Ground state energy of the hydrogen atom inside penetrable spherical cavities; variational approach

R. A. Rojas, N. Aquino* and E. Castaño

Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa,
Av. San Rafael Atlixco 186, Col. Vicentina, Iztapalapa, Ciudad de México, 09340, México.
**e-mail: naa@xanum.uam.mx*

Received 22 August 2022; accepted 15 September 2022

In this work we calculate the ground state energy of the hydrogen atom confined in a sphere of penetrable walls of radius R_c. Inside the sphere the system is subject to a Coulomb potential, whereas outside of it the potential is a finite constant V_0. The energy is obtained as a function of R_c and V_0 by means of the Rayleigh-Ritz variational method, in which, the trial function is proposed as a free particle wave function within a finite square well potential but including an exponential factor that takes into account the electron-nucleus Coulomb attraction. For an impenetrable sphere, $V_0 = \infty$, the energy grows fast as R_c approaches zero. On the other hand, when the height of the barrier V_0 is finite, the energy increases slowly as R_c goes to zero. We also compute the Fermi contact term, nuclear magnetic screening, polarizability, pressure and tunneling as a function of R_c and V_0. As expected, these physical quantities approach the corresponding values of the free hydrogen atom as R_c grows. We also discuss the pressure-induced ionization of the hydrogen atom. The present results are found in good agreement with those previously published in the literature.

Keywords: Confined hydrogen atom; penetrable confinement; polarizability; nuclear magnetic screening; pressure-induced ionization; tunneling.

DOI: https://doi.org/10.31349/RevMexFisE.20.010205

1. Introduction

There are few examples in quantum mechanics for which the Schrödinger equation has exact solutions. Otherwise, one ought to resort to approximate methods. Of these, one of the most widely used is the Rayleigh-Ritz variational method, often simply referred to as the variational method. This method is mainly used in problems that do not have analytical solutions or when they are very laborious and difficult to obtain, or in cases where approximate values of the energy and wave functions are only required. The variational method has been utilized since the early days of quantum mechanics and it has successfully been applied to the study of free systems and those subject to any form of spatial constraint (confined). The quantum confined systems are of much interest due to its wide variety of applications for modeling physical phenomena such as potential wells, wires and quantum dots, electronic structure of atoms and molecules subject to external high pressures, specific heats of crystalline solids under high pressures, atoms trapped in cavities, nanopores and into fullerenes, among others [1-25]. Recent progress on the field of confined atoms and molecules can be reviewed in Ref. [24]. As for example, much emphasis has been placed in the study of Shannon entropies [19-22], as well as the study of spectroscopy of confined atomic systems [18] and the use of various methods for solving these problems. A large list of applications can be found in reviews and books on the subject [1-8,24]. Only few articles have been published with a pedagogical point of view, addressing the study of the confined harmonic oscillator (CHO) and the confined hydrogen atom (CHA) [26-32].

Over 80 years ago, Michels *et al.* [10] proposed the CHA model in which a nucleus of positive charge is clamped at the center of an impenetrable sphere of radius R_c with an electron moving inside. The impenetrable walls were proposed to simulate, in first approximation, the potential exerted by other charges surrounding the hydrogen atom. Michels *et al.* [10] were chiefly interested in studying how the polarizability of the hydrogen atom changes when subjected to high pressures. However, it is known that this type of confinement overestimates the observable effects, and therefore, it has been suggested that a soft confinement (a cavity with penetrable walls) would be a model with a more realistic physical meaning.

In the late 70's, Ley-Koo and Rubinstein [11] used the model of a hydrogen atom confined in a spherical box with penetrable walls to explain the experimentally obtained result for the hyperfine splitting of atomic hydrogen in α-quarz. Although they found analytic solutions for the corresponding Schrödinger equation, the energy values were obtained numerically by solving a transcendental equation. They also computed the nuclear magnetic screening, the Fermi contact term, polarizability and pressure as a function of R_c and V_0. Montgomery and Sen [12] improved the theoretical development of Rubinstein and Ley-Koo [11], whereas other authors used the variational method with a different trial wave function to solve this problem [25, 26].

The pedagogically oriented articles addressing studies on the confined hydrogen atom are rather scarce in the literature, as we mentioned above, and furthermore, in most of them, the physical system is assumed to be confined within an impenetrable cavity [26-30]. The purpose of present work is to study the confined hydrogen atom inside a soft spherical box by using the Rayleigh-Ritz variational method, where the trial function consists of a modified free-particle-in-a-box solution. We calculate some physical properties such as the hyperfine splitting, nuclear magnetic screening, polarizability, pressure and tunneling through the barrier as a function of the position and the potential height.

This work is organized as follows: in Sec. 2 we provide some details on the calculation of the confined hydrogen atom ground state energy and some physical properties as a function of R_c and V_0 by using the Rayleigh-Ritz variational method. In Sec. 3 results are shown and compared with those reported in the literature. Finally, in Sec. 4 we give our conclusions.

2. Methodology

The confined hydrogen atom Hamiltonian in atomic units is given by

$$H = -\frac{1}{2}\nabla^2 + V_c. \tag{1}$$

The potential energy associated with the soft spherically confined hydrogen atom is given by a Coulomb term inside the box ($0 < r \leq R_c$, where R_c is the confinement radius), and a barrier of constant height V_0 outside the box ($r > R_c$).

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

For the ground state of the system we use the following trial function,

$$R_i\left(r\right) = A e^{-\alpha r} j_0\left(\frac{\gamma\pi r}{R_c}\right), \quad 0 \leq r \leq R_c, \tag{3}$$

and

$$R_e\left(r\right) = B\frac{e^{-\beta r}}{r}, \quad r > R_c, \tag{4}$$

where A and B are normalization constants and α, β and γ are variational parameters. j_0 refers to the zeroth order spherical Bessel function [33].

Factor $e^{-\alpha r}$ takes into account the nucleus-electron Coulomb interaction. If $\alpha = 0$, Eqs. (3) and (4) correspond to the wave function for a free particle in a finite spherical well [35, 36].

The radial wave function and its first derivative are continuous in all space, in particular at $r = R_c$. By requiring continuity of the radial wave functions through the boundary R_c, one has

$$R_i\left(R_c\right) = R_e\left(R_c\right), \tag{5}$$

which leads to a relation between A and B

$$B = A\, R_c j_0\left(\gamma\pi\right) e^{(\beta-\alpha)R_c}. \tag{6}$$

Continuity of the first derivative of the wave function can be written in terms of the logarithmic derivative at R_c, for the inner wave function,

$$\frac{R_i^{'}(R_c)}{R_i(R_c)} = -\frac{\gamma\pi}{R_c}\frac{j_1(\gamma\pi)}{j_0(\gamma\pi)} - \alpha, \tag{7}$$

and the outer wave function,

$$\frac{R_e^{'}(R_c)}{R_e(R_c)} = -\beta - \frac{1}{R_c}. \tag{8}$$

Continuity of both logarithmic derivatives through R_c, leads to

$$\beta = \alpha + \frac{\gamma\pi j_1\left(\gamma\pi\right)}{R_c j_0\left(\gamma\pi\right)} - \frac{1}{R_c}. \tag{9}$$

Therefore, only two independent variational parameters are needed. On the other hand, one should bear in mind that for any physically acceptable wave function, β must be > 0.

The energy functional in the variational method is given by:

$$E(\alpha,\gamma) = \frac{\langle R|T|R\rangle + \langle R|V_c|R\rangle}{\langle R|R|\rangle}, \tag{10}$$

in which, the overlap integral is

$$\langle R|R\rangle = \int_0^{R_c} R_i^* R_i r^2 dr + \int_{R_c}^{\infty} R_e^* R_e r^2 dr. \tag{11}$$

The kinetic energy integral is given by:

$$\langle R|T|R\rangle = \int_0^{R_c} R_i^*\left(-\frac{1}{2}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}R_i\right)\right)r^2 dr + \int_{R_c}^{\infty} R_e^*\left(-\frac{1}{2}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}R_e\right)\right)r^2 dr, \tag{12}$$

and the potential energy integral by:

$$\langle R|V_c|R\rangle = \int_0^{R_c} R_i^*\left(-\frac{1}{r}\right) R_i r^2 dr + \int_{R_c}^{\infty} R_e^* V_0 R_e r^2 dr. \tag{13}$$

The optimal energy is obtained by minimizing the energy functional with respect to variational parameters α and γ. The optimization was carried out by using the command **FindMinimum** of Mathematica 11.

Physical properties

Once obtained the optimal ground state energy and the corresponding variational parameters α, β and γ, we can calculate some physical properties. Those we have chosen to calculate in this report are:

1. The hyperfine splitting A, given by the Fermi contact term [11, 25]

$$A = (2/3)\, gBg_nB_n|R(0)|^2. \tag{14}$$

2. The nuclear magnetic screening [11, 25], given by the diamagnetic screening constant

$$\sigma = \frac{e^2}{3\mu c^2}\left\langle r^{-1}\right\rangle. \tag{15}$$

3. The polarizability in the Buckingham's approximation [37]

$$\alpha_d = \frac{2}{3}\left[\frac{6\left\langle r^2\right\rangle^3 + 3\left\langle r^3\right\rangle^2 - 8\left\langle r\right\rangle\left\langle r^2\right\rangle\left\langle r^3\right\rangle}{9\left\langle r^2\right\rangle - 8\left\langle r\right\rangle^2}\right]. \tag{16}$$

4. The pressure computed by

$$P = -\frac{1}{4\pi R_c^2}\frac{dE}{dR_c}. \tag{17}$$

5. The tunneling probability of the electron given by the right hand integral in Eq. (11)

$$p\left(r > R_c\right) = \int_{R_c}^{\infty} R_e^* R_e r^2 dr. \tag{18}$$

3. Results

In Table I are shown the optimal values for the variational parameters α and γ, and the ground state energy eigenvalues E of the system, for different radii R_c and barrier heights $V_0 = 0,\ 2$ and 5 Hartrees. These eigenvalues are compared with those reported by Marín and Cruz [25], who also utilized the variational method but with a different trial function. We also compare our values with those of Ley-Koo and Rubinstein [11], whose results can be considered exact up to the reported numerical accuracy. As can be seen, there exists a good agreement between the eigenvalues obtained by the Rayleigh-Ritz variational method by using the here proposed trial function and the results previously reported by other authors [11, 25].

TABLE I. Ground state energy E of the confined hydrogen atom inside a penetrable spherical box of radius R_c and barrier height V_0. Distances are given in Bohrs and energies in Hartrees. Energies obtained in this work in comparison with those reported by Marín and Cruz [25] and Ley-Koo and Rubinstein [11].

R_c	α	γ	E	Ref. [25]	Ref. [11]
			$V_0 = 0$		
0.83155	0.9207	0.3504	−0.0312	−0.0313	−0.0313
1.00000	0.9027	0.4001	−0.1249	−0.1250	−0.1250
2.04918	0.8946	0.4967	−0.4362	−0.4366	−0.4367
4.08889	0.9714	0.3749	−0.4978	−0.4979	−0.4980
5.77827	0.9959	0.1884	−0.4999	−0.4999	−0.4999
			$V_0 = 2$		
0.50746	0.8700	0.4306	1.9606	1.9607	1.9606
0.59179	0.8388	0.4891	1.7149	1.7149	1.7147
1.00791	0.7635	0.6382	0.5014	0.5003	0.5000
4.90402	0.9296	0.6550	−0.4966	−0.4973	−0.4980
5.75669	0.9641	0.5410	−0.4989	−0.4992	−0.4995
			$V_0 = 5$		
0.42945	0.8202	0.5068	4.5915	4.5927	4.5914
0.50502	0.7859	0.5638	3.8585	3.8593	3.8580
1.55982	0.6858	0.8006	−0.0195	−0.0247	−0.0247
5.06334	0.9089	0.7534	−0.4959	−0.4971	−0.4980
5.49360	0.9307	0.7077	−0.4975	−0.4983	−0.4990

The energy eigenvalues $E(R_c)$ grow as the box radius decreases; however, in order for the electron to remain in an atomic bound state the energy must be $E < V_0$. At the same time, this gives rise to the fact that, for a fixed value V_0, the electron remains in a bound state only for boxes whose radius $R_c > R_{crit}$, where R_{crit} is the critical radius at which $E = V_0$. For $V_0 = \infty$ the energy grows, apparently without limit, as $R_c \to 0$.

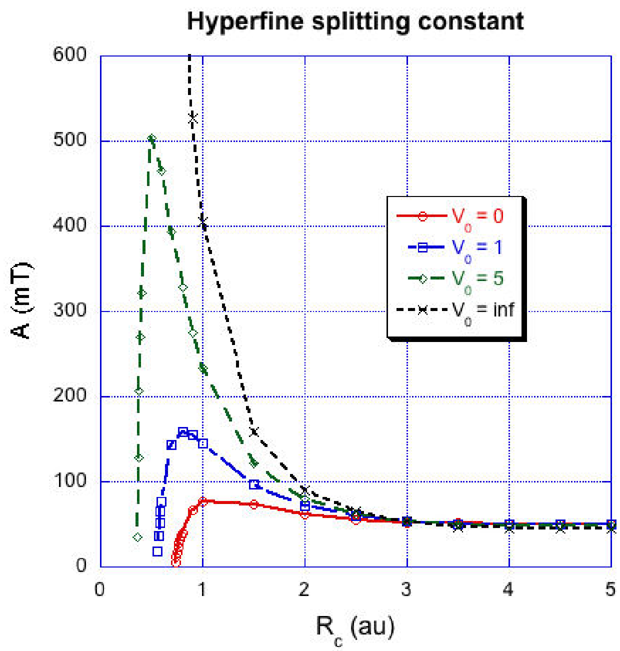

FIGURE 1. Hyperfine splitting constant A (in units 12.690565 mT) as function of R_c (Bohrs) for $V_0 = 0,\ 1,\ 5,\ \infty$, Hartrees.

For boxes of certain particular radii the energy eigenvalues are higher for higher values of V_0, that is, for less penetrable walls. As R_c increases, the energy eigenvalues asymptotically approach those of the free hydrogen atom.

For most of the confinement radii and barrier heights, the calculated energies with the trial function used in this work are equal or they are slightly higher than those obtained by Marín and Cruz [25]. Just for small radii and very high barriers we obtain lower energies.

In Figs. 1 to 4 we show the behavior of the hyperfine splitting A, nuclear magnetic screening σ, polarizability α, pressure P and tunneling probability as a function of R_c, respectively, for different values of V_0.

For a fixed value of V_0 and large confinement radii, A and σ tend asymptotically to the free hydrogen atom values ($A = 50.762$ mT and $\sigma = e^2/3\mu a_0 c^2$). As the confinement radius decreases, these quantities grow monotonically up to a maximum value, and then this quantity decreases fast as R_c approaches to the critical radius $R_{\rm crit}$. For a fixed confinement radius these quantities become larger for higher values of V_0. For $V_0 = \infty$, A and σ grow apparently without limit, as $R_c \to 0$. The corresponding behavior is shown in Figs. 1 and 2.

In the calculations of the polarizability we used Buckingham approximation [37] because it gives better results than the Kirkwood approximation [12], even for large values of R_c. As the confinement radius increases both approximations tend to the same value.

For a finite V_0 and large radii the polarizability tends asymptotically to the corresponding value of the free hydrogen atom, $\alpha_d = 0.5927 \times 10^{-24}$ cm^3. For a decreasing confinement radius the polarizability attains a minimum value and then grows fast up to radius R_c reaches the critical con-

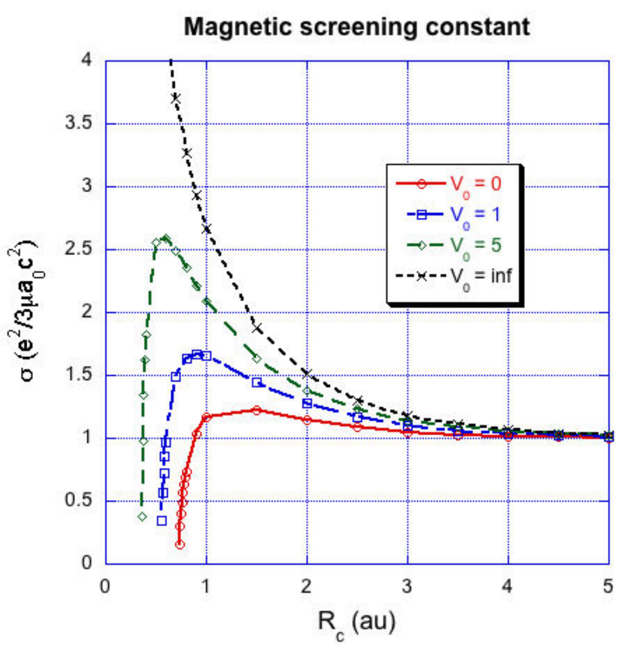

FIGURE 2. Magnetic screening constant (in units $e^2/(3\mu a_0 c^2)$) as a function of R_c (Bohrs) for $V_0 = 0,\ 1,\ 5,\ \infty$, Hartrees.

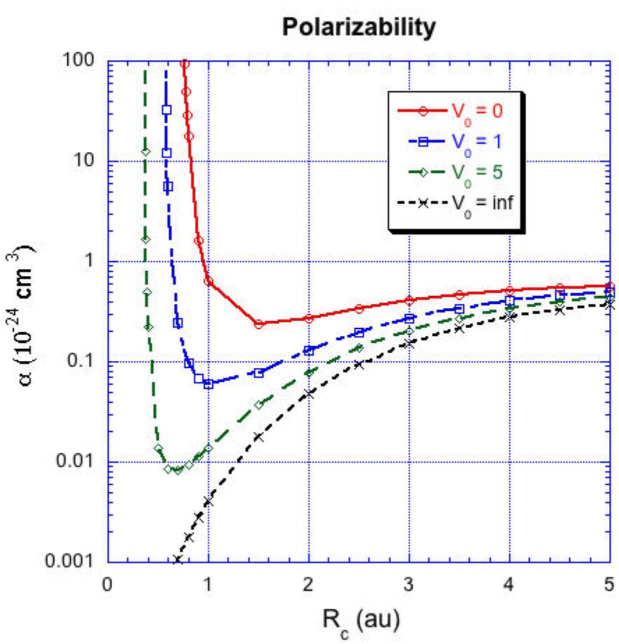

FIGURE 3. Polarizability α_d (in units 10^{-24} cm^3) as a function of R_c (Bohrs) for $V_0 = 0,\ 1,\ 5,\ \infty$, Hartrees.

finement radius R_{crit}. On the other hand, for an impenetrable box, the polarizability tends to zero as R_c correspondingly approaches zero. Opposite to what happens with the Fermi contact term and the diamagnetic screening constant, for less penetrable walls, the polarizability diminishes. For $V_0 = \infty$, the polarizability approaches to zero as $R_c \to 0$. In Fig. 3 we show the behaviour of the polarizability as a function of R_c for few values of V_0.

In previous papers [11, 25], the pressure was computed via the virial theorem

$$P = \frac{1}{4\pi R_c^3}\left(2E - \langle V\rangle\right). \tag{19}$$

This formula is correct for the confinement in an impenetrable sphere. Fernández and Castro pointed out [34] that virial theorem for systems with sectionally defined potentials, like that of the Eq. (2), must be reformulated. In any case, the correct way to compute the pressure is given by Eq. (17).

The derivative involved in Eq. (17) is difficult to obtain in an analytic way because we decided to compute that numerically. The differentiation was performed using the five term centered difference formula [38],

$$\left.\frac{dE}{dR_c}\right|_{r=R_c} = \frac{-E\left(R_c+2h\right)+8E\left(R_c+h\right)-8E\left(R_c-h\right)+E\left(R_c-2h\right)}{12h}, \tag{20}$$

with a step size $h = 0.01$.

Figure 4 we show the behaviour of the pressure as a function of R_c for few values of V_0. For a finite value of V_0 the pressure grows as R_c diminishes, it reaches its maximum value and then diminishes. For an impenetrable box, the pressure shows a different behaviour because this grows without limit as $R_c \to \infty$.

Figure 5 we show the behavior of the energy as a function of the pressure for $V_0 = 5\ au$. At low pressure the energy increases slowly but it grows fast as the pressure approaches to the critical pressure P_{crit}, which corresponds to the pressure on the system at the critical radius R_{crit}. When the external pressure reaches the critical pressure P_{crit}, the system is *ionized*. This critical pressure P_{crit} is different for different values of V_0.

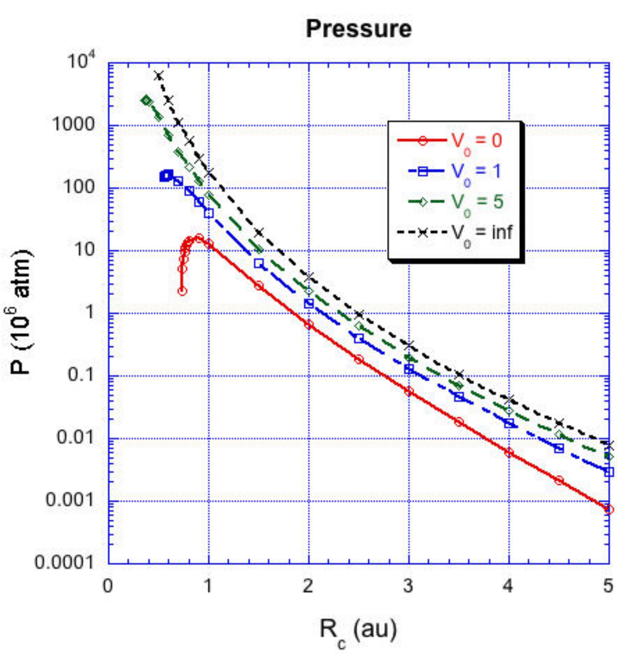

FIGURE 4. Pressure $P(10^6$ atm) as a function of R_c (Bohrs) for $V_0 = 0,\ 1,\ 5,\ \infty$, Hartrees.

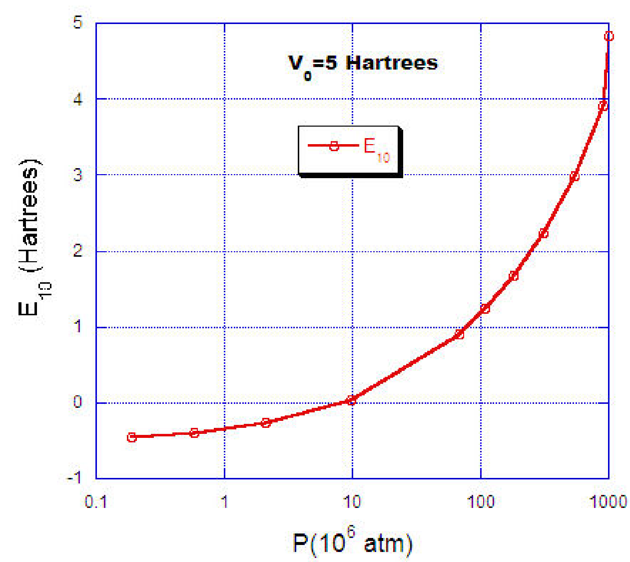

FIGURE 5. Ground state energy of the confined hydrogen atom for $V_0 = 5$ Hartrees as a function of the pressure P.

The Eq. (18) gives the probability to find the electron in the classically forbidden region, and a measure of the tunneling into that region [31]. In Fig. 6 we show the tunneling probability of the electron as function of barrier height, and confinement radius. For a finite value of V_0, as the system is more confined, small R_c, the tunneling probability grows approaching to 1, and decreases fast as the confining radius increases.

4. Conclusions

The present results, as well as those obtained by Marín and Cruz [25], show the usefulness of the direct variational method when studying confined quantum systems, judging

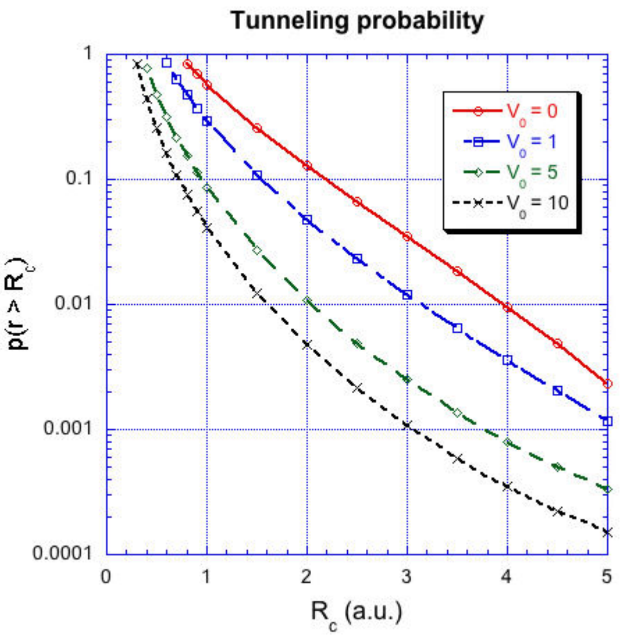

FIGURE 6. Tunneling probability as function of R_c (Bohrs) for $V_0 = 0,\ 1,\ 5,\ 10$, Hartrees.

by the here obtained energy eigenvalues, which are fairly good and the utilized method is easy to handle, unlike, for instance, the one employed by Ley-Koo and Rubinstein, through which, even if exact results could be obtained, it is computationally more difficult to use by comparison.

The behavior of the physical properties of the hydrogen atom confined by penetrable and impenetrable walls is different, this is more evident for small values of V_0, as it is shown in Figs. 1-4 and 6.

Quantum systems inside soft boxes are more realistic and flexible to analyze than those based on impenetrable confinement models, since they allow the description of van der Waals attraction forces produced by neighboring molecules, which may be accomplished by making a proper choice of the barrier height V_0.

The wave function proposed in this work is very similar to that of a free particle in a spherical box [35, 36], where an exponential term is added to account for the nucleus-electron Coulomb interaction in the inner region, so that, the here obtained energies show, expectedly, an improvement for small confinement radii and large barrier heights.

All calculations in this work were performed with Mathematica 11.0, exhibiting no convergence problems, as long as we consider β values > 0.

Montgomey *et al.* [31] point out that when the electronic energy reaches the height of the barrier, pressure-induced ionization occurs. This effect can occur in the atmosphere of gas giant planets [39] and stars [40], where the matter is subject to extreme pressures. The majority of the matter in these systems is hydrogen from the dissociation of molecular hydrogen. The pressure-induced ionization occurs when the individual identities of hydrogen atoms or molecules disappear due to the overlap of the wave functions and a metallic phase is formed. For the formation of the metallic hydrogen are necessary pressures of orders of several hundreds of GPa. In this paper we explained in a pedagogical way the pressure-induced ionization.

Acknowledgments

We thank A. Flores-Riveros and H. E. Montgomery Jr. for their useful comments.

1. F. M. Fernández and E. A. Castro, *Tratamiento hipervirial de sistemas mecano-cuánticos acotados*, Kinam **4** (1982) 193-223.
2. P. O. Fröman, S. Yngve, N. J. Fröman, *The energy levels and the corresponding normalized wave functions for a model of a compressed atom*, J. Math. Phys. **28** (1987) 1813.
3. S. J. Yngve, *The energy levels and the corresponding normalized wave functions for a model of a compressed atom*, J. Math. Phys. **29** (1988) 931 .
4. W. Jaskólski, *Confined many-electron systems*, Phys. Rep. **271** (1996) 1.
5. A. L. Buchachenko, *Compressed atoms*, J. Phys. Chem. **105** (2001) 5839.
6. J. P. Connerade, V. H. Dolmatov and P. A. Lakshmi, *The filling of shells in compressed atoms*, J. Phys. B: At. Mol. Opt. Phys. **33** (2000) 251.
7. J. R. Sabin, E. Brändas and S. A. Cruz, Editors, *Advances in Quantum Chemistry*, vol. **58** (Academic Press, Amsterdam 2009).
8. K. D. Sen, Editor, *Electronic Structure of Quantum Confined Atoms and Molecules* (Springer, New York 2014).
9. L. Bányai and S. W. Koch, *Semiconductor Quantum Dots* (World Scientific, Singapore 1993)
10. A. Michels, J. de Boer and A. Bijl, *Remarks concerning molecular interaction and their influence on the polarizability*, Physica **4** (1937) 981-994.
11. E. Ley-Koo and S. Rubinstein, *The hydrogen atom within spherical boxes with penetrable walls*, J. Chem. Phys. **71** (1979) 351.
12. H. E. Montgomery Jr. and K. D. Sen, *Dipole polarizabilities for a hydrogen atom confined in a penetrable sphere*, Phys. Lett. A **376** (2012) 1992-1996.
13. A.L. Frapiccini and D.M. Mitnik, *Study of hydrogen confined in onion shells*, Eur. Phys. J. D **75** (2021) 41. `https://doi.org/10.1140/epjd/s10053-021-00060-4`.
14. N. Aquino, V. Granados and H. Yee-Madeira, *The Einstein model and the heat capacity of solids under high pressure*,

Rev. Méx. Fís. **55** (2009) 125-129 ; H. de Oliveira Batael, E. D. Filho, J. Chahine and J. F. da Silva, *Efects of quantum confinement on thermodynamic properties*, Eur. Phys. J. D **75** (2021) 52. https://doi.org/10.1140/epjd/s10053-021-00057-z.

15. R. Jha, S. Giri and P.K. Chattaraj, *Does confinement alter the ionization energy and electron affinity of atoms?*, Eur. Phys. J. D **75** (2021) 88. https://doi.org/10.1140/epjd/s10053-021-00106-7.
16. E. P. Wigner and H. B. Huntington, *On the possibility of a metallic modification of hydrogen*, J. Chem. Phys. **3** (1935) 764.
17. K.D. Sen, V.I. Pupyshev, and H.E. Montgomery, *Advances in Quantum Chemistry,* **57**, (Academic Press, Amsterdam 2009). p. 25-77
18. A. N. Sil, S. Canuto, and P.K. Mukherjee, *Advances in Quantum Chemistry* **58**, (Academic Press, Amsterdam 2009) p. 115-175 .
19. K. D. Sen, *Characteristic features of Shannon information entropy of confined atoms*, J. Chem. Phys., **123** (2005) 074110.
20. N. Aquino, A. Flores-Riveros and J. F. Rivas-Silva, *Shannon and Fisher entropies for a hydrogen atom under soft spherical confinement*, Phys. Lett. A. **377** (2013) 2062-2068.
21. M. Rodríguez-Bautista, R. Vargas, N. Aquino and J. Garza, Electron-density delocalization in many-electron atoms confined by penetrable walls: A Hartree-Fock study, Int. J. Quantum Chem. (2017) e25571. https://doi.org/10.1002/qua.25571.
22. C. R. Estañón, N. Aquino, D. Puertas-Centeno and J. S Dehesa, *Two–dimensional confined hydrogen: An entropy and complexity approach,* Int. J. Quantum Chem. (2020) e26192. https://doi.org/10.1002/qua.26192.
23. M. A. Martínez-Sánchez, N. Aquino, R. Vargas and J. Garza, *Exact solution for the hydrogen atom confined by a dielectric continuum and the correct basis set to study many electron atoms under similar confinements*, Chem. Phys. Lett., **90** (2017) 14.
24. E. Ley-Koo, *Recent progress in confined atoms and molecules: Super integrability and symmetry breakings*, Rev. Mex. Fís. **64** (2018) 326-363.
25. J. L. Marín and S. A. Cruz, *Use of the direct variational method for the study of one and two–electron atomic systems confined by spherical penetrable boxes*, J. Phys. B: At. Mol. Opt. Phys. **25** (1992) 4365-4371.
26. J. L. Marín and S. A. Cruz, *Enclosed quantum systems: use of direc variational method*, Am. J. Phys. **59** (1991) 931-935.
27. J. L. Marín, R. Rosas and A. Uribe, *Analysis of asymmetric confined quantum systems by the direct variational method*, Am. J. Phys. **63** (1995) 460-463.
28. F. M. Fernández, *Variational treatment of the confined hydrogen with a moving nucleus*, Eur. J. Phys. **31** (2010) 611.
29. Djajaputra and R. B. Cooper, *Hydrogen atom in a spherical well: linear approximation* Eur. J. Phys. **21** (2000) 261-267.
30. N. Aquino and R. A. Rojas, *The confined hydrogen atom: a linear variational approach*, Eur. J. Phys. **37** (2016) 015401.
31. J. Hunt, J. Martin, V. Rosing, J. Winner and H. E. Montgomery Jr., *Pressure-induced ionization of hydrogen: A computational project*, Chem. Educator **19** (2014) 384.
32. W. S. Nascimento, F. V. Prudente, *Sobre un studo da entropía da Shannon no contexto da mecánica cuantica: uma aplicacao ao oscilador harmonico libre e confinado,* Quim. Nova **39** (2016) 757-764.
33. NIST Digital Library of Mathematical Functions, http://dlmf.nist.gob/10.
34. F. M. Fernández and E. A. Castro, *The virial theorem for systems subjected to sectionally defined potentials*, J. Chem. Phys. **75** (1981) 2908.
35. A. S. Davydov, *Quantum Mechanics*, (Pergamon Press, New York, 1965), Chapter VI.
36. B. H. Bransden and C. J. Joachain, *Quantum mechanics*, 2^{nd} edition (Pearson Prentice Hall, England, 2000), pp. 347-349.
37. R. A. Buckingham, *The quantum theory of atomic polarization I -Polarization by a uniform field*, Proc. Roy. Soc. A, **160** (1937) 94.
38. S. C. Chapra and R. P. Canale, *Numerical methods for engineers*, fifth edition (McGraw Hill, 2006), Chapter 23.
39. G. Chabrier, D. Saumon, W. B. Hubbard and J. I. *The molecular-metallic transition of hydrogen and the structure of Jupiter and Saturn*, Lunine, Astrophys. J., **391** (1992) 817.
40. F. Palla, E. E. Salpeter and S. W. Stahler, *Primordial star formation: the role of molecular hydrogen*, The Astrophysical J. **271** (1983) 632.