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# Effects of size on the spectrum and stability of a confined on-center Hydrogen atom

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**Abstract.** In this work we studied the problem of the stability of confined atoms when they are released from confinement. We analyzed the confined Hydrogen atom inside a cage modelled by a square-well potential, in particular the effects of size on the energy and the electronic structure of the confined atom, by considering different internal radii of the confining cage. Starting from the confined wave function, we clarified the effect on the probability transition between different confined states, and characterized the stability of the atom when released from in term of both, the ionization probability and the transition probability to a bound state of the free atom. The values of the different atomic properties calculated present oscillations when they are studied as a function of the size of the confining cage. This behaviour can be explained in terms of the shell structure of the atom.

*Keywords:* confined systems, electronic structure, ionization probability

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## 1. Introduction

The study of confined systems has attracted considerable interest in recent years due to their promising applications in a wide range of disciplines due to the changes in the physical and chemical properties of a system when it becomes confined. An extensive list of examples can be found, for instance, in [1–4] and the references therein. Some of these applications extend from fields such as optoelectronics [5–11] and the design of nonlinear optical (NLO) materials [12] or, plasma Physics [13–15], to the development of qubits for quantum computing [16], or photovoltaics [17–20], where artificial photosynthesis has been the focus of several works [21, 22]. Hydrogen storage and transportation also deserve special mention, both of which have attracted particular attention owing to the use of this gas as an effective, eco-friendly and clean alternative to fossil fuels [23–25].

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For this reason, over the last few decades, fullerenes (especially  $C_{60}$ ) have emerged as a promising cheap and lightweight system for Hydrogen storage [24, 26–30]. The isomerization of the  $sp^2$ -hybridized carbon network [31] allows us to use fullerenes as storage cages not only for Hydrogen, but for atoms, ions and molecules in general [32, 33]. Moreover, their unique structure and electronic properties make fullerenes useful for applications with NLO materials [34, 35], where the change of the catalytic activity of the confined systems makes use of their fluxional behaviour [36], or in biomedicine [37] for drug design and delivery [38–40].

Consequently, in view of the importance of the subject, many theoretical works on confined systems can be found in the literature [41–54]. Different models of confinement have been proposed to study the properties of confined atoms and molecules, most of which use a potential barrier to model the confinement. Among the models proposed are the infinite [55–58] or finite [59–61] spherical barrier, the harmonic potential [51], a parabolic confinement [62], the gaussian potential [63–67], the square-well potential [32, 68–71], a combination of Woods-Saxon potentials [60, 72, 73], and Lorentzian functions [74]. In the case of fullerenes, the use of the square-well potential or a combination of Woods-Saxon potentials provides suitable results in agreement with experiment [75]. Although some atomic properties can be better described by diffuse potentials [73], others, like energy levels or photoionization spectra of enclosed species, are not affected by the square-well discontinuity [73, 75].

One key question that needs to be addressed is the stability of the encapsulated system when removed from confinement as regards some of the above applications, for example, for a possible use as nanocontainers. Owing to the fact that energy levels of the confined system are different from those of the free system, stability could not to be taken for granted. If it is considered that the confining cavity exerts pressure on the confined atom, which disappears once the atom leaves the cavity, atomic conditions may change in such a way that the atom can become unstable and ionize or, in the case of molecules, instabilities may lead to dissociation or ionization. Despite the importance of this issue, little information is available in the literature [57, 61]. In this work we study the problem of the stability of an atom when it is released from a confining environment, which is closely related to how the electronic structure of the encapsulated species changes. The stability is characterized here in terms of the ionization probability of the confined atom when removed from its cage.

As an initial approach to the subject of stability, we first studied the Hydrogen atom confined by a square-well potential to model an endofullerene [71, 73]. In spite of its simplicity, it contains relevant physical information of the problem and can help to model other more complex and realistic confinement situations. Thus, we first analyze the effects of size on the spectrum and electronic structure of the atom in order to understand the results obtained for the stability.

The structure of this work is as follows: section (2) includes a description of the model and the theoretical approach to studying the confined Hydrogen atom inside the cage. In section (3), we show and discuss the results obtained here. Finally, our

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 conclusions are presented in section (4). Atomic units are used throughout this work.

## 2. Methodology

The Hamiltonian for a Hydrogen atom confined by a spherically symmetric potential,  $V_c(r)$ , can be written as

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r} + V_c(r). \quad (1)$$

A square-well potential is employed to model the confining attractive environment

$$V_c(r) = \begin{cases} -V_0 & \text{if } r_0 \leq r \leq r_0 + \Delta, \\ 0 & \text{otherwise,} \end{cases} \quad (2)$$

where  $r_0$  is the inner radius of the well,  $\Delta$ , the width, and  $V_0$  the depth of the well. The effects of size are studied here by considering different values of the parameter inner radius for fixed  $\Delta$  and  $V_0$  values.

In this work, we have obtained confined stationary states which, due to the spherical symmetry of the problem, are in the form

$$\Psi_{nlm}^c(\mathbf{r}) = \frac{u_{nl}^c(r)}{r} Y_{lm}(\Omega), \quad (3)$$

with  $Y_{lm}(\Omega)$  the Spherical Harmonics and  $u_{nl}^c(r)$  the reduced radial function, which is calculated by solving the radial Schrödinger equation

$$\frac{d^2 u_{nl}^c(r)}{dr^2} + \left[ 2E_{nl}^c + \frac{2Z}{r} - \frac{l(l+1)}{r^2} - 2V_c(r) \right] u_{nl}^c(r) = 0 \quad (4)$$

with the usual boundary conditions for bound states;  $E_{nl}^c$  is the energy of the confined state.

In this work, we solved the radial Schrödinger equation, (4), by using the analytic continuation method [57, 61, 76–78]. The basic idea is to expand the solution around each tabular point,  $r_t$ , in a power series. Thus, the solution around the origin is written as a Frobenius series [79],

$$u(r) = \sum_{j=0}^{\infty} b_j r^{l+j+1}, \quad (5)$$

while for the other tabular points,  $r_t \neq 0$ ,  $t = 1, 2, \dots$ , it produces

$$u(r) = \sum_{j=0}^{\infty} c_{tj} (r - r_t)^j. \quad (6)$$

In practice, the series are truncated at a given  $N$  value that governs the accuracy of the method; the reduced radial wave function is therefore written as a piece-wise polynomial function. When the proposed solution around the origin, (5), is substituted into the radial Schrödinger equation, (4), a three term recursion relationship is obtained for the  $b_j$  coefficients. This equation is solved by using both the regularity and normalization conditions to initialize the recursion. The values of the  $c_{tj}$  coefficients

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are also calculated by employing the three term recursion relationship obtained by substituting the proposed solution, (6), into the radial Schödinger equation, (4). The recursion is initialized at any given  $r_t$  value by using the solution at  $r_{t-1}$  and applying the condition of the continuity of the radial function and its first derivative.

Here, equally-spaced tabular points with step size  $\sim 10^{-4}$  and polynomial expansions of degree  $N = 20$  have been employed. These parameters lead to accuracies of 18 decimal digits in the eigenvalues. All of the recursion relationships involve the energy eigenvalue  $E_{nl}^c$ . A shooting method is used to compute the eigenvalue, carrying out inward and outward integrations and imposing the continuity of the log derivative at an intermediate point [57].

Once the wave functions were known, we calculated physically relevant magnitudes for the problem such as the Dipole Oscillator Strength (DOS) or the ionization probability. The DOS is related to the transition probability from the ground state to an excited state. Owing to the spherical symmetry of the problem considered, the DOS between the ground state,  $1s$ , and the excited state,  $np$ , can be reduced to

$$f_{np,1s} = \frac{2}{3}(E_{np} - E_{1s}) \left| \int_0^\infty dr u_{np}^c(r) r u_{1s}^c(r) \right|^2 \quad (7)$$

which is known as the mean Dipole Oscillator Strength [79].

The ionization probability can be obtained as

$$P_I = \int_0^\infty dE |C^{nl}(E)|^2, \quad (8)$$

where  $|C^{nl}(E)|^2 dE$  represents the probability that the electron, which is initially in the  $\Psi_{nlm}^c$  confined state, becomes ionized with energy between  $E$  and  $E + dE$  when released from the cage. If we employ the sudden approximation [80], the  $C^{nl}(E)$  functions can be calculated as

$$C^{nl}(E) = \int_0^\infty dr u_{El}^f(r) u_{nl}^c(r), \quad (9)$$

where  $u_{El}^f(r)$  is the reduced radial function of the ionized H atom with energy  $E$  and angular momentum  $l$ . The ionization probability can also be written in terms of  $P_B$ , the probability that the atom remains in a bound state when removed from confinement,

$$P_I = 1 - P_B, \quad (10)$$

where  $P_B$  is calculated as

$$P_B = \sum_{n'=1}^{\infty} |C_{n'}^{ml}|^2, \quad C_{n'}^{ml} = \int_0^\infty dr u_{n'l}^f(r) u_{nl}^c(r). \quad (11)$$

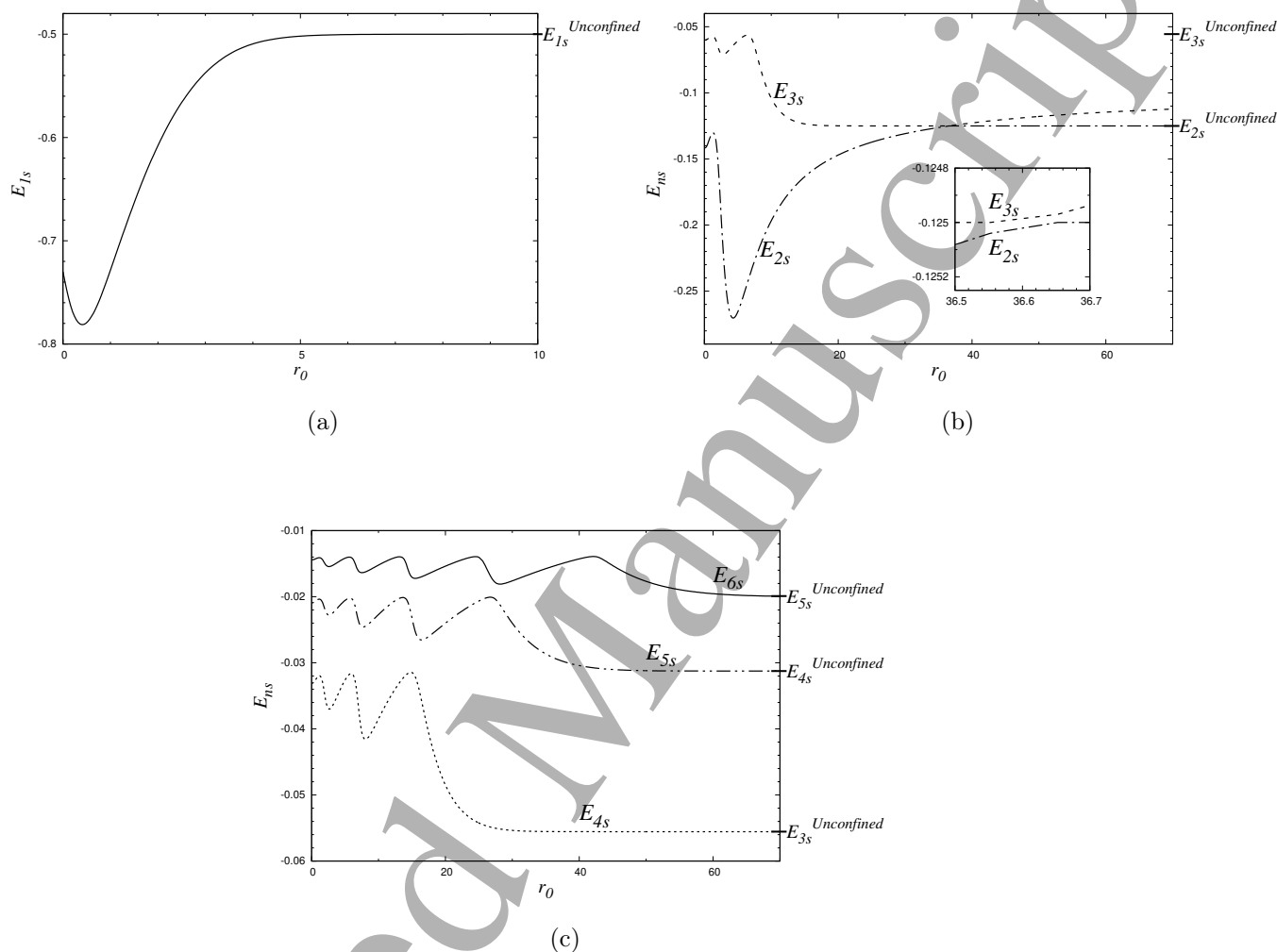
### 3. Results and discussion

In figure 1, we study the effects of size on the single particle spectrum of the confined H atom. We plot the energy of the  $1s$  to  $6s$  states as a function of the inner radius of the square-well,  $r_0$ , for fixed values of potential depth,  $V_0 = 0.422$ , and width,  $\Delta = 1.25$ ,

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generally used to model a  $C_{60}$  fullerene [73, 75]. Here, we can distinguish three different kinds of behaviours for the orbital energies. For the ground state, the effect of the confinement is significant only for  $r_0 \lesssim 5$ . The energy initially decreases and presents a minimum at  $r_0 \approx 0.5$ , and then increases, reaching the value of the free atom at  $r_0 \approx 5$ . The behaviour of the energy of the  $2s$  and  $3s$  orbitals is different from that of the other orbitals. Cage effects for the  $2s$  energy are relevant for sizes up to  $r_0 \approx 40$ , with a maximum and minimum for lower values of the confinement radius, and reaches the free orbital value as  $r_0$  increases. The  $3s$  orbital does not reach the free atom value as  $r_0$  rises (for the sizes studied here) and presents two maxima and one minimum for small confinement sizes. Finally, for inner radii between 36.5 and 36.7, as can be seen in the inset of figure 1(b), the energies of the  $2s$  and  $3s$  orbitals are very similar but do not cross. The behaviour for the other excited bound states is different, showing a series of maxima and minima as a function of  $r_0$ , see figure 1(c), where we plot the energy for the  $4s$ ,  $5s$  and  $6s$  orbitals, which are representative of the other excited states. For  $ns$  orbitals with  $n \geq 4$ , the asymptotic value of the energy as the cage size increases is that of the free  $(n-1)s$  orbital,  $E_{ns} = -1/(2(n-1)^2)$  for  $n \geq 4$ , and the number of maxima is  $n-1$ , *i.e.*, the number of nodes of the radial function. The data of such figures can be found in the supplementary material.

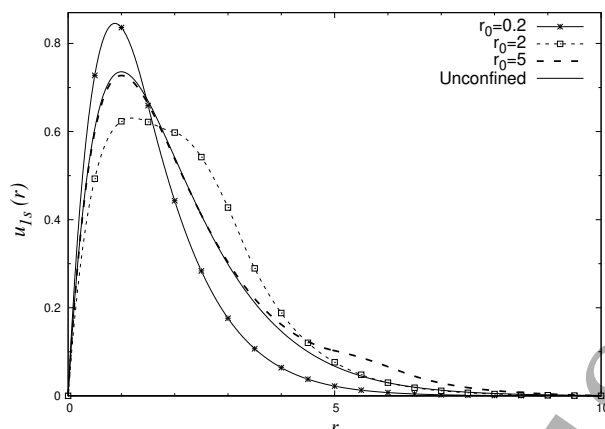
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**Figure 1.** (a) Energy of the 1s orbital as a function of inner square-well radius,  $r_0$ ; (b) same for 2s and 3s; (c) same for 4s, 5s and 6s states

In order to understand the behaviour of the orbital energies, we studied the confined radial functions. In figure 2 we plot the reduced radial orbital of the ground state for several representative values of the cage size,  $r_0$ , and the free orbital for the sake of comparison. For  $r_0 = 0.2$ , the effect of the cage is to trap charge in the well, reducing the potential energy and increasing the kinetic energy, with a net effect of a total energy lowering. As the well radius increases, the charge distribution becomes more spread and the total energy increases, but it is still smaller than the energy of the free atom. For cage sizes larger than  $r_0 \approx 5$ , the effect of the well on this orbital is negligible.

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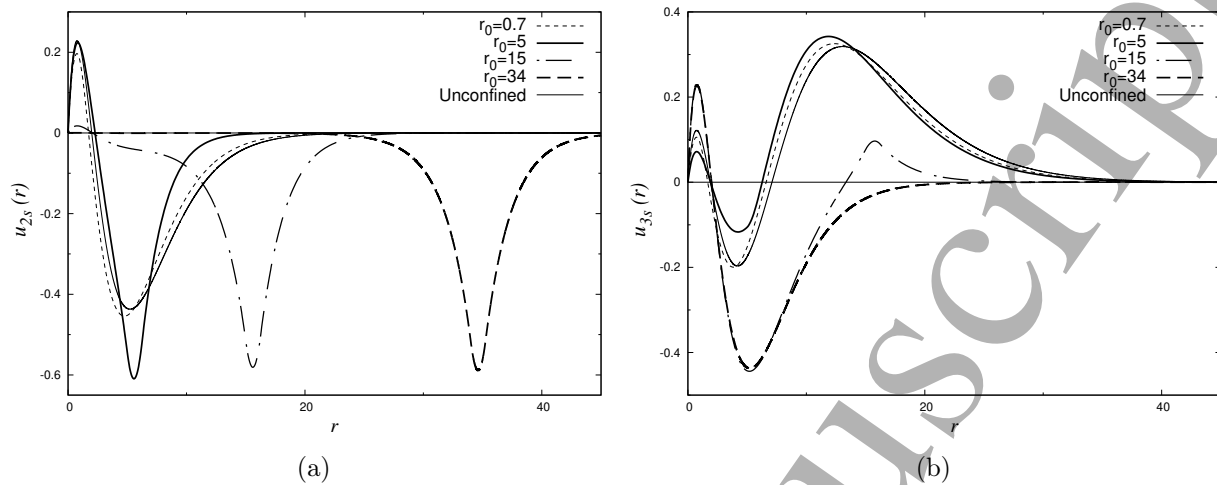
**Figure 2.** Reduced radial function,  $u(r)$ , of the  $1s$  orbital for  $r_0 = 0.2, 2$  and  $5$ . The free orbital is also plotted

In figure 3(a), we plot the reduced radial function of the  $2s$  orbital for several representative values of the cage size,  $r_0$ . The unconfined orbital is also plotted. For  $r_0 \lesssim 1$  the effect of the cage is small and consists of reducing the charge distribution and increasing the energy. When the well is located in the second shell position of the unconfined atom,  $r_0 \approx 5$ , *i.e.* the second maximum of the charge distribution, the energy reaches a minimum and most of the electric charge is located within the well. As  $r_0$  increases, as is illustrated in the figure for  $r_0 = 15$ , the first shell tends to disappear and the orbital resembles that of the ground state of the well, with a minor contribution of the Coulomb interaction with the atomic nucleus. Thus, for  $r_0 = 34$  the confined  $2s$  radial function presents a node which is indistinguishable within the scale of the figure, making the first shell negligible. As the inner radius of the cage increases, the energy of the orbital increases due to decreased nuclear attraction. This situation holds for cage sizes of  $r_0 \lesssim 36$ .

In figure 3(b), we plot the reduced radial function of the  $3s$  orbital for the same cage sizes as in figure 3(a). For  $r_0 \lesssim 5$ , confinement does not affect this orbital much. The charge is compressed towards the nucleus, increasing the kinetic energy and lowering the potential energy. This competition leads to the oscillatory behaviour shown in figure 1(c); the minimum corresponds to a well located in the region of the first shell, while the two maxima appear when the well is in a zone with almost no charge. For  $5 \lesssim r_0 \lesssim 36.5$ , the third atomic shell gradually vanishes and the charge density shrinks toward the nucleus in such a way that the confined  $3s$  orbital behaves like the free  $2s$  orbital. Thus, for  $r_0 = 34$ , the third node of the  $3s$  cannot be observed within the scale of the figure. As a result, the energy of the confined  $3s$  orbital approaches the energy of the  $2s$  orbital of the free H atom and the confined  $2s$  orbital for this radius. Although the electronic structure of these orbitals is very different, their energies are very close for  $r_0 \approx 36.5$ , see inset of figure 1(b).

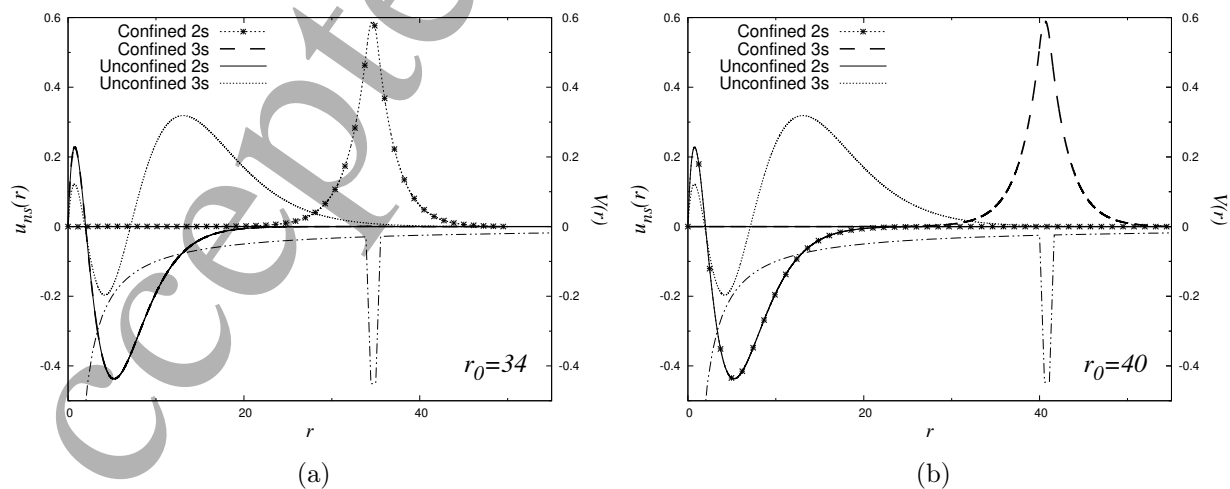


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**Figure 3.** (a) Reduced radial function,  $u(r)$ , of the 2s state for  $r_0 = 0.7, 5, 15$  and 34. The free state is also shown. (b) Same for 3s state

For  $r_0 \gtrsim 36.5$ , confinement effects on the 2s orbital become negligible, see figure 1b, and the confined and unconfined 2s orbitals practically overlap, while the electron cloud of the 3s orbital is located within the well. This is illustrated in figure 4, which shows the radial function of these orbitals for  $r_0 = 34$  and  $r_0 = 40$ . The radial functions for the unconfined H atom are also plotted for the sake of comparison. It is worth remembering that the orbitals of the excited states have the right number of nodes, although they cannot be seen within the scale of the figure. As the size of the cage increases, the effect of confinement on the 1s and 2s orbitals becomes negligible while the 3s orbital continues to be trapped within the well. For this reason, the asymptotic energy of this orbital is not the energy of the free orbital - see figure 1(b).

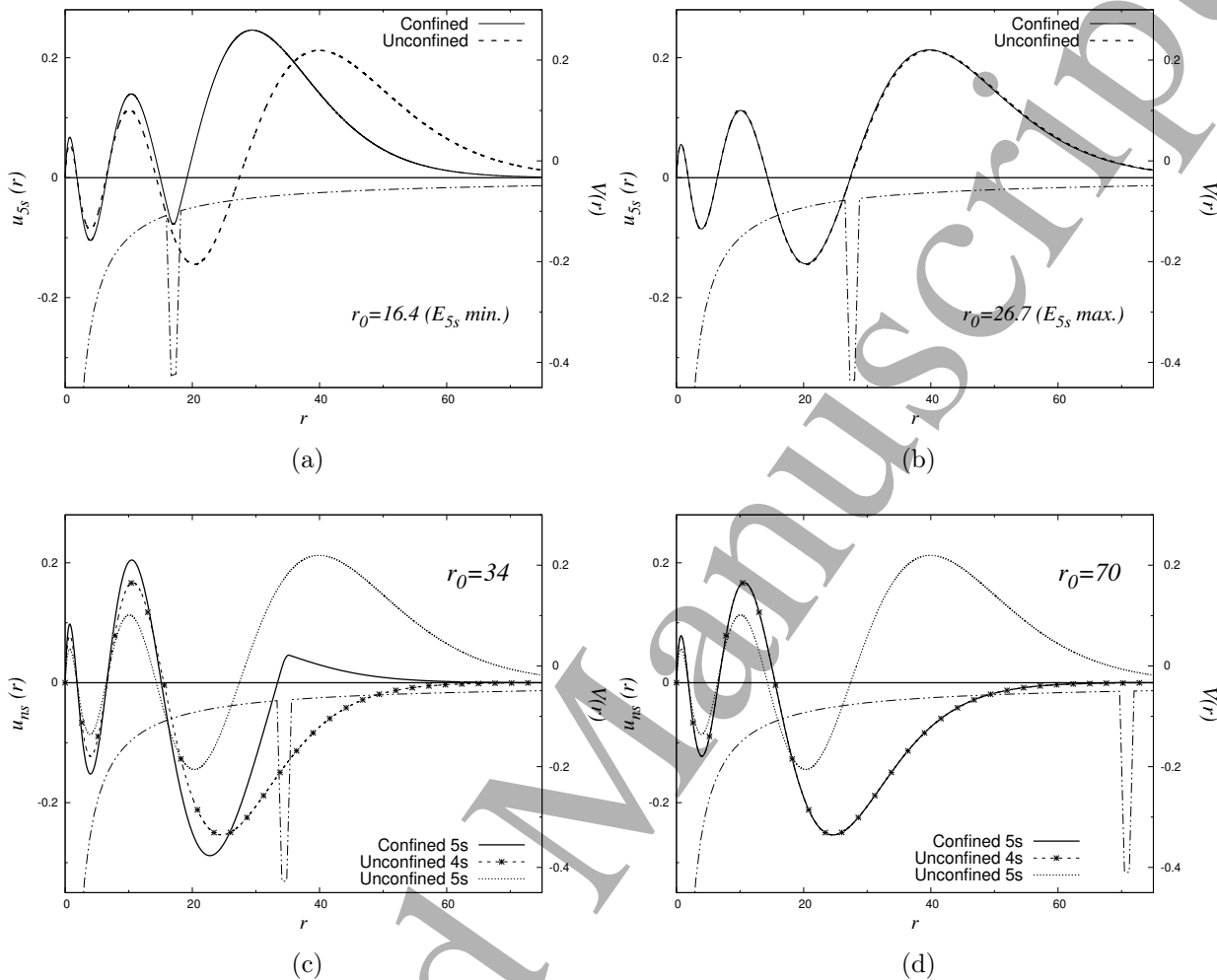


**Figure 4.** (a) Reduced radial functions,  $u(r)$ , of the 2s and 3s orbitals for  $r_0 = 34$ . The effective potential and the free states are also plotted. The free 2s and confined 3s orbitals overlap. (b) Same for  $r_0 = 40$ . Free 2s and confined 2s orbitals overlap

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Figure 5 shows the effect of the cage on the  $5s$  orbital for several representative  $r_0$  values, which illustrates the behaviour of higher excited states. As was the case of previous orbitals, when the well was located at a maximum point of the free atom charge distribution, the energy decreases, while the opposite occurs when it is near a node. In the latter case, the state is practically unmodified by the confining potential and its energy is similar to that of the free atom. This explains the sawtooth structure of the energy as a function of  $r_0$  for these states, with a number of maxima equal to the number of nodes of the radial function - see figure 1(c). In figure 5(c), we plot the reduced radial function for  $r_0 = 34$ , the location of the outermost shell of the free  $5s$  orbital. In this case, the effect of confinement is to shrink the charge towards the nucleus by diminishing the charge in the outermost shell. This effect is enhanced as larger  $r_0$  values are considered - see figure 5(d), where we plot the reduced radial function for  $r_0 = 70$ . For this radius the outermost shell is located in the well and is negligible, therefore the node is not visible within the scale of the figure. The confined  $5s$  orbital therefore behaves in the same way as the unconfined  $4s$  orbital. This is the same behaviour as in other  $ns$  confined states that approach the free  $(n - 1)s$  orbitals for cage sizes larger than the outermost shell.

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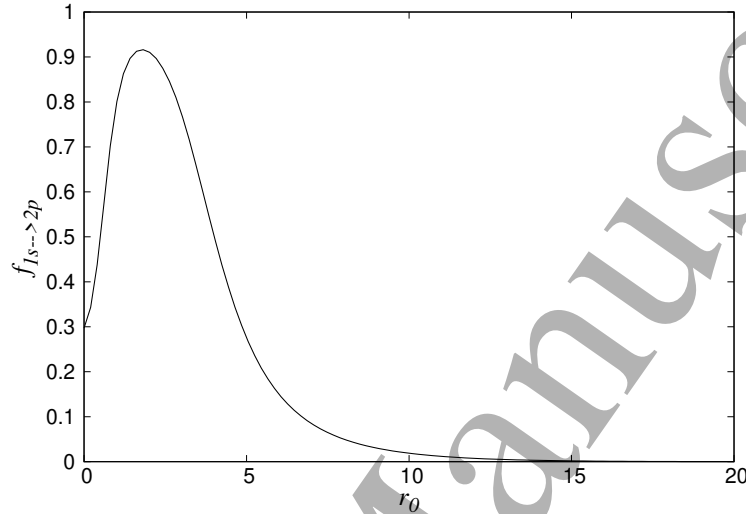


**Figure 5.** (a) Reduced radial function,  $u(r)$ , of free and confined 5s orbital for  $r_0 = 16.4$ , corresponding to minimum in the orbital energy. The potential is also shown. (b) The same for  $r_0 = 26.7$ , which provides a maximum value of the orbital energy. (c) Same for  $r_0 = 34.0$ ; the 4s free orbital is also plotted. (d) Same as (c) for  $r_0 = 70.0$ .

These changes in the charge distribution within the cage give rise to substantial modification of certain atomic properties. One important case is the transition probability between confined bound states. Here, we consider the probability of a transition between the ground and the  $2p$  state, which is representative for other transitions. The value of the Dipole Oscillator Strength for this transition for the free atom is  $f_{1s \rightarrow 2p} = 0.4162$  [81]. For the confined atom with potential parameters  $r_0 = 6.01$ ,  $V_0 = 2$  and  $\Delta = 1.25$ , a set of parameters which has been previously studied in [73], we obtained  $f_{1s \rightarrow 2p} = 0.6825$ , in agreement with the results reported in the aforementioned work. In figure 6, we study the effects of size due to confinement for this magnitude. The DOS presents a maximum value of around 0.9 for cage sizes of  $r_0 \approx 1.8$ , which disappears as  $r_0$  increases. The reason for this behaviour lies in the different charge distribution of the orbital when the atom is in the cage. For  $r_0 \approx 1$ , the two orbitals

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1s and 2p are practically superimposed, while at large distances, the confined 1s is near the nucleus while the 2p is trapped in the well. It is worth noting that the excitation energy for  $r_0 = 1.8$  is  $E_{2p}^c - E_{1s}^c = 0.361$ , similar to, but smaller than, the excitation energy of the free atom, 0.375.



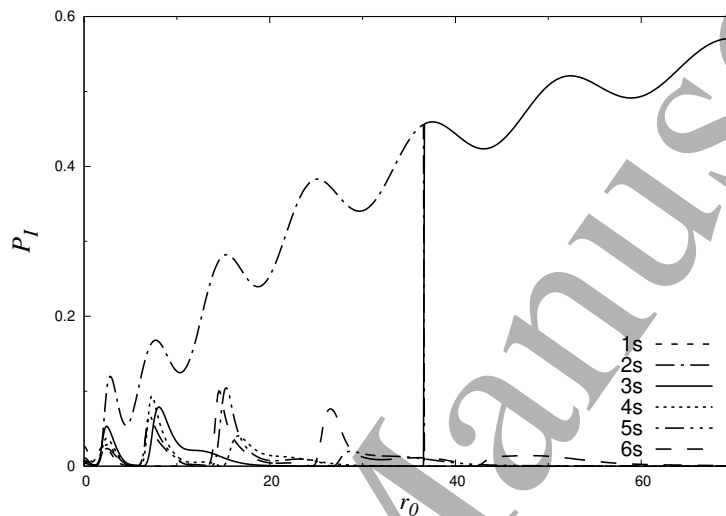
**Figure 6.** Dipole Oscillator Strength for the  $1s \rightarrow 2p$  transition as a function of  $r_0$

Finally, we studied the effects of confinement on the stability of the atom when it is released from confinement. Figure 7 shows the effects of size on the ionization probability of the 1s to 6s confined orbitals. The ionization probability exhibits oscillatory behaviour as a function of  $r_0$ . The maximum ionization probability is shown by the orbital trapped within the well, *i.e.* 2s for  $r_0 \lesssim 36.5$  and 3s for larger inner radii. For the trapped orbital, the ionization probability increases with the cage size, reaching values above 0.5. The ionization probability decreases abruptly for the 2s orbital when it leaves the well, while the opposite occurs for the confined 3s orbital. The ionization probability of the other orbitals is below 0.1. Furthermore, it is worth noting that the excitation energy of a confined orbital is smaller than the ionization energy of the free atom.

This behaviour of the ionization probability is different from that obtained in previous works where other confinement models were considered. In [57] a spherical hard wall potential, which accounts only for size effects, was studied. The probability of ionization in that case was very high and practically constant for small sizes and decreased monotonically as the cavity size increased. In [61] stability of confined H when confinement is removed was analyzed by considering a model of a penetrable spherical barrier, which accounts not only for the size of the confinement but also for the strength of the potential. The ionization probability for that model showed sharply peaked local maxima at some values of the confinement radius, which are originated by the tunnelling and re-tunnelling of the electronic cloud of the atom across the barrier. In both cases, the behaviour of the ionization potential in terms of the confinement size is different

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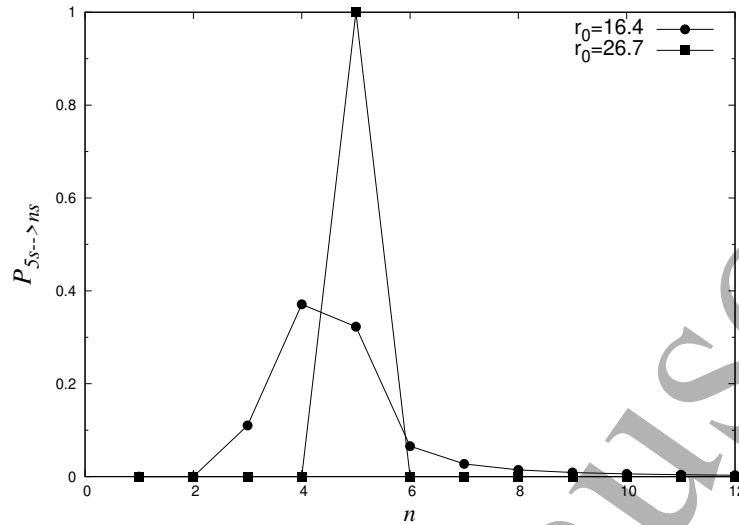
to that here found. The physical origin of the behaviour of the ionization probability for the attractive potential here considered lies in the fact that the electronic charge is located within the well for some values of the confinement radius. Therefore, the stability of the atom when confinement is removed presents an important dependence not only on the size of the cavity but also on the form of the potential.



**Figure 7.** Ionization probability of the 1s – 6s states as a function of  $r_0$

The probability that the atom remains in an excited bound state provides complementary information about the stability of confined species when they are released from confinement. In figure 8 we show  $P_{5s \rightarrow ns}$ , the probability that, starting from a confined 5s state, the final free state is  $ns$ . These results are representative for the other confined initial bound states. We show the results for two different confinement radii,  $r_0 = 16.4$  and  $r_0 = 26.7$ , corresponding respectively to a minimum and a maximum of the orbital energy as a function of  $r_0$  respectively. For  $r_0 = 16.4$  we find a non-negligible probability for the different final free states; however, for a confinement radius of  $r_0 = 26.7$ , practically the only possible final state is the 5s. The former cage size corresponds to a well located in the neighborhood of an atomic electronic shell, see figure 5(a), while in the latter case, the well is in the region between the shells and hardly modifies the atomic orbital at all - see figure 5(b). This behaviour is generally seen in other orbitals, in such a way that the shell structure of the free atom governs the stability of the system when it is released from confinement. Thus, when the well is located in the neighborhood of an electron shell, the final state is a mixed state, while when the well is in a charge distribution node, the final state has the same quantum number as the initial one. For cage radii larger than the outermost electron shell of the confined  $ns$  state, the final state is the free  $(n - 1)s$  state.

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**Figure 8.** Transition probabilities to bound  $ns$  states of the free atom for an initial  $5s$  orbital for  $r_0 = 16.4$  and  $r_0 = 26.7$ . Lines are used as visual guides

#### 4. Conclusions

Here we studied the stability of a confined Hydrogen atom when removed from confinement by a cage. A square-well potential has been used to model the cage. We obtained the ionization and excitation probabilities for different initial states and studied the effects of size. For the confinement potential model studied here, the  $2s$  orbital is trapped in the well for radii of the cage,  $r_0$ , smaller than 36.6, while the  $3s$  remains inside the well for larger cage radii. This leads to a high ionization probability if the initial state is trapped in the well, reaching values above 0.5 for the  $3s$  state, while the ionization probability for the other confined orbitals exhibits oscillatory behaviour as a function of the cage radius, with maximum values of 0.1.

The energies of the confined states present a series of local maxima and minima as a function of the cage size, in such a way that when the well is located in an unconfined electronic shell, the energy is at a minimum, while the opposite occurs when the well is near the nodes of the radial function. Thus, the energy of the  $ns$  orbital with  $n > 3$  as a function of the cage radius, presents a sawtooth structure with  $n - 1$  maxima and asymptotically converges to the energy of the free  $(n - 1)s$  state, because the  $3s$  orbital is located in the well for large radii. For the attractive environment model considered here, the ground state energy of one electron in the well, without nuclear attraction, is between the  $2s$  and  $3s$  orbital energies of the free Hydrogen atom. If other parameters of the confining potential are considered, the atomic orbital with unconfined energy just above that of the ground state of the well is trapped for large confinement sizes and presents the greatest ionization probability. Thus, the stability and the behaviour of other properties of the confined atom are governed by the shell structure of the free atom with respect to the size of the cage.

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