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A Confined Hydrogen Atom in Higher Space Dimensions

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Abstract We compute ground state energies for the N-dimensional hydrogen atom confined in an impenetrable spherical cavity. The obtained results show their dependence on the size of the cavity and the space dimension N. We also examine the value of the critical radius of the cavity in different dimensions. Furthermore, the number of bound states was found for a given radius S, in different space dimensions.

Keywords Quantum mechanics · Formalism · Bound states · Atoms in cavities

1 Introduction

Quantum confinement effects on the physical properties of a system has been a subject of great importance in physics [1–8]. The hydrogen atom confined to bounded regions has long been investigated by many authors [9–11]. Recently, parabolically confined hydrogen atom has been discussed [12]. Different methods have been used in the study of the confined hydrogen atom: Baye and Sen used the Lagrange-mesh method [13], Costa et al. used the woods- Saxon potential [14], Guimaraes et al. considered the finite element method [15]. Over the past two decades, the generalization of the three-dimensional quantum problems to higher dimensions received a considerable development in theoretical and mathematical physics. For example, the N-dimensional analogy of the hydrogen atom has been investigated extensively over the years [16–18]. In addition, the generalization to higher dimensions is useful in random walks [19], in Casimir effect [20], in harmonic oscillator [20–22], and in mathematical physics [23–26].

In the present paper, we consider an N-dimensional hydrogen atom that is confined in an impenetrable spherical cavity. The paper is organized as follows: In Sect. 2, we present the solution to the confined hydrogen atom in a spatial dimension N. In Sect. 3, we calculate

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the ground state energies for the confined hydrogen atom in different space dimensions and different radii of the confining cavity. In Sect. 4, we examine number of bound states for the confined hydrogen atom in different dimensions and we further calculate the critical radius of the cavity at which the binding energy becomes zero. Section 5 is devoted for conclusions and results.

2 The N-dimensional Hydrogen Atom

We consider a hydrogen atom that is confined at the center of an N-dimensional spherical cavity of radius S. It is assumed that the walls of the cavity to be impenetrable. The potential to be considered is

$$V(r) = \begin{cases} \dfrac{-ze^z}{4\pi\varepsilon_0 r}, & 0 \le r \le S \\ \infty, & \text{elsewhere} \end{cases} \tag{1}$$

In the approach by Stillinger [27], and later by He [28], the Schrödinger equation is solved in dimension N, for central potentials $V(r)$ only, by first writing the N-dimensional Laplacian operator ∇^2 in the form

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{(N-1)}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Omega^2 \tag{2}$$

where r is the radial coordinate and Ω^2 is the Laplace operator on the unit hyper-sphere R^{N-1}. Using separation of variables, the Schrödinger equation splits into radial and angular differential equations with the latter having solutions that are independent of the form of the central potential. The eigenvalues of Ω^2 are $-\ell(\ell+N-2)$, with ℓ being a non-negative integer, and thus the Laplacian operator ∇^2 becomes,

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{(N-1)}{r}\frac{\partial}{\partial r} - \frac{\ell(\ell+N-2)}{r^2} \tag{3}$$

The radial part solution, $R(r)$, satisfies

$$r^{1-N}\frac{d}{dr}\left(r^{N-1}\frac{dR}{dr}\right) - \frac{\ell(\ell+N-2)}{r^2}R + \frac{2\mu}{\hbar^2}\left(\frac{ze^2}{4\pi\varepsilon_0 r} - E\right)R = 0 \tag{4}$$

Considering $E < 0$ for bound states and defining λ and ρ as

$$\lambda = \frac{\hbar}{a_0}\frac{1}{\sqrt{-2\mu E}} \tag{5}$$

$$\rho = \frac{2}{\lambda a_0} r \tag{6}$$

with $a_0 (= \frac{4\pi\varepsilon_0\hbar^2}{z\mu e^2})$ is Bohr radius, (4) becomes,

$$\frac{d^2R}{d\rho^2} + \left(\frac{N-1}{\rho}\frac{dR}{d\rho}\right) - \frac{l(l+N-2)}{\rho^2}R + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)R = 0 \tag{7}$$

Writing the solution, $R(r)$ in the form

$$R(r) = \rho^{\ell} e^{-\rho/2} W(\rho) \tag{8}$$

enables us to write (7) as

$$\frac{d^2W}{d\rho^2}+\left(\frac{2\ell+N-1}{\rho}-1\right)\frac{dW}{d\rho}+\left(\frac{\lambda-\ell-(N-1)/2}{\rho}\right)W(\rho)=0. \tag{9}$$

The above differential equation is just the Kummer-Laplace differential equation whose standard form is given by

$$z\frac{d^2W}{dz^2}+(b-z)\frac{dW}{dz}-aW(z)=0 \tag{10}$$

and whose solution, regular at the origin, is the confluent hypergeometric function, ${}_1F_1(a,b,z)$ given by

$${}_1F_1(a,b,z)=\sum\frac{(a)_nz^n}{(b)_n(n)!} \tag{11}$$

where the Pochhammer symbol $(a)_n$ is defined by [29]

$$(a)_n=a(a+1)(a+2)(a+3)\cdots(a+n-1). \tag{12}$$

Comparing (9) with (10) and with the identification

$$a=\ell+\frac{N-1}{2}-\lambda \tag{13}$$

$$b=2\ell+N-1 \tag{14}$$

allows us to write the solution of (9), up to a multiplicative constant, as ${}_1F_1(\ell+(N-1)/2-\lambda,2\ell+N-1,\rho)$. With the help of (8), the desired solution to (7) immediately follows, namely

$$R(r)=A\rho^{\ell}e^{-\rho/2}{}_1F_1\left(\ell+\frac{N-1}{2}-\lambda,2\ell+N-1,\rho\right) \tag{15}$$

with A is a normalization constant.

3 The Ground State Energies for the Confined Hydrogen Atom

Our purpose here is to investigate the effect of the size of the cavity and the space dimension on the ground state energy of the confined hydrogen atom. Since the cavity is assumed to be impenetrable, the confluent hypergeometric function ${}_1F_1(a,b,z)$ must vanish at the surface of the cavity, *i.e.* at $r=S$. Therefore, (6) implies that $\lambda=2S/\rho a_0$, and thus we are seeking (for $\ell=0$) the roots of ${}_1F_1(\frac{N-1}{2}-\frac{2S}{\rho a_0},(N-1),\rho)$. Letting χ_n be the nth root of ${}_1F_1$ which means that $\rho=\chi_n$, gives us

$$\lambda=\frac{2S}{a_0\chi_n} \tag{16}$$

Hence (5) yields the bound-state energy eigenvalues, namely

$$E_n=\frac{-\hbar^2}{2\mu a_0^2}\frac{1}{\lambda^2}=\frac{-\hbar^2}{2\mu}\frac{\chi_n^2}{4S^2} \tag{17}$$

Upon using the value of the ground-state energy in three dimensions [30] which is $E_0 = -\frac{\hbar^2}{2\mu a_0^2} = -13.6$ eV, (17) becomes

$$E_n = \frac{\chi_n^2 a_0^2}{4S^2} E_0 \tag{18}$$

For later comparison between the energies of the confined hydrogen atom and the free one, we write the energy of the free hydrogen atom in N dimensions [31], namely

$$E_{n\,\text{free}} = \frac{E_0}{(n + \frac{(N-3)}{2})^2} \tag{19}$$

It must be noticed that in searching for the roots χ_n of ${}_1F_1(\frac{N-1}{2} - \frac{2S}{\rho a_0}, (N-1), \rho)$ one must choose the root with the largest value, χ_1 which yields the ground-state energy (E_1) as seen from (18). It may be instructive to write down the ground-state eigen-functions ($n = 1$) for the confined hydrogen atom by using (15) with $\ell = 0$, the result is

$$R(r) = A \exp(-\chi_1 r/2S)\, {}_1F_1\left(\frac{N-1}{2} - \frac{2S}{a\chi_1}, (N-1), \frac{\chi_1}{S} r\right) \tag{20}$$

The search for the root with largest value (χ_1) is carried out using Mathematica software. We have located the zeros of ${}_1F_1$ for $\ell = 0$ with different radii of the cavity for a given space dimension N. Once the zeros are found, the ground-state energies in eV are computed by using (18). Our results are shown, for $N = 3$ to 10, in Tables 1–3.

These results show that, for a given N, as the radius of the cavity decreases the ground-state energy become less negative (*i.e.* increases). This is so because as the cavity radius decreases, more collisions will occur between the electron and the cavity surface and thus an increase in the kinetic energy which makes the particle less bounded. Alternatively, as the cavity radius decreases the surface gets closer to the position where the electron radial distribution function is maximum, and hence the confinement effect is expected to become more profound. Another feature of the results is that as the cavity radius increases, the ground-state energy of the confined hydrogen atom decreases and its limiting value becomes equal to that for the free hydrogen atom in N dimensions which can be easily calculated from (19). One more observation about our results is that confinement effects become more profound in higher dimensions. For example, for a cavity radius, $S = 9a_0$, Table 1 shows that the ground-state energies (eV) in space dimensions $N = 3, 4, 5, 6$ are respectively -13.998, -5.944, -3.105, -1.250 while the corresponding values for the free hydrogen atom are -13.6, -6.044, -3.4, -2.176. The results in Tables 1–3 are displayed in Figs. 1 and 2. These figures clearly show that the ground-state energies shift considerably (slightly) for small (large) size confinement and their limiting values coincide with those for the free hydrogen atom in the given dimension.

4 Bound States and Critical Cage

In this section, we consider the effect of confinement and dimensionality of space on number of bound states of the confined hydrogen atom. To that end, we choose two values for the cavity radius ($S = 22a_0$ and $44a_0$). The number of bound states is determined by number of zeros of the confluent hyper-geometric function which we search for by using Mathematica software. As before, once the zeros are located, the bound-state energies are calculated

Table 1 Ground-state energies for different values of S, and for specific values of N, for $\ell = 0$

$N = 3$			$N = 4$			$N = 5$		
S (a_0)	E (eV)	χ_1	S (a_0)	E (eV)	χ_1	S (a_0)	E (eV)	χ_1
14	−13.599999	27.999999	13	−6.042	17.33	13	−3.35	12.9
13	−13.599999	25.999999	12	−6.04	16	12	−3.34	11.9
12	−13.59999	23.99999	11	−6.03	14.65	11	−3.28	10.8
9	−13.5998	17.9999	10	−6.014	13.3	10	−3.2	9.7
6	−13.5802	11.9913	9	−5.944	11.9	9	−3.105	8.6
4	−12.93	7.8	8	−5.913	10.55	8	−2.83	7.3
3	−11.43	5.5	7	−5.81	9.15	7	−2.34	5.81
2	−3.4	2	6	−5.46	7.6	6	−1.51	4
1.95	−2.434	1.65	5	−4.81	5.95	5.5	−0.81	2.68
1.9	−1.3789	1.21	4	−3.055	3.8	5.3	−0.44	1.9
1.85	−0.3576	0.6	3.5	−1.11	2	5.1	−0.0265	0.45
1.845	−0.2041	0.542	3.4	−0.431	1.21	5.09	−0.0019	0.12
1.84	−0.11003	0.331	3.33	−0.31	1.01	5.0885	−0.00045	0.058
1.8375	−0.0533	0.23	3.3	−0.0195	0.25	5.08835	−9.2E−05	0.0265
1.8365	−0.02913	0.17	3.2995	−0.0161	0.227	5.08834	−8.2E−05	0.025
1.8355	−0.00568	0.075	3.2985	−0.01012	0.18	5.08833	−4.5E−05	0.0185
1.83525	−8.5E−05	0.0092	3.2975	−0.0045	0.12	5.088329	−4.4E−05	0.0184
1.8352	−3.4E−05	0.0058	3.297	−0.00109	0.059	5.088328	−4.4E−05	0.0182
1.835175	−3.1E−05	0.0055	3.2969	−0.0005	0.04	5.088308	−3.3E−05	0.000013
1.835247	−1.19E−06	0.00401	3.29683	−0.00017	0.0103			

using (18). The lowest bound-state energy is the ground-state ($n = 1$) and the next ones are excited states ($n = 2, 3, \ldots$). These calculations are carried out for dimensions $N = 3$ to 10. It is tempting to compare these energy values with those for the free N-dimensional hydrogen atom. Our results, for $\ell = 0$, are shown in Table 4 for $S = 22a_0$ and in Table 5 for $S = 44a$.

The results in Tables 4 and 5 show interesting features: firstly, for a given S the number of bound states decreases as N increases and this is due to the extra repulsive term in the effective potential in higher dimensions whose role was emphasized by AL-Jaber [31]. Secondly, the larger the cavity radius the higher number of bound states since the confinement effect is small for large confining cavity. Thirdly, upon comparing the bound-state energies for the confined case with those for the free one, we note that while the ground-state energies are very close the excited-state energies have a difference which increases as we go to higher excited states. This is explained by the fact that the radial distribution function has a maximum at a point that gets closer to the cavity surface as we go to higher excited states and thus the confinement effects become profound.

It is illuminating to consider the special case $a = -1$. Here, (11) implies that ${}_1F_1(a, b, z)$ has only one zero, whose value is $\chi = b$ as (12) shows, and thus we have only one bound state. Therefore, for $\ell = 0$, we get $\chi = (N - 1)$ and thus (13) and (16) yield the cavity radius and (18) yields the binding energy, namely

$$S = \frac{N^2 - 1}{4} a_0 \tag{21}$$

Table 2 Ground-state energies for different values of S, and for specific values of N for $\ell = 0$

$N = 6$			$N = 7$			$N = 8$		
S (a_0)	E (eV)	$x_{\lambda\ell}$	S (a_0)	E (eV)	$x_{\lambda\ell}$	S (a_0)	E (eV)	$x_{\lambda\ell}$
23	−2.176	18.4	35	−1.51104	23.333	54	−1.21	31
21	−2.176	16.8	30	−1.5103	19.995	37	−1.11	21.1
19	−2.162	15.15	26	−1.507	17.309	36	−1.092	20.45
17	−2.144	13.5	23	−1.497	15.23	32	−1.088	18.1
14	−2.1	10.9	20	−1.481	13.2	27	−1.078	15.2
13	−2.012	10	17	−1.37224	10.8	20	−0.973	10.7
12	−1.92	9.01	16	−1.355	10.1	17.8	−0.85	8.9
11	−1.754	7.9	15	−1.28	9.2	17	−0.791	8.2
10	−1.55	6.75	14	−1.17	8.2	16	−0.689	7.2
9	−1.25	5.45	13	−1.103	7.15	15	−0.581	6.2
8	−0.73	3.7	12	−0.85	6	14	−0.391	4.75
7.5	−0.293	2.2	11	−0.58	4.55	13.5	−0.306	4.05
7.35	−0.152	1.55	10	−0.196	2.4	12.5	−0.096	2.1
7.25	−0.055	0.92	9.75	−0.07	1.4	12.4	−0.019	0.92
7.235	−0.038	0.76	9.65	−0.019	0.68	12.385	−0.0138	0.79
7.225	−0.026	0.63	9.635	−0.0092	0.5	12.38	−0.118	0.73
7.215	−0.0198	0.55	9.625	−0.0038	0.32	12.37	−0.0091	0.64
7.205	−0.00802	0.35	9.62	−0.0014	0.195	12.355	−0.00451	0.45
7.2025	−0.00443	0.26	9.6175	−7.1E−05	0.044	12.351	−0.00304	0.369
7.20125	−0.0035	0.23	9.6174	−1.7E−05	0.015	12.34	−2.2E−11	0.0001
7.2005	−0.00289	0.21	9.617375	−5.1E−06	0.118			
7.197687	−2.1E−11	0.000018	9.61737	−2.2E−06	0.0078			
			9.617368	−7.8E−07	0.00461			
			9.617367	−5.E−07	0.0037			
			9.6173665	−1.19E−11	0.0000018			

$$E = \frac{4}{(N+1)^2} E_0 \tag{22}$$

It is interesting to note that the above bound state energy coincides with the energy of the first excited state ($n = 2$) for the free hydrogen atom as can easily be checked using (19). One can also observe that in the infinite dimensional space ($N \to \infty$) the binding energy vanishes and the cavity radius becomes infinite which means that the hydrogen atom is not anymore confined. This implies that we can not confine a hydrogen atom in the infinite dimensional space.

An important point to discuss below is to find the minimum cavity size that can allow a bound state. Our previous results show that as the cavity radius decreases, the binding energy diminishes and therefore, there is a critical value, S_c, for the cavity radius at which the binding energy becomes zero. The critical cage radius of hydrogen is relevant to the study of partition function of atomic hydrogen and also to ionization of its ground state. Here we search for the smallest cavity radius, for a given dimension N, at which the bound state energy approaches zero. We carry the calculations for $N = 2$ to 10, and present our results in Table 6. For the three dimensional case, our results give $S_c = 1.835247 a_0$. Som-

Table 3 Ground-state energies for different values of S, and for specific values of N for $\ell = 0$

$N = 9$			$N = 10$		
S (in a_0)	E (eV)	$x_{\lambda\ell}$	S (in a_0)	E (eV)	$x_{\lambda\ell}$
44	−0.84923	21.99	77.5	−0.672	34.444
40	−0.84745	19.97	54	−0.671	23.99
26	−0.7985	12.6	42	−0.6597	18.5
20	−0.544	8	31	−0.5998	13
18	−0.378	6	25	−0.4604	9.2
16	−0.114	2.93	23	−0.362	7.5
15.5	−0.025	1.33	20	−0.1464	4.15
15.4	−0.00703	0.7	19	−0.0396	2.05
15.38	−0.00345	0.49	18.9	−0.027	1.68
15.375	−0.00208	0.38	18.7	−0.00233	0.49
15.374	−0.002	0.373	18.685	−0.00043	0.21
15.37	−0.0013	0.295	18.684	−0.00039	0.165
15.369	−0.00011	0.275	18.6816	−4.77E−09	0.00007
15.365	−3.E−05	0.145			
15.364	−1.E−05	0.085			
15.3630	−1.44E−08	0.001			

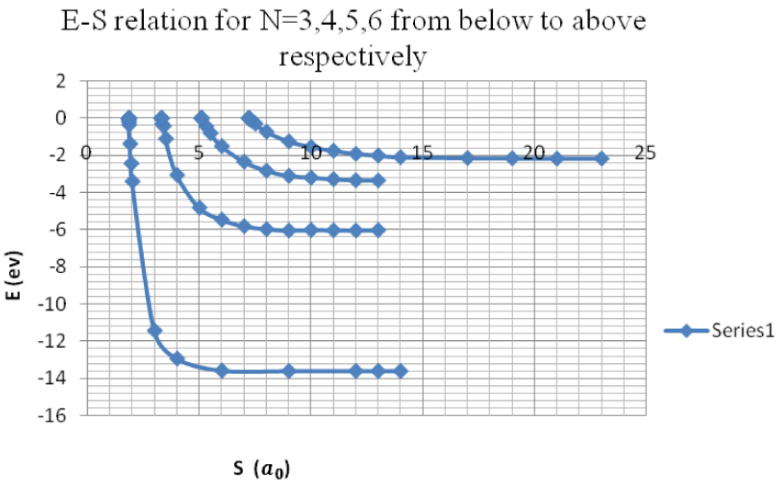

Fig. 1 Relation between ground-state energies of a confined H-atom and the radius of the cavity for a given space dimensions for $\ell = 0$

merfield and Welker [10] obtained a critical value $1.835a_0$ while Dingle [32] obtained the value $1.8354a_0$. Our results show that the value of the critical cage increases as the space dimension N, increases. This is so because as the dimension increases the particle is repelled further away from the nucleus which is due to the extra repulsive term in the effective potential. We display these results in Fig. 3.

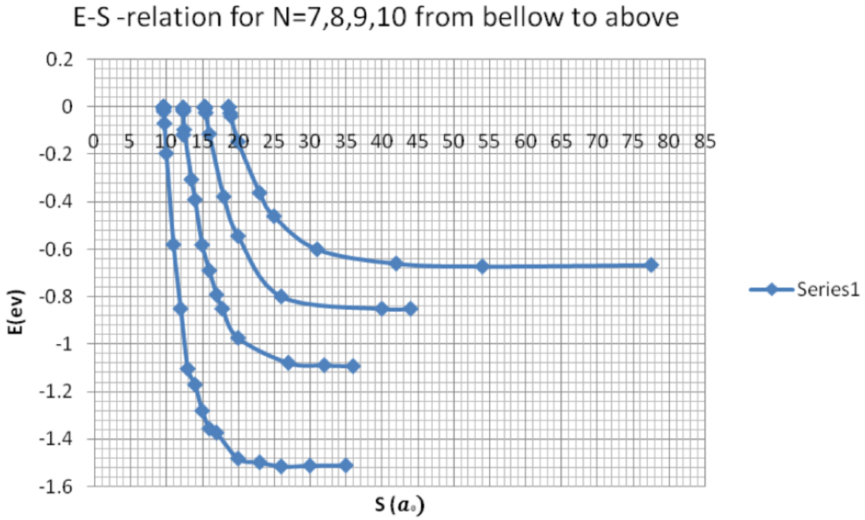

Fig. 2 Relation between ground-state energies of a confined H-atom and the radius of the cavity for given space dimensions for $\ell = 0$

Table 4 Bound-state energies for confined and free hydrogen atom for $\ell = 0$, $S = 22a_0$

N	n	$E\ (\mathrm{eV})_{n\ \mathrm{confined}}$	$E\ (\mathrm{eV})_{n\ \mathrm{free}}$
3	1	−13.6	−13.6
3	2	−3.3999	−3.4
3	3	−1.426	−1.511
4	1	−5.99	−6.044
4	2	−2.164	−2.176
4	3	−0.79	−1.11
5	1	−3.4	−3.4
5	2	−1.46	−1.511
5	3	−0.13	−0.85
6	1	−2.151	−2.176
6	2	−0.897	−1.11
7	1	−1.48	−1.511
7	2	−0.374	−0.85
8	1	−1.03	−1.11
9	1	−0.65	−0.85
10	1	−0.31	−0.67

5 Conclusions and Results

Investigations on the behavior of confined atoms has been of great interest especially after the discovery of fullerenes and other structures that are capable of quantum confinement of atoms such that their electronic states are considerably altered. Due to the recent knowledge about nanoscale devices there is currently intense scientific research in a wide range of confining systems to which quantum mechanical formalism may be applied.

Table 5 Bound-state energies for confined and free hydrogen atom for $\ell = 0$, $S = 44a_0$

N	n	E (eV)$_{n\,\text{confined}}$	E (eV)$_{n\,\text{free}}$
3	1	−13.6	−13.6
3	2	−3.4	−3.4
3	3	−1.49	−1.511
3	4	−0.8432	−0.85
3	5	−0.40	−0.544
4	1	−6.04440	−6.0444
4	2	−2.176	−2.176
4	3	−1.098	−1.11
4	4	−0.641	−0.672
4	5	−0.15	−0.45
5	1	−3.4	−3.4
5	2	−1.51	−1.511
5	3	−0.8448	−0.85
5	4	−0.42	−0.544
6	1	−2.15	−2.176
6	2	−1.1100	−1.1101
6	3	−0.641	−0.672
6	4	−0.20	−0.45
7	1	−1.51	−1.511
7	2	−0.8473	−0.85
7	3	−0.46	−0.544
8	1	−1.098	−1.11
8	2	−0.65	−0.672
8	3	−0.274	−0.45
9	1	−0.8492	−0.85
9	2	−0.4493	−0.544
9	3	−0.072	−0.377
10	1	−0.666	−0.672
10	2	−0.344	−0.45

In the present paper, we considered a hydrogen atom that is confined to an impenetrable spherical cavity in N dimensions. The energy eigenvalues for the ground-state ($\ell = 0$) for different cavity radii were computed for a given space dimension. This was achieved by searching for the zeros of the hyper-geometric function ${}_1F_1(a, b, z)$ at which the wave function vanishes at the surface of the confining cavity. It was shown that as the cavity radius decreases, the ground-state energy becomes less negative (*i.e.* increases) which is due to the increase collisions between the electron and the surface. We also showed that the limiting value for the ground-state energy for the confined hydrogen atom approaches that for the free N-dimensional hydrogen atom when the cavity radius becomes very large. The effect of space dimension on the ground-state energy has also been discussed and was shown that confinement effects become more profound as N increases. Our results revealed that the number of bound states decreases either as the cavity size decreases for a given N or as the space dimension increases for a given cavity radius. This is because that in either of these cases there are more collisions between the electron and the cavity surface. An interesting case ($a = -1$) shows that there is only one bound state, for a given dimension, whose en-

Table 6 Critical cage radius for different space dimensions

N	χ	S_c (a_0)
2	0.000008	0.72289
3	0.00401	1.835247
4	0.0103	3.29683
5	0.000013	5.088308
6	0.000018	7.197867
7	0.000018	9.617366
8	0.000045	12.340784
9	0.001	15.3630
10	0.0007	18.6816

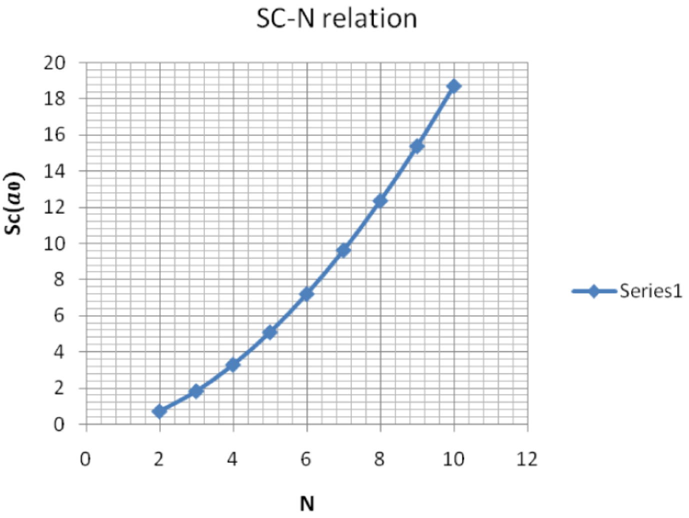

Fig. 3 Relationship between critical radius and space dimension

ergy coincides with the first exited-state energy ($n = 2$) for the free hydrogen atom in that dimension. It has also been shown that in the limit of infinite dimension ($N \to \infty$) the cavity radius becomes infinite and thus the hydrogen atom becomes a free one. Furthermore, it has been shown that as the size of the confining cavity is lowered, there ultimately comes a point where the electron becomes delocalized (binding energy becomes zero) and behaving like a particle in a sphere. This minimum radius (called the critical cage) was calculated for space dimensions $N = (2\text{–}10)$. Our results show that the critical cage increases as the space dimension increases. This is so because the particle is repelled further away from the nucleus, due the extra repulsive term in the effective potential, as the space dimension increases and thus the critical cage is expected to increase.

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