psi_{n_{00}}$ are an orthonormal set of wave functions with the form

$$\psi_{n_{00}}(r,\theta,\phi) = R_{n_0}(r) Y_0^0(\theta,\phi). \tag{21}$$

Substituting (21) in (20) we obtain

$$E_{n0}^{(1)} = \frac{1}{2r_0} \int\limits_0^{r_0} |R_{n0}(r)|^2 \left[\left(\frac{r}{r_0} \right)^2 - 3 + \frac{2r_0}{r} \right] r^2 dr. \tag{22}$$

In the region $r \leq r_0$, taking in account that for a proton, $r_0 \ll 1$,

$$R_{nl}(r) \cong R_{nl}(0). \tag{23}$$

Equation (22) then becomes

$$E_{n0}^{(1)} = \frac{r_0^2}{10} |R_{n0}(0)|^2. \tag{24}$$

In this work we will use the most recent measured proton radius $r_0 = 0.8335$ femtometers ($1.575086726 \times 10^{-5}$ bohrs) [24].

4. Shannon entropy

Claude E. Shannon in 1948 introduced the so called Shannon entropy in his paper "A Mathematical Theory of Communication" [27]. The quantum version of Shannon entropy S_r, in configuration space is defined as

$$S_r = -\int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r}, \tag{25}$$

where $\rho(\vec{r})$ is probability density of the electron, in atomic units.

The Shannon entropy in quantum computation means the absolute limit of the best possible lossless compression of any communication, under some particular constraints [33]. On the other hand, the Shannon entropy has a wide variety of applications in Physics and Chemistry [34]. Usually, it is interpreted as the uncertainty associated with the particle position, which is related with the degree of localization (delocalization) of the particle. In chemistry, the Shannon entropy is associated with the delocalization of an electron in aromatic compounds [35].

Panos *et al*. [36], computed and plotted S_r as a function of the atomic number, Z, for many-electron atoms. They found that the curve $S_r(Z)$ has relative minimum values for the closed shell atoms as He, Ne, Ar and Kr. They interpreted this fact as the electronic density of those atoms is more compact (localized) than their near neighbors. Recently, this interpretation for the Shannon entropy was used successfully in the study of many-electron atoms confined in soft spherical cavities [37,38]. In this work we will adopt this interpretation for the Shannon entropy.

5. Results

In Tables I-III, we show the corrections to the ground-state energy of CHA, taking into account a nucleus with finite size. The correction to the energy is small compared with the energy of the unperturbed confined atom. As the confinement radius R_c grows, $E_{10}^{(1)}$ approaches the value of the first-order correction of the free hydrogen atom, $E_{10\text{free}}^{(1)} = 0.9923592777 \times 10^{-10}$ hartrees, according to Eq. (24).We can see that there is a change in the value of the energy correction that depends on R_c and V_0. This behavior can be seen more clearly in Fig. 1, where we have plotted the ratio between the correction of the ground state energy of CHA due to the finite nucleus, relative to the correction for the free hydrogen atom. It should be noted that this ratio is independent of the value of r_0 and depends only on the ratio of the wave functions evaluated at the origin

$$\frac{E_{10}^{(1)}}{E_{10\text{free}}^{(1)}} = \frac{|R_{10}(0)|^2}{|R_{10\text{free}}(0)|^2}, \tag{26}$$

where $R_{\text{free}}(r)$ and $R_{10}(r)$ are the radial wave functions of the free hydrogen atom and the CHA, respectively.

For a spherical cavity with impenetrable walls, the correction to the energy grows rapidly as R_c tends to zero because by reducing R_c the electron is closer to the nucleus without the possibility to escape. In Fig. 1 we can see that for a value of $R_c = 1$, the energy correction $E_{10}^{(1)}$ to the ground state of the CHA is 10 times greater than in the free hydrogen atom.

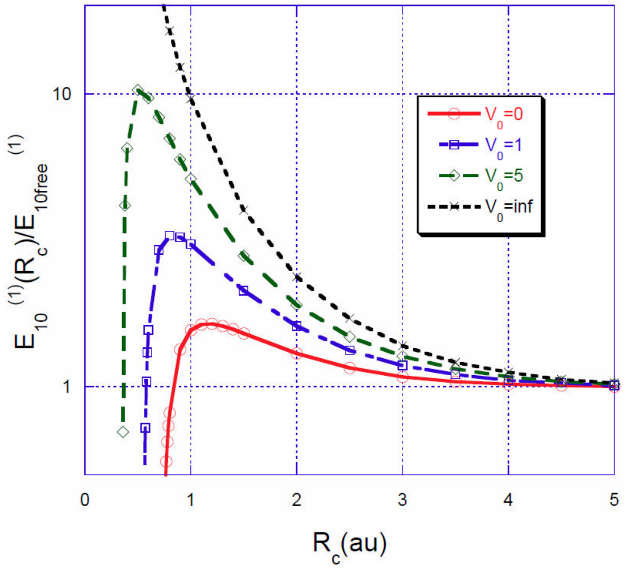

FIGURE 1. Ratio $E_{10}^{(1)}(R_c)/E_{10\text{free}}^{(1)}$ of the energy correction of CHA to the free hydrogen atom as a function of R_c.

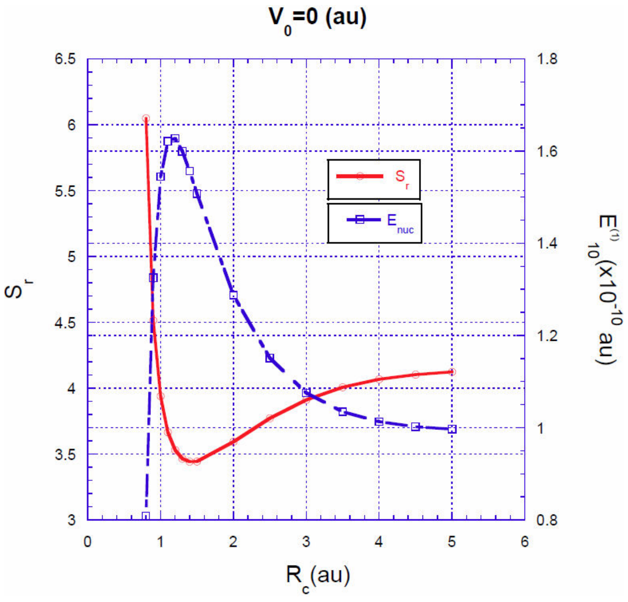

FIGURE 2. Energy correction $E_{10}^{(1)}$ and Shannon entropy S_r as a function of R_c for $V_0 = 0$ hartrees.

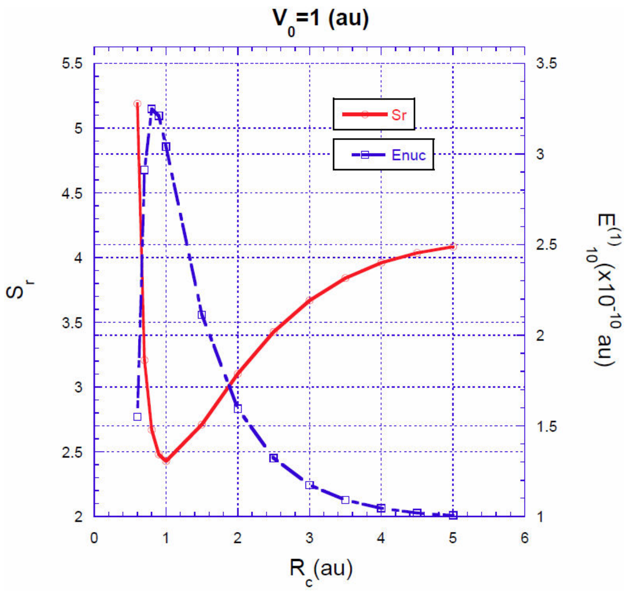

FIGURE 3. Energy correction $E_{10}^{(1)}$ and Shannon entropy S_r as a function of R_c for $V_0 = 1$ hartrees.

This value is in complete agreement with that calculated by Goldman and Joslin [6]. They found that for very small values of R_c and very excited states, the correction of the energy, $E_{10}^{(1)}$, can be several orders of magnitude greater than the value for the free atom.

For a fixed value of the barrier height V_0, the situation is quite different. The energy correction $E_{10}^{(1)}\,(R_c)$ grows as R_c decreases, and it reaches its maximum value at a confinement radius that we call $R_{c_{\max}}$. As R_c continues to decrease, the energy correction, $E_{10}^{(1)}(R_c)$, decreases also, approaching zero as R_c approaches a critical radius, at which the total energy of the electron is equal to the height of the barrier V_0.

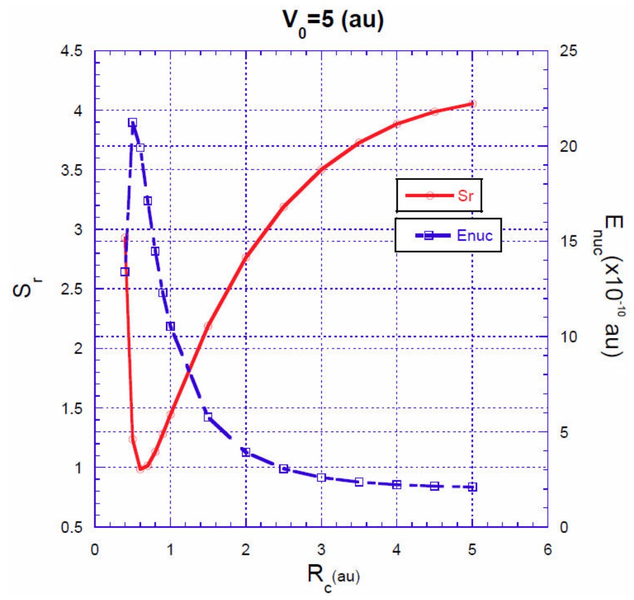

FIGURE 4. Energy correction $E_{10}^{(1)}$ and Shannon entropy S_r as a function of R_c for $V_0 = 5$ hartrees.

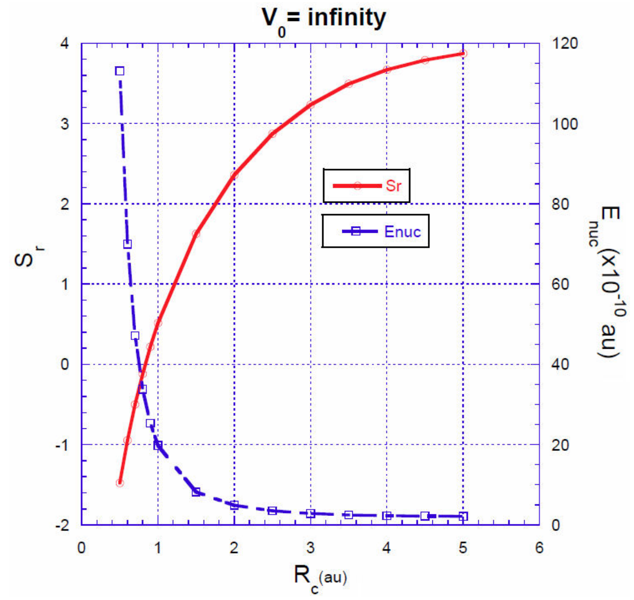

FIGURE 5. Energy correction $E_{10}^{(1)}$ and Shannon entropy S_r as a function of R_c for a spherical impenetrable of radius R_c.

Intuitively, one expects that the energy correction $E_{10}^{(1)}$ be higher in a small size cavity, in which the electron is closer the nucleus, *i.e.* a cavity in which the electronic density is more compact. One way to quantify the compactness of the electronic density is by means of the Shannon entropy [27-38], as was mentioned above. This idea is supported in the interpretation of localization-delocalization associated with the Shannon entropy, S_r. A small value of S_r, means that the electron density is more localized around the nucleus [30-32,36-38]. At R_c^*, where the entropy curve, $S_r(R_c)$, has a minimum value, the electron density is more compact around the nucleus, and thus the contribution to the energy correction

$E_{10}^{(1)}(R_c)$ is greater. In Figs. 2 to 5 we plot the energy correction $E_{10}^{(1)}(R_c)$ and the Shannon entropy $S_r(R_c)$ for a few values of V_0 as a function of R_c. In Fig. 2 we plot together $E_{10}^{(1)}(R_c)$ and $S_r(R_c)$, as a function of the confinement radius, R_c, for $V_0 = \infty$. We see that when R_c decreases, S_r also decreases. This means that the electron density around the nucleus increases and there is an increase in $E_{10}^{(1)}$. This behavior continues as R_c diminishes.

In Figs. 3-5 we show the energy correction $E_{10}^{(1)}(R_c)$ and the Shannon entropy S_r for fixed values of V_0. In all figures, we see that the curve of the energy correction $E_{10}^{(1)}(R_c)$ reaches a maximum value at a confinement radius $R_{c_{\max}}$ which depends on the value of V_0. We can also see that the curve of the Shannon entropy $S_r(R_c)$ reaches its minimum value at a confinement radius R_c^*, $i.e.$, in a spherical box of radius R_c^* the electron density is more compact around the nucleus. From Figs. 3-5 we can see that $R_{c_{\max}} < R_c^*$. This result can be interpreted in the following way. As R_c decreases, the value of S_r also decreases, and the density becomes more compact up to a maximum value at R_c^*. As R_c continues to decrease, S_r begins to increase and the electron starts to be delocalized, the wave function increases its value at the origin and inside the barrier. If R_c continues decreasing, the value of the wave function at the origin decreases quickly, but it grows fast inside the barrier. This process continues until ionization take place.

6. Conclusions

In this work we calculated the energies and wave functions, with high numerical precision, for the ground state of the hydrogen atom confined in a penetrable spherical cavity. We also calculated the energy correction due to a nucleus of finite size for the CHA as a function of R_c and V_0. For finite barriers, the curves of the energy correction reach a maximum value, while the curves of the Shannon entropy as a function of $R_c reach$ a minimum value. The maximum of the energy correction is always close to the position at which the Shannon entropy has its minimum value, *i.e.* at the position in which the electron density is most compact.

Acknowledgments

One of us (RAR) is grateful to Universidad Autónoma Metropolitana for providing the funds through a PhD studies scholarship.

---

1. A. Michels, J. de Boer and A. Bijl, *Physica* **4** (1937) 981.
2. E. Ley-Koo and S. Rubinstein, *J. Chem. Phys.* **71** (1979) 351.
3. D. Suryanarayana and J. A. Weil, *J. Chem. Phys.* **64** (1976)510.
4. J. A. Weil, *J. Chem. Phys.* **71** (1979) 2803.
5. F. M. Fernández and E. A. Castro, *Kinam* **4** (1982) 193; P. O. Fröman, S. Yngve and N.J. Fröman, *J. Math. Phys.* **28** (1987) 1813; S. Yngve, *J. Math Phys.* **29** (1988) 931; W. Jaskálski, *Phys. Rep.* **271** (1996) 1; A. L. Buchachenko, *J. Phys. Chem.* **105** (2001) 5839; J. P. Connerade, V. H. Dolmatov and P. A. Lakshmi, *J. Phys. B* **33** (2000) 251; J. R. Sabin, E. Brändas and S. A. Cruz (eds) *The Theory of Confined Quantum Systems*, Parts I and II Advances in Quantum Chemistry **vol 57**, (Amsterdam: Academic2009); K. D. Sen (ed) *Electronic Structure of Quantum Confined Atoms and Molecules* (Heidelberg: Springer2014) and references therein.
6. S. Goldman and C. Joslin, *J. Phys. Chem.* **96** (1992) 6021.
7. N. Aquino, *Adv. Quantum Chem.* **57** (2009) 148.
8. N. Aquino, G. Campoy and H. E. Montgomery, *Int. J. Quantum Chem.* **107** (2007) 1548.
9. H. E. Montgomery and K. D. Sen, *Phys. Lett. A* **376** (2012) 1992.
10. J. Hunt, J. Martin, V. Rosing, J. Winner and H. E. Montgomery, *Chem. Educator* **19** (2014) 384.
11. R. Cabrera-Trujillo and S. A. Cruz, *Phys. Rev. A* **87** (2013) 012502.
12. M. Rodríguez-Bautista, C. Díaz-García, A. M. Navarrete-López, R. Vargas and J. Garza, *J. Chem. Phys.* **143** (2015) 34103.
13. M. A. Martínez-Sánchez, M. Rodríguez-Bautista, R. Vargas and J. Garza, *Theor. Chem. Acc.* **135** (2016) 207.
14. A. Ray, P. Das, S. K. Saha, A. Goswami and A. De, *Phys. Lett. B* **679** (2009) 106.
15. W. K. Hensley, W. A. Basset and R. J. Huizenga, *Science Lett.* **181** (1973) 1164.
16. L. Liu, C. Huh, *Earth and Planetary Science Lett.* **180** (2000) 163.
17. A. Ray, P. Das, N. Aquino and M. Lozano Unpublished data
18. NIST Digital Library of Mathematical Functions. http://dlmf.nist.gov/, Release 1.0.18 of 2017-09-18 F.W.J. Olver *et al*., eds, Sec. 13.
19. E. Ley-Koo, E. Castaño, D. Finotello, E. Nahmad-Achar and S. Ulloa, *Am. J. Phys.* **48** (1980) 949.
20. Pyarelal and P. L. Bhatnagar, http://www.insa.nic.in/writereaddata/UpLoadedFiles/PINSA/Vol18_1952_3_Art06.pdf
21. A. A. Sokolov, Y. M. Loskutov and I. M. Ternov, *Quantum Mechanics* (Holt Rinehart and Winston, Inc: New York 1966) p. 334.
22. C. Cohen-Tannoudji, *Quantum Mechanics* **vol. 2** (John Wiley and Sons Inc: New York 1977) p.1141.
23. B. H. Bransden and C. J. Joachain, *Physics of atoms and molecules* (Longman Group UK, Ltd: London 1990) p. 245.
24. A. Beyer *et al*., *Science* **358** (2017) 79.
25. A. Adamu and Y. H. Ngadda, *Int. J. Theo. Math. Phys.* **7** (2017) 9.

26. B. Holdomand and R. Koniuk, arXiv:1710.01697v1, 2017 [physics.atom-ph].
27. C. E. Shannon, *Bell Syst. Tech. J.*, **27** (1948) 379-473; **27** (1948) 623-656. Reprinted in C. E. Shannon; W. Weaver, *The Mathematical Theory of Communication*; Illinois Press: Urbana, 1949); pp. 29-125 and http://cm.belllabs.com/cm/ms/what/shannonday/paper.html
28. K. D. Sen, *J. Chem. Phys.* **12** (2005) 074110 and references therein.
29. A. Nagy, K. D. Sen and H. E. Montgomery, *Phys. Lett. A* **373** (2009) 2552.
30. I. Bialinicki-Birula and L. Rudnicki, Statistical Complexity, Applications in Electronic Structure(Springer:London, 2011) Chapter 1.
31. H. G. Laguna, H. H. Corso, and R. P. Sagar, *J. Math. Chem.* **50** (2012) 233. H. G. Laguna, H. H. Corso, E. Castaño and R. P. Sagar, *J. Math. Chem.* **51** (2012) 179.
32. N. Aquino, A. Flores-Riveros and F. J. Rivas-Silva, *Phys. Lett. A* **377** (2013) 2062, and references therein.
33. M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press, Cambridge, U. K. (2005).
34. S. R. Gadre, *Phys. Rev. A* **30** (1984) 620.
35. Z. Chen, C. S. Wannere Corminboeuf, R. Pucha, P. V. R. Schleyer, *Chem. Rev.* **105** (2005) 3842.
36. K. D. Sen (Ed.), Statistical Complexity, *Applications in Electronic Structure*, (Springer, London, 2011), Chap. 3.
37. M. A. Martínez-Sánchez, N. Aquino, R. Vargas and J. Garza, *Chem. Phys. Lett.* **90** (2017) 14.
38. M. Rodríguez-Bautista, R. Vargas, N. Aquino and J. Garza, *Int. J. Quantm Chem.* (2017); e25571. https://doi.org/10.1002/qua.25571