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Confined Hydrogen Atom in HigherSpace Dimension under Pressure

ذرة الهيدروجين المحصورة والمضغوطة في فضاء متعدد الأبعاد

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Abstract

We investigated the Schrödinger equation for the confined H-atom in an impenetrable spherical cavity in N-dimensional space. We found that the wave functions are dimension-dependent and have the same form as the wave functions of the free hydrogen atom in N- dimensions. Moreover, we investigated the ground state energies for this case, where we found that those energies depend on the radius of the cavity (S), and the dimensionality of the space (N). On the other hand, we investigated the average pressure exerted by the confined H-atom in an impenetrable spherical cavity in N-dimensional space on the wall of the cavity. We found that the values of the pressure depends on both N, and S such as: for a given N, as the radius of the cavity decreases, the pressure increases up to a maximum value called P_{max} , suddenly after which, the value of the pressure decreases to zero. The value of P_{max} depends on N, where we found that it decreases as N increases. In addition to that, the value of the radius of the cavity ($S_{P_{max}}$) at which the pressure has its maximum value (P_{max}) increases as N increases.

Keywords: Quantum mechanics, Formalism, Atoms in cavities Average Pressure, Ground state energy.

ملخص

لقد قمنا بحل معادلة شرودنجر لذرة الهيدروجين المحصورة في فجوة كروية محكمة في فضاء عدد أبعاده N، حيث وجدنا أن الاقترانات الموجية الناتجة تعتمد على عدد أبعاد الفضاء الذي توجد فيه ولها نفس شكل الاقترانات الموجية لذرة الهيدروجين الحرة في فضاء عدد أبعاده N. وكذلك درسنا الطاقة التى تمتلكها ذرة الهيدروجين المحصورة في فجوة كروية محكمة وفي فضاء متعدد الأبعاد في المستوى الأرضي، حيث وجدنا أن قيم الطاقة تعتمد على نصف قطر الفجوة (S) وعلى عدد أبعاد الفضاء (N). ومن ناحية أخرى درسنا معدل الضغط الذي تؤثر به ذرة الهيدروجين المحصورة في فجوة كروية محكمة في فضاء عدد أبعاده N، على جدران الفجوة. ولقد وجدنا أن متوسط الضغط يعتمد على كل من N و S كما يلي:- لكل قيمة محددة من قيم N، فان الضغط يزداد بنقصان نصف قطر الفجوة (S) حتى يصل الى قيمة قصوى أسميناها (P_{max})،ثم فجأة بعد ذلك تتناقص قيمة الضغط الى الصفر. ان قيمة P_{max} تعتمد على عدد الأبعاد N . بالاضافة الى ذلك فان قيمة نصف قطر الفجوة ($S_{P_{max}}$) ، والتي تكون عندها قيمة معدل الضغط أكبر ما يمكن (P_{max})،هي أيضا تزداد بازدياد N .

1. Introduction

The idea of higher dimensional space is important in many aspects in physics and mathematics, in cosmology, group theory, many body problem, super symmetry, and the problem of unifying the four forces in nature.

Quantum confinement means confinement on a scale comparable to the atomic size, where confined atoms can be considered as atoms under pressure [1].

The potential of this problem can be expressed as:

$$V(r) = \begin{cases} \dfrac{-ze^2}{4\pi\varepsilon_0 r} , & 0 \le r \le S \\ \infty , & \text{elsewhere} \end{cases}$$

S is the radius of the cavity.

The Schrödinger equation for the confined H-atom in an impenetrable spherical cavity in N dimensional space has been investigated, and the wave functions for this case are obtained. It is found that the radial wave functions have the form given by the following equation: [1]

$$R_{\lambda l}(\rho) = A'\rho^{l} e^{\left(-\frac{\rho}{2}\right)} {}_1F_1\left(l+\frac{N-1}{2}-\lambda;\ 2l+N-1;\ \rho\right)$$

And the energy eigen values can be computed from this equation: [1]

$$E_n = \frac{{x_n}^2 {a_0}^2}{4S^2} E_0$$

Where x_n is the n[th] root of the wave function, which is the last intercept that coincides with the surface of the walls of the cavity and hence indicates the ground state energy for each value of S where $x_n = \frac{2}{a_0\lambda} S$, from which $\lambda = \frac{2S}{a_0\ x_n}$.

a_0 is the Bohr radius and E_0 is the ground state energy for the free hydrogen atom in three dimensions [1].

The recent development in nanotechnology has generated intensive research activity in modeling spatially confined quantum systems, when an atom or a molecule is trapped inside any kind of microscopic cavity, or is placed in a high pressure environment, it experiences special confinement that affects its physical and chemical properties.[2]

An atomic system under very high pressure simulates a confined system. The interaction of the atom with the surroundings was suggested to be replaced by a uniform pressure on a sphere within which the atom is considered to be enclosed. [2]

This paper investigated the effect of the higher space dimensions N, and the radius of the cavity S, where the hydrogen atom is enclosed, on the pressure that is exerted on the walls of the cavity.

2. Theory

The problem of the confined hydrogen atom in higher space dimensions is solved [1], and the energy eigen values of the ground state are obtained.

Knowing the dependence of the ground state energy on the radius of the cavity (S), [1] allows us to calculate the average pressure needed to 'compress' a hydrogen atom in the ground state in a certain size of the cavity. The energy eigen values can be computed from the relation

$$E_n = \frac{x_n{}^2 \, a_0{}^2}{4S^2} E_0 \tag{1}$$

And It is known that $P = \frac{-dE}{dV}$ (2)

Substitute for the value of E_n in eqn. (2), then,

$$P = \frac{-d}{dV}\left(\frac{X_n{}^2 a_0{}^2}{4S^2}\right)E_0 \tag{3}$$

But $dV = A\, dS$, then

$$P = \frac{-d}{A\, dS} E_n = \frac{-1}{A}\frac{dE_n}{dS} \tag{4}$$

Now, in N dimensions the area of the hyper sphere is,

$$A_N(S) = \frac{2(\pi)^{N/2}}{\left(\frac{N}{2}-1\right)!} S^{N-1} \tag{5}$$

and $P_N = \frac{-1}{\frac{2(\pi)^{N/2}}{\left(\frac{N}{2}-1\right)!} S^{N-1}} \frac{dE_n}{dS}$ (6)

$$= \frac{-\left(\frac{N}{2}-1\right)!}{2(\pi)^{N/2}\,S^{N-1}}\,\frac{2x_n{}^2 a_0{}^2}{4S}\,\frac{-1}{S^2}\,E_0 \quad (7)$$

$$= \frac{\left(\frac{N}{2}-1\right)!}{2(\pi)^{N/2}\,S^{N-1}}\,\frac{2x_n{}^2 a_0{}^2}{4S}\,\frac{1}{S^2}\,E_0 \quad (8)$$

Finally

$$P_N = \frac{\left(\frac{N}{2}-1\right)!}{\pi^{N/2}}\,\frac{x_n{}^2 a_0{}^2}{4S^{N+2}}\,E_0 \quad (9)$$

When N=3,

$$P_{N-3} = \frac{\left(\frac{1}{2}\right)!}{\pi^{3/2}}\,\frac{x_n{}^2 a_0{}^2}{4S^5}\,E_0 = \frac{\sqrt{\pi}}{2\pi^{3/2}}\,\frac{x_n{}^2 a_0{}^2}{4S^5}\,E_0 = \frac{1}{8\pi}\,\frac{x_n{}^2 a_0{}^2}{S^5}\,E_0 \quad (10)$$

Equation (9) shows the dependence of the pressure exerted on the confined H-atom on the space dimension N, where more pressure is exerted on it with increasing N.

3. Results and Discussion

In this part of the study, we represented the relation between the pressures exerted by the H-atom on the wall of the cavity due to the change of its radius for each value of N from 3 to 10 in graphs.

This relation is interesting, where it is noticed that when the radius of the cavity is increased, the pressure decreases and approaches zero. This implies that the cavity effect becomes negligible and the particle acts like a free one. On the other hand, when the radius of the cavity decreases the pressure increases gradually up to a certain maximum value called P_{max} . This maximum value corresponds to a certain cavity radius which we call $S_{p\ max}$. If the radius of the cavity becomes less than $S_{p\ max}$, the pressure will decrease rapidly until it approaches zero again within a very short range of S values. We suggest that this is because, as S decreases, one is moving away from maximum distribution function, and the probability of finding the particle within this region becomes small. (Radial distribution function gives the probability of finding the particle in a distance **r** from a certain point in space),

Table (1): Relation between the Pressure Exerted on a Confined Hydrogen Atom and the Radius of the Cavity when l=0, N=3.

S× a_0 (m)	P(eV/a_0^3)
14.00000	0.0007889
13.00000	0.0009852
12.00000	0.0012526
9.000000	0.0029691
6.000000	0.0100064
5.000000	0.0172469
4.000000	0.0326881
3.000000	0.0679767
2.500000	0.0930108
2.400000	0.0945503
2.000000	0.0676413
1.950000	0.0532823
1.900000	0.0341165
1.850000	0.0088524
1.845000	0.0059292
1.840000	0.0029282
1.837500	0.0013974
1.836500	0.0007794
1.835500	0.0001502
1.835250	0.0000022
1.835200	0.0000016
1.835175	0.0000079
1.835170	0.0000079

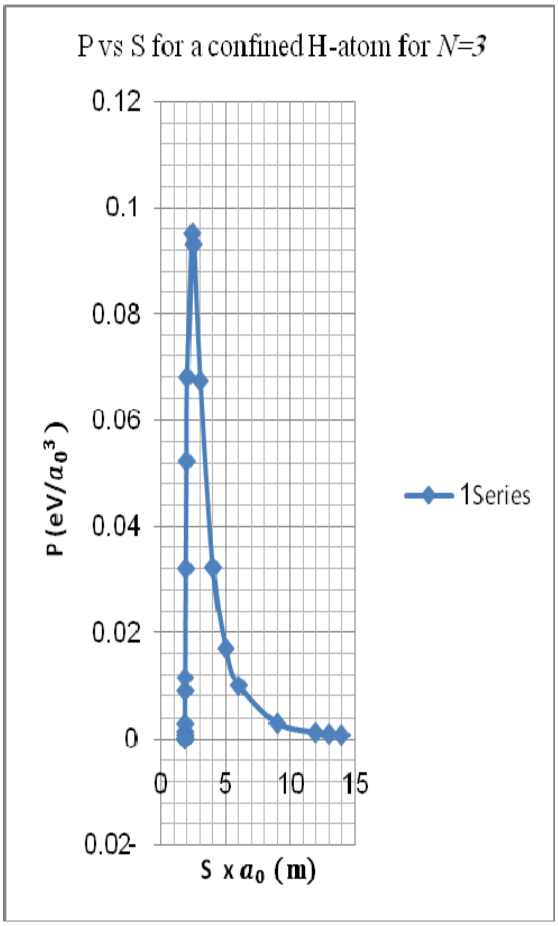

Fig.(1): Relation between the Pressure Exerted on the Confined H-Atom in a Cavity and its Radius for l = 0 and N=3.

One can notice here that the pressure is maximum at S=2.4a_0.

Table (2): Relation between the Pressure Exerted on a Confined Hydrogen Atom and the Radius of the Cavity when *l*=0,N=4.

S X a_0 (m)	P(eV/a_0^4)
13.0000	0.000022
12.0000	0.000026
11.0000	.0000422
10.0000	0.000061
9.00000	0.000094
8.00000	0.000150
7.00000	0.000245
6.00000	0.000430
5.00000	0.000781
4.00000	0.001210
3.50000	0.000750
3.40000	0.000330
3.35000	0.000250
3.30000	0.000170
3.29950	0.000014
3.29850	8.7E-06
3.29750	3.81E-06
3.29700	9.34E-07
3.29690	4.3E-07
3.29685	1.4E-07

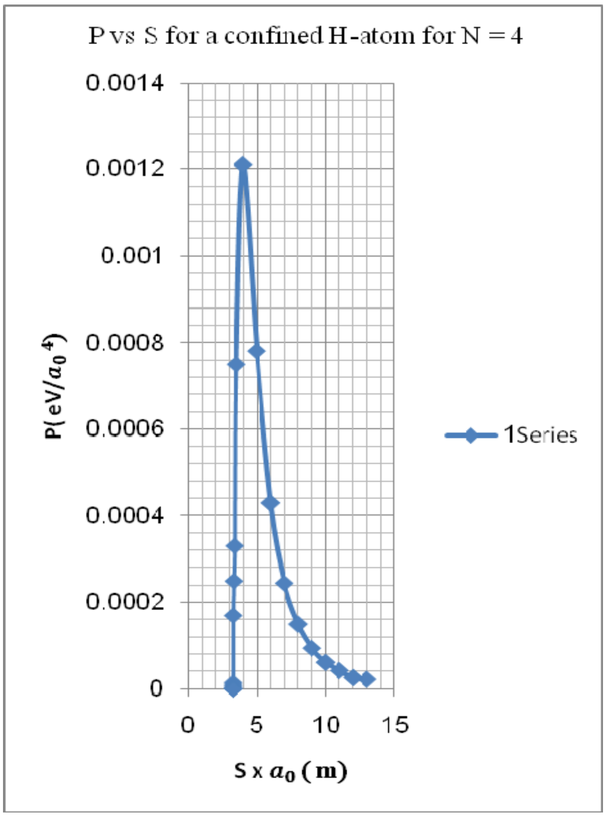

Fig.(2): Relation between the Pressure Exerted on a Confined H-atom and the Radius of the Cavity when *l* = 0 for N=4.

Table (3): Relation between the Pressure Exerted on a Confined Hydrogen Atom and the Radius of the Cavity when *l*=0,N=5.

S × a_0 (m)	P (eV/a_0^5)
13.00000	0.00000046
12.00000	0.00000068
11.00000	0.00000103
10.00000	0.00000162
9.000000	0.00000270
8.000000	0.00000440
7.000000	0.00000706
6.000000	0.00000985
5.500000	0.00000813
5.300000	0.00000520
5.100000	0.00000311
5.090000	0.00000003
5.088500	5.25E-08
5.088350	1.4E-09
5.088340	1.22E-09
5.088330	6.7E-10
5.088329	6.61E-10
5.088328	6.46E-10
5.088327	6.3E-10

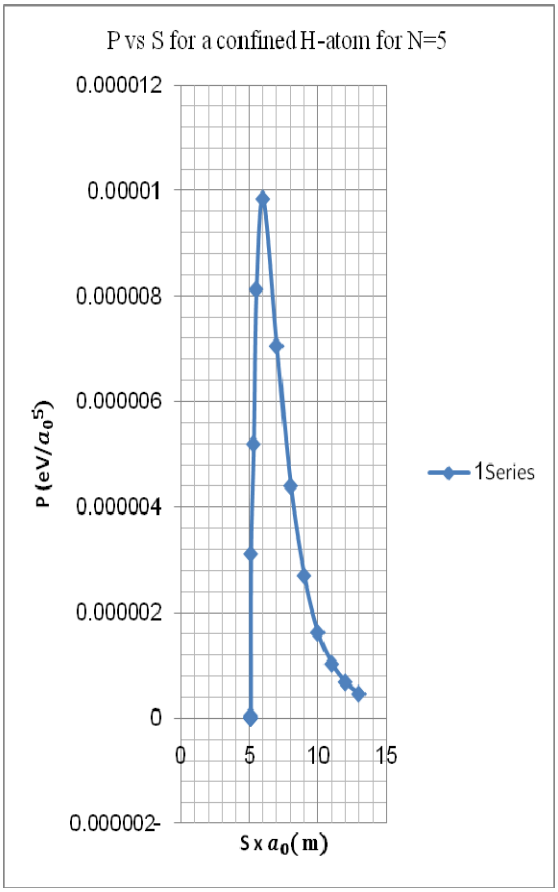

Fig. (3): Relation between the Pressure Exerted on a Confined H-Atom and the Radius of the Cavity when *l* = 0, N=5.

Table (4): Relation between the Pressure Exerted on a Confined Hydrogen Atom and the Radius of the Cavity for l=0,N=6.

S× a_0	P x 10^{-8}(eV/$a_0{}^6$)
23.0000	0.0095
21.0000	0.0160
19.0000	0.0297
17.0000	0.0573
14.0000	1.7656
13.0000	2.6885
12.0000	4.1406
11.0000	6.3852
10.0000	9.9923
9.00000	15.133
8.00000	17.895
7.50000	10.603
7.35000	6.1862
7.25000	2.4318
7.23500	1.6909
7.22500	1.1723
7.21500	0.9035
7.20500	0.3670
7.20250	0.2050
7.20125	0.1605
7.20050	0.0134
7.20025	0.0098

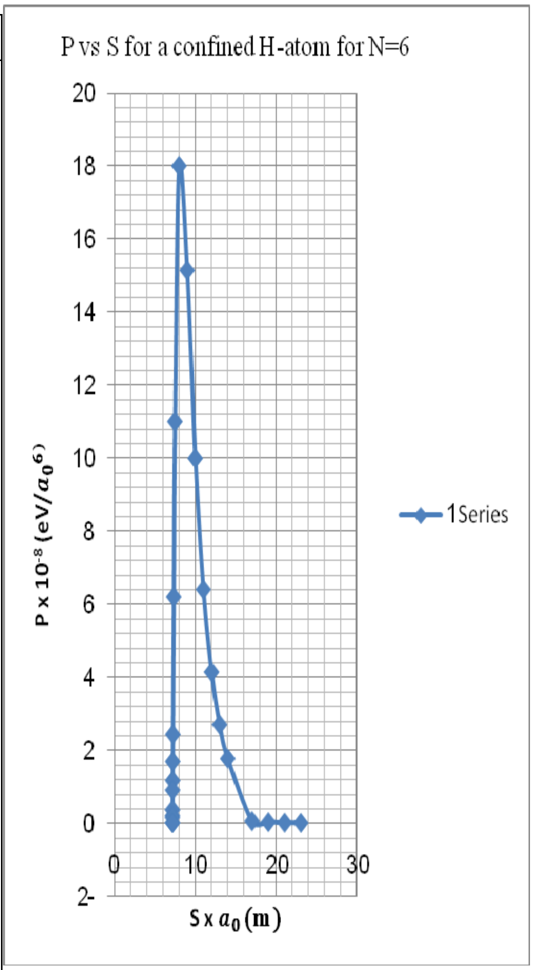

Fig (4): Relation between the Pressure Exerted on a Confined H-Atom and the Radius of the Cavity when l = 0, N=6.

Table (5): Relation between the Pressure Exerted on a Confined Hydrogen Atom and the Radius of the Cavity for l=0,N=7.

$S \times a_0$ (m)	$P \times 10^{-10}(eV/a_0{}^7)$
35.00000	0.01420
30.00000	0.04176
26.00000	0.11451
23.00000	0.26477
20.00000	0.69968
17.00000	2.02222
16.00000	3.05201
15.00000	4.52666
14.00000	6.69111
13.00000	9.91163
12.00000	14.3448
11.00000	18.0514
10.00000	11.8433
9.750000	5.06102
9.650000	1.31007
9.635000	0.71827
9.625000	0.29697
9.620000	0.11079
9.617500	0.00565
9.617400	0.00066
9.617375	0.00039
9.617370	0.00018
9.617368	0.00006
9.617367	0.00004
9.617367	0.00002

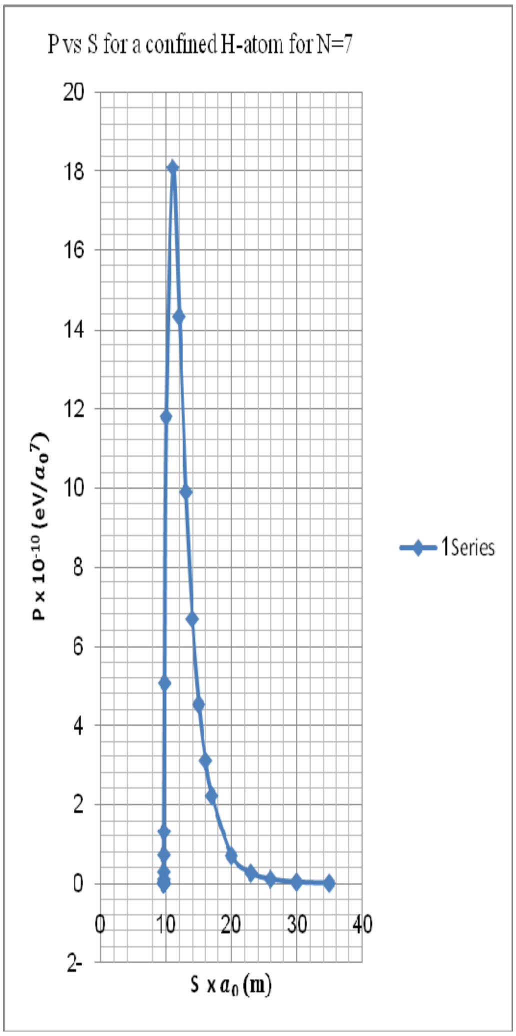

Fig (5): Relation between the Pressure Exerted on a Confined H-Atom and the Radius of the Cavity when l = 0, N=7.

Table (6): Relation between the Pressure Exerted on a Confined Hydrogen Atom and the Radius of the Cavity for *l*=0,N=8.

$S \times a_0$ (m)	$P \times 10^{-12}$(eV/$a_0{}^8$)
54.00	0.00096
37.00	0.01940
36.00	0.02396
32.00	0.06094
27.00	0.23501
20.00	2.34156
17.80	5.19539
17.00	6.98518
16.00	9.87425
15.00	13.9608
14.00	16.3360
13.50	17.1085
12.500	9.91693
12.400	2.06252
12.385	1.53933
12.380	1.31971
12.370	1.02259
12.355	0.05120
12.351	0.03452
12.350	0.03110

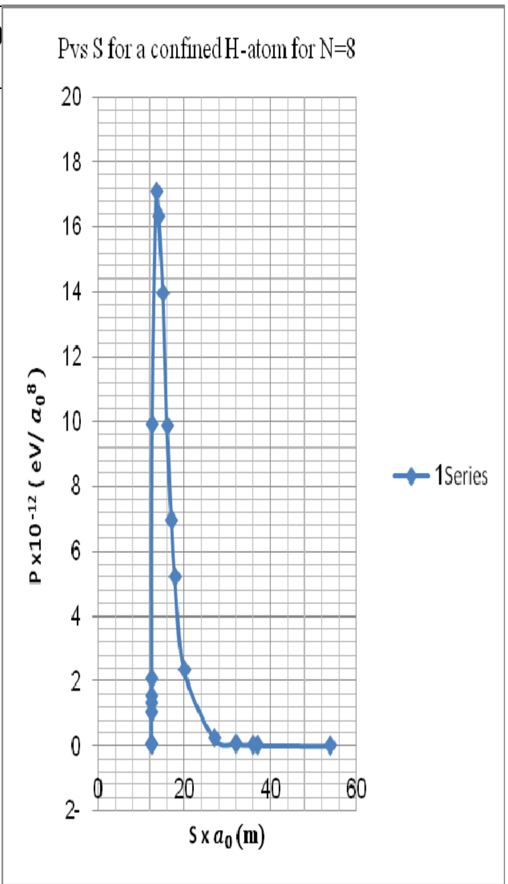

Fig (6): Relation between the Pressure Exerted on a Confined H-Atom in a Cavity and the Radius of the Cavity when *l* = 0, N=8.

Table (7): Relation between the Pressure Exerted on a Confined Hydrogen Atom and the Radius of the Cavity for l=0,N=9.

$S \times a_0$ (m)	$P \times 10^{-16}$($eV/a_0{}^9$)
65.0000	0.0069
46.0000	0.1553
44.0000	0.2316
40.0000	0.5469
30.0000	6.8913
29.0000	9.3323
26.0000	24.772
23.0000	63.767
20.0000	178.97
18.0000	320.80
17.0000	377.03
16.0000	279.47
15.5000	81.655
15.4000	24.288
15.3800	12.073
15.3750	7.2867
15.3740	7.0257
15.3700	4.4072
15.3690	3.8326
15.3650	1.0686
15.3640	0.3675
15.3635	0.0344

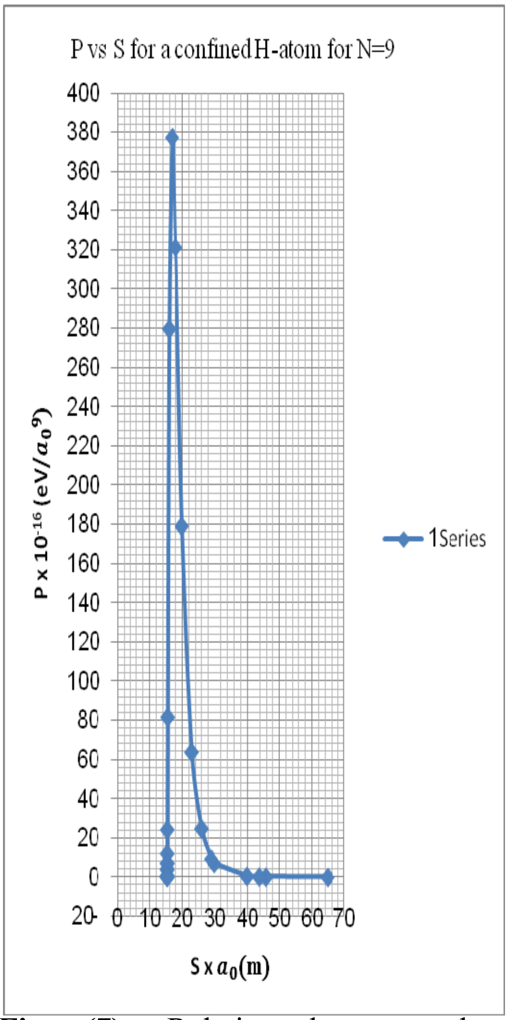

Fig. (7): Relation between the Pressure Exerted on a Confined H-Atom in a Cavity and the Radius of the Cavity when l = 0, N=9.

Table (8): Relation between the Pressure Exerted on a Confined Hydrogen Atom and the Radius of the Cavity for l=0,N=10.

S× a_0 (m)	P× 10^{-18}(eV/$a_0{}^{10}$)
77.500	0.00668
54.000	0.24983
42.000	3.02896
31.000	57.2121
25.000	378.649
23.000	683.432
20.000	1121.19
19.000	506.298
18.900	362.258
18.700	35.0134
18.685	6.49326
18.684	4.01117
18.682	0.72287

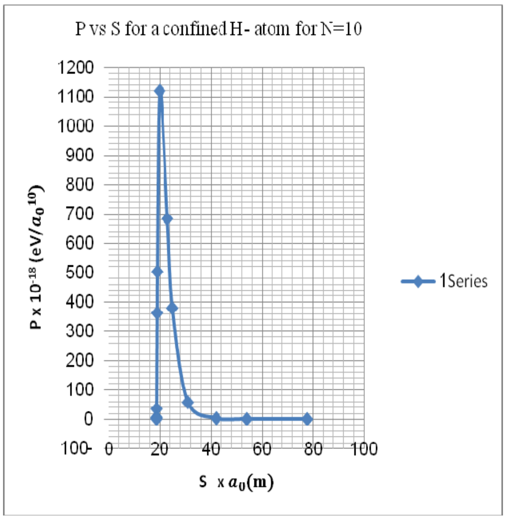

Fig. (8): Relation between the Pressure Exerted on a Confined H-Atom in a Cavity and the Radius of the Cavity for l = 0, N=10.

Table (9): Relation between the Values of S, where the Pressure is Maximum and N.

$S_{P\,max} \times \square_0$ (m)	N
2.4	3
4.0	4
6.0	5
8.0	6
11.0	7
13.5	8
17.0	9
20.0	10

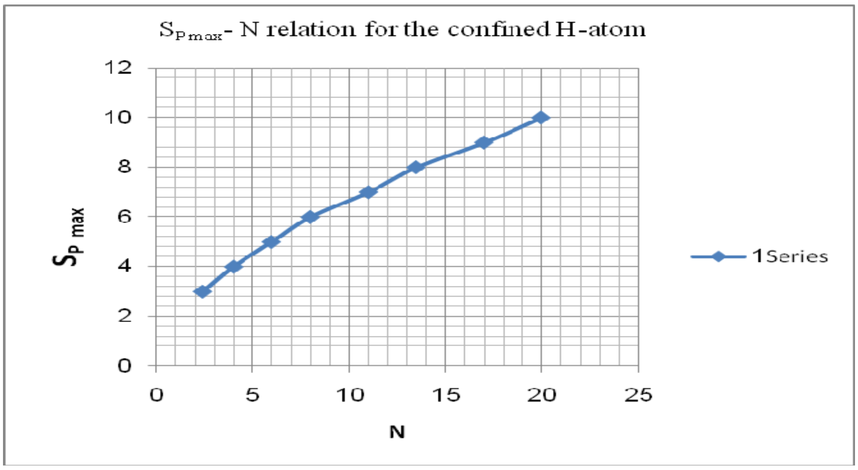

Fig. (9): Relation between the Radius of the Cavity at which the Pressure has a Maximum Value, and N for the Ground State of a Confined H-atom.

We examined the relation between the radius at which pressure is maximum, $S_{p\ max}$, and N, see fig. (9) above. We found that as N increases $S_{p\ max}$ increases. This is due to the dependence of the radial distribution function on space dimension N.

4. Conclusions:

The pressure exerted on the wall of the cavity due to enclosing the H-atom inside a cavity of radius S depends on N and S. It is found that for a given N, the pressure increases as the radius decreases, up to a certain value, and then starts to decrease; this value of P is a maximum. The value of this pressure decreases with increasing N, and the value of the radius of the cavity at which the pressure is maximum increases as N increases.

As I mentioned before, this study is only for the ground-state energy (l=0). As a future study I am looking forward to extending this work for different values of *l,* and to examine the effect of confinement, for $l > 0$, on physical properties of the confined hydrogen atom.

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