



Pressure Ionization, Polarizability and Screening Constants in Confined Hydrogen Like Ions of Astrophysical Importance

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Abstract. An extensive non-relativistic study of the confined Hydrogenic ions of Astrophysical importance like CVI, NVII and OVIII is made in the framework of a simple model of a spherical penetrable box. The detailed calculations of the energy eigenvalues of these ions have been performed. The variation of the energy levels with the spatial restrictions in the form of the variation in the confinement radii or size of the box and the strength of the penetrable wall is investigated. The solution of the radial Schrodinger equation is done numerically using the highly efficient Numerov method which is generally employed to solve the second order ordinary differential equations without the first order term. A point worth mentioning is that with the decrease in confinement radius, the bound state transformed into continuum states, resulting Pressure ionization which we find in Astrophysical Objects under extreme pressure. We also find effect of confinement on several useful quantities like polarizability and Screening constants.

Keywords. Confined atoms, Pressure ionization, Polarizability, Numerov method

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1. Introduction

The study of spatially confined quantum systems has gained substantial attention over the years. Numerous physical phenomena occur in the environment which could be considered as cavities such as atoms and molecules under high pressure, and chemical reactions inside zeolite molecular sieves or fullerenes. With the arrival of modern experimental techniques that have allowed the fabrication of semiconductor nanostructures, such as quantum wells and quantum dots, it has permitted us to explore the limits of dimension and confinement [8].

When compared with free systems, the systems subjected to tight spatial confinement changes drastically in their physical and chemical properties. Since the confined systems have a number of applications, the interest in the study of such systems has increased. A primary area of investigation has been atoms and molecules subjected to high pressure. Models having atoms at the center of spherical penetrable and impenetrable boxes and at off-centre in the spherical box have been used to model the interior of the giant planets Jupiter and Saturn [7] and to study ionized plasma properties [2].

This model of a compressed atom was first proposed by Michels *et al.* [12] to simulate the effect of pressure on an atom, whereas its astrophysical importance was recognized by Sommerfeld and Welker [15]. Several methods have been employed for the study of the confined atoms. For example, Goldman and Joslin [5] and also De Groot and Ten Seldam [6] used the exact solution of the problem. Aquino [1] applied a power series to solve the Schrodinger equation, whereas Laughlin *et al.* [9, 10] employed algebraic methods and perturbation theory to derive the wavefunctions.

Since 1937, Michels *et al.* [12] confined hydrogen atom (CHA) model is acknowledged as the starting point for studying atoms and molecules subject to high pressures. A year after Michels *et al.* [12] work, Sommerfeld and Welker [15] put forward the formal solution to the problem in terms of confluent hypergeometric functions. However, the energy eigenvalues could not be obtained analytically and thus had to be found numerically.

The study of Carbon (CVI), Nitrogen (NVII) and Oxygen (OVIII) atoms are very crucial to understand chemical evolution of galaxies, as these elements are present in different amounts and produced by various mechanisms in diverse stellar mass ranges. Oxygen is mainly present in massive stars and due to explosion, it is ejected into interstellar medium. Carbon and Nitrogen are present in the stars with relatively medium and low masses [4]. In the present paper we study the effect of pressure on CVI, NVII and OVIII through confinement, and also explore its consequence on the energy spectrum of these atoms. The result from solution of time-independent Schrodinger equation using Numerov method has been examined for various values of penetrable wall. The theory and method are presented in Section 2 while the results are discussed in Section 3.

2. Theory and Method

The quantum mechanical non-relativistic Hamiltonian for the confined Hydrogenic atom (in Rydberg units) has the following structure:

$$H = -\frac{d^2}{dr^2} + V(r).$$

The potential taken is of the form of a spherical box with penetrable walls.

$$V(r) = \begin{cases} -\frac{2Z}{r}, & r < r_c, \\ V_c, & r \geq r_c. \end{cases}$$

As the height of the wall, V_c , increases the penetrability of the box decreases and in the limit of V_c tends to infinity the box becomes completely impenetrable. We seek the solutions of time-independent Schrodinger equation:

$$H\Psi(r) = E\Psi(r),$$

where E and $\Psi(r)$ are the stationary state energies and wave function.

We have used the Numerov method to solve the radial part of the Schrodinger equation. Developed by B. V. Numerov, it is a specialized method to solve ordinary differential equations of second order which do not contain the first order differential term. Therefore, the method is particularly useful for the solution of one-dimensional Schrodinger equation or radial Schrodinger equation in three dimensions, as we can easily eliminate the term with first order derivative from it with a minor substitution.

Starting with the differential equations of the form:

$$\frac{d^2y}{dx^2} = P(x) + Q(x)y.$$

The use of the centered difference equation

$$y_{n+1} - 2y_n + y_{n-1} \approx 2 \left(\frac{h^2}{2} \frac{d^2y}{dx^2} + \frac{h^4}{4!} \frac{d^4y}{dx^4} + O(h^6) \right)$$

with $y_n = y(x_n)$ gives the Numerov expression

$$y_{n+1} = \frac{2y_n - y_{n-1} + \frac{h^2}{12}(P_{n+1} + 10F_n + F_{n-1})}{1 - \frac{Q_{n+1}h^2}{12}} + O(h^6),$$

where $F = P(x) + Q(x)y$. The Numerov method is highly efficient as we achieve an error of $P(h^6)$ with the evaluation of P and Q only once per step in comparison to Runge Kutta method which needs the evaluation of functions six time for every step.

We discretize the space into a number of points in the form of a logarithmic grid. The Spatial step size is given by:

$$\Delta r = \frac{\log(Z * r_{\max}) - r_{\min}}{N},$$

where r_{\max} = maximum value of grid point and r_{\min} = minimum value of the grid point and N is the total number of grid points.

On calculating the energy eigenvalues and wavefunctions using Numerov method, we can calculate various other quantities like pressure, polarizability and diamagnetic screening constant. The pressure is given by:

$$P = -\frac{1}{4\pi r_c^2} \frac{dE}{dr_c} = \frac{1}{4\pi r_c^3} (2E - \langle V \rangle).$$

The polarizability is given by:

$$\alpha = \frac{4}{9a_0} \langle r^2 \rangle^2$$

and the diamagnetic screening constant is given by:

$$\sigma = \frac{e^2}{2\pi c^2} \langle 1/r \rangle.$$

In a confined atom these properties depend on the confinement radius as well as the height of the penetrable wall.

3. Result and Discussion

In this paper we have studied the effect of confinement on Hydrogen like, one electron ions. We have made calculations for the energy eigenvalues of the confined CVI, NVII, OVIII. The energies are calculated for different radii of the spherical box and at different strengths of the penetrability of the wall.

As a test of our method, we have computed the energy eigenvalues for the ground state of confined Hydrogen atom and compare our results with those of Ley-Koo and Rubinstein [11]. Our results are found to be in excellent agreement with them. Table 1 shows the comparison of our results with their results.

Table 1. Comparison of energy eigenvalue of ground state of Hydrogen atom with the results of Ley-Koo and Rubinstein [11] for different confinement radii and for $V_c = 0$ and 4

r_c	$V_c = 0$		r_c	$V_c = 4$	
	Energy			Energy	
	Ley-Koo <i>et al.</i> [11]	Our results		Ley-Koo <i>et al.</i> [11]	Our results
5.77827	-0.9998	-0.999800	5.75669	-0.9990	-0.99900207
4.87924	-0.9990	-0.998996	4.02695	-0.9842	-0.98423818
4.08889	-0.9960	-0.996018	2.45668	-0.8264	-0.82618937
3.45203	-0.9881	-0.988074	1.00791	1.0000	1.00145982
1.25921	-0.5102	-0.510220	0.59179	3.4294	3.42894867

We now perform the calculations for the CVI, NVII, OVIII atoms. Figure 1 to Figure 3 show the variation of energy eigenvalues as a function of confinement length for ground, first and second excited states of CVI.

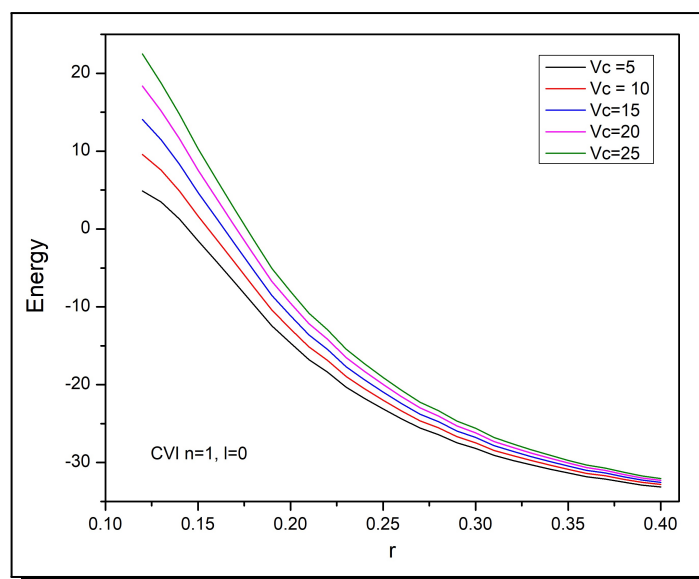


Figure 1. Variation of energy eigenvalue as a function of confinement radius for the ground (1s) state of CVI with different value of V_c

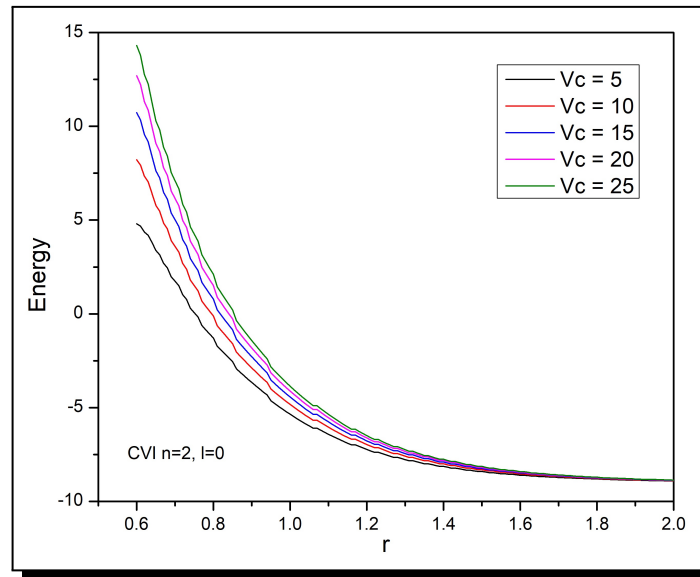


Figure 2. Variation of energy eigenvalue as a function of confinement radius for the 2s state of CVI with different value of V_c

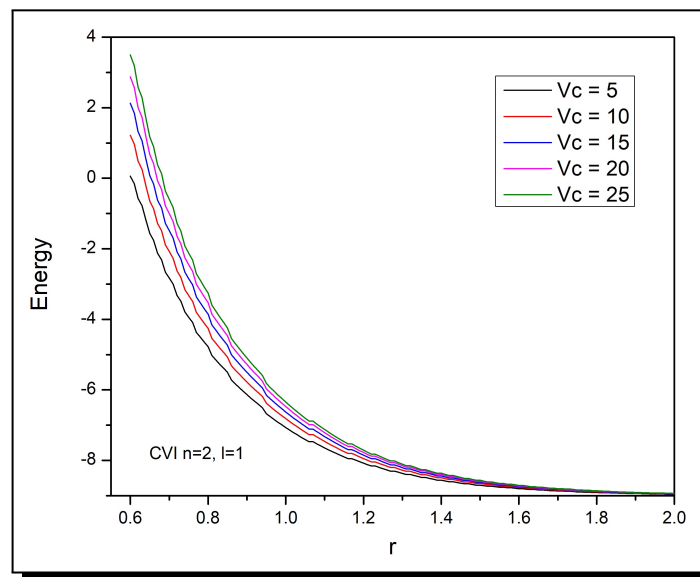


Figure 3. Variation of energy eigenvalue as a function of confinement radius for the 2p state of CVI with different value of V_c

It is observed that the energy of ions in ground state is large enough that there is certain probability to penetrate through barrier potential (or confinement radius), however this tendency becomes smaller with increase in height of potential wall. For excited atoms, this behavior is likely absent as the atom does not carry enough energy. Hence, it seems that the ground state atoms have certain existence beyond confinement region, whereas excited atoms more likely are completely confined within spherical box of radius equivalent to confinement length. Moreover, for sufficiently large confinement radius, the effect of potential wall height on the atom is ignorable and energy eigenvalue turn out to be unaffected.

Tables 2 to Table 7 show the variation in the energies of the ground and excited states for different values of confinement radii. These values are calculated at five different levels of penetrability for the NVII and OVIII atoms.

Table 2. Energy eigenvalue as a function of Confinement radii for 1s state of NVII for different heights of penetrable wall

r_c	Energy				
	$V_c = 5$	$V_c = 10$	$V_c = 15$	$V_c = 20$	$V_c = 25$
0.105	4.68921	9.29337	13.7496	18.0664	22.2516
0.115	2.12686	6.0746	9.8855	13.5679	17.1296
0.125	-1.61359	1.81633	5.1191	8.3031	11.376
0.135	-6.12541	-3.15747	-0.307	2.4342	5.0736
0.145	-10.37114	-7.7657	-5.2694	-2.8741	-0.5726
0.155	-14.67589	-12.39734	-10.2196	-8.1349	-6.1362
0.165	-18.29704	-16.27255	-14.3419	-12.4976	-10.7326
0.175	-21.78133	-19.98857	-18.2828	-16.6567	-15.1037
0.185	-24.54433	-22.92878	-21.3946	-19.9347	-18.5428
0.195	-27.66131	-26.2406	-24.8947	-23.6167	-22.4007
0.205	-30.0779	-28.80565	-27.6028	-26.4629	-25.38
0.215	-31.88706	-30.72503	-29.6282	-28.5903	-27.6057
0.225	-33.99029	-32.95593	-31.9816	-31.0614	-30.19
0.235	-35.54599	-34.60609	-33.7223	-32.8888	-32.1006
0.245	-36.98996	-36.13809	-35.3384	-34.5854	-33.8743

Table 3. Energy eigenvalue as a function of Confinement radii for 2s state of NVII for different heights of penetrable wall

r_c	Energy				
	$V_c = 5$	$V_c = 10$	$V_c = 15$	$V_c = 20$	$V_c = 25$
0.55	4.00636	6.9869	9.3432	11.2802	12.9159
0.65	-0.83887	0.73149	1.9982	3.0515	3.9473
0.75	-4.62037	-3.65115	-2.8717	-2.2252	-1.6765
0.85	-7.34081	-6.7264	-6.2361	-5.8317	-5.4901
0.95	-9.03533	-8.62601	-8.302	-8.0364	-7.813
1.05	-10.15637	-9.88047	-9.6638	-9.4872	-9.3392
1.15	-10.88355	-10.69536	-10.5486	-10.4295	-10.3301
1.25	-11.34912	-11.21885	-11.1178	-11.0362	-10.9682
1.35	-11.67966	-11.59238	-11.525	-11.4708	-11.4257
1.45	-11.88202	-11.82248	-11.7767	-11.7399	-11.7094
1.55	-12.02204	-11.98287	-11.9528	-11.9287	-11.9088
1.65	-12.10419	-12.07774	-12.0575	-12.0413	-12.0278
1.75	-12.16016	-12.14292	-12.1297	-12.1192	-12.1104
1.85	-12.19688	-12.18608	-12.1778	-12.1712	-12.1657
1.95	-12.21687	-12.20981	-12.2044	-12.2001	-12.1965
2.05	-12.23002	-12.22555	-12.2221	-12.2194	-12.2171

Table 4. Energy eigenvalue as a function of Confinement radii for 2p state of N VII for different heights of penetrable wall

r_c	Energy				
	$V_c = 5$	$V_c = 10$	$V_c = 15$	$V_c = 20$	$V_c = 25$
0.45	3.71655	5.69525	7.2833	8.6184	9.7702
0.55	-2.02364	-0.93891	-0.0477	0.7057	1.3558
0.65	-5.82287	-5.15218	-4.6049	-4.1454	-3.7512
0.75	-8.10732	-7.6638	-7.3054	-7.0069	-6.7524
0.85	-9.63485	-9.34125	-9.1065	-8.9124	-8.7481
0.95	-10.55843	-10.35765	-10.1985	-10.0679	-9.9578
1.05	-11.16062	-11.02307	-10.9149	-10.8266	-10.7525
1.15	-11.54729	-11.45269	-11.3788	-11.3187	-11.2685
1.25	-11.79248	-11.72687	-11.6759	-11.6346	-11.6001
1.35	-11.96465	-11.92084	-11.8869	-11.8595	-11.8368
1.45	-12.06867	-12.03901	-12.0161	-11.9977	-11.9823
1.55	-12.13957	-12.12028	-12.1054	-12.0935	-12.0835
1.65	-12.18048	-12.16763	-12.1577	-12.1498	-12.1432
1.75	-12.20788	-12.19963	-12.1933	-12.1882	-12.1839
1.85	-12.22553	-12.22045	-12.2165	-12.2134	-12.2108
1.95	-12.23496	-12.23169	-12.2292	-12.2271	-12.2255
2.05	-12.24106	-12.23903	-12.2375	-12.2362	-12.2351

Table 5. Energy eigenvalue as a function of Confinement radii for 1s state of OVIII for different heights of penetrable wall

r_c	Energy				
	$V_c = 5$	$V_c = 10$	$V_c = 15$	$V_c = 20$	$V_c = 25$
0.105	-0.65039	3.07951	6.7051	10.2317	13.6641
0.115	-6.69524	-3.51573	-0.4321	2.5608	5.4678
0.125	-12.79385	-10.04748	-7.3896	-4.8151	-2.3194
0.135	-19.1004	-16.73946	-14.4597	-12.2561	-10.1242
0.145	-24.53685	-22.4775	-20.493	-18.5786	-16.7298
0.155	-29.74033	-27.95216	-26.2326	-24.5771	-22.9813
0.165	-33.93804	-32.35996	-30.8453	-29.3896	-27.9887
0.175	-37.84925	-36.4622	-35.1334	-33.8586	-32.634
0.185	-41.44886	-40.23508	-39.0746	-37.9633	-36.8975
0.195	-44.20123	-43.1192	-42.0864	-41.0989	-40.1532
0.205	-46.72666	-45.76561	-44.8498	-43.9755	-43.1395
0.215	-49.0273	-48.1771	-47.3683	-46.5974	-45.8612
0.225	-50.70943	-49.941	-49.211	-48.516	-47.8532
0.245	-54.00173	-53.39648	-52.8232	-52.2791	-51.7614
0.265	-56.39461	-55.9122	-55.4565	-55.025	-54.6155
0.285	-58.11623	-57.72578	-57.3578	-57.0101	-56.6807
0.305	-59.52761	-59.21594	-58.9229	-58.6465	-58.3851
0.325	-60.51809	-60.26435	-60.0262	-59.8019	-59.5902
0.345	-61.33036	-61.12642	-60.9353	-60.7557	-60.5863

Table 6. Energy eigenvalue as a function of Confinement radii for 2s state of OVIII for different heights of penetrable wall

r_c	Energy				
	$V_c = 5$	$V_c = 10$	$V_c = 15$	$V_c = 20$	$V_c = 25$
0.5	3.00412	5.76655	8.0548	9.9991	11.6824
0.6	-3.44142	-2.0066	-0.8054	0.2218	1.1149
0.7	-8.35041	-7.52233	-6.8331	-6.2465	-5.7385
0.8	-11.24602	-10.72559	-10.296	-9.9325	-9.6193
0.9	-13.1181	-12.7895	-12.5205	-12.2944	-12.1005
1	-14.1963	-13.97961	-13.8035	-13.6562	-13.5304
1.1	-14.93155	-14.79434	-14.6835	-14.5913	-14.5128
1.2	-15.36907	-15.28209	-15.2122	-15.1542	-15.1051
1.3	-15.62491	-15.56944	-15.525	-15.4883	-15.4571
1.4	-15.77275	-15.73685	-15.7082	-15.6845	-15.6644
1.5	-15.86888	-15.84668	-15.829	-15.8144	-15.802
1.6	-15.92163	-15.90753	-15.8963	-15.887	-15.8792
1.7	-15.95934	-15.95149	-15.9452	-15.9401	-15.9357
1.8	-15.97555	-15.97059	-15.9666	-15.9634	-15.9606
1.9	-15.98734	-15.98461	-15.9824	-15.9806	-15.9791

Table 7. Energy eigenvalue as a function of Confinement radii for 2p state of OVIII for different heights of penetrable wall

r_c	Energy				
	$V_c = 5$	$V_c = 10$	$V_c = 15$	$V_c = 20$	$V_c = 25$
0.39	4.48254	6.75109	8.5984	10.1794	11.5653
0.49	-3.66539	-2.55843	-1.6185	-0.8037	-0.0865
0.59	-8.76562	-8.11868	-7.5731	-7.1035	-6.6927
0.69	-11.57261	-11.15931	-10.8141	-10.5193	-10.2631
0.79	-13.3771	-13.11521	-12.8986	-12.7151	-12.5567
0.89	-14.42435	-14.25463	-14.1155	-13.9983	-13.8977
0.99	-15.02188	-14.90834	-14.8159	-14.7384	-14.6722
1.09	-15.4264	-15.35397	-15.2953	-15.2464	-15.2047
1.19	-15.66505	-15.61912	-15.5821	-15.5513	-15.5251
1.29	-15.80319	-15.77402	-15.7506	-15.7311	-15.7146
1.39	-15.8821	-15.86336	-15.8483	-15.8358	-15.8253
1.49	-15.93278	-15.92131	-15.9121	-15.9045	-15.898
1.59	-15.96372	-15.95707	-15.9517	-15.9473	-15.9436
1.69	-15.97961	-15.97564	-15.9725	-15.9698	-15.9676
1.79	-15.98908	-15.98682	-15.985	-15.9835	-15.9822
1.89	-15.99376	-15.9924	-15.9913	-15.9904	-15.9896
1.99	-15.99656	-15.99578	-15.9952	-15.9946	-15.9942

It is observed that for a fixed size of the box, and for a particular energy level, the energy eigenvalue increases as the penetrability decreases i.e., when the value of V_c increases. On the other hand, if the confinement radius is sufficiently long, the ions behave just like the

free ions and effect of confinement is not seen. Here it is interesting to observe that as per the prediction of Ley-Koo and Rubinstein [11], this increase in the energy eigenvalues is not unlimited however the maximum value of the energy eigenvalue can be equal to the barrier height only.

The increase in the energy eigenvalues is more for the ground state as compared to the 2s and 2p states. Also, increase in the energy eigenvalues is more for the 2s state than the corresponding increase for the 2p states. To summarize the increase in the energy eigenvalues is more for lower values of the quantum numbers n and l . For every energy level there is a critical value of confinement radius below which the electron becomes free.

We have also calculated the Pressure, polarizability and Diamagnetic screening constant. As a test of our calculations, we have calculated these quantities for the ground state of confined hydrogen atom for $V_c = 0$. Table 8 shows the comparison of our results with those Ley-Koo and Rubinstein [11]. As can be seen our results are in excellent agreement with them.

Table 8. Comparison of polarizability, diamagnetic screening constant and pressure for ground state of Hydrogen atom with the results of Ley-Koo and Rubinstein [11] for different confinement radii

r_c	Polarizability (10^{-24} cm^3)		Diamagnetic Screening constant		Pressure (10^6 atm)	
	Ley-Koo <i>et al.</i> [11]	Our result	Ley-Koo <i>et al.</i> [11]	Our result	Ley-Koo <i>et al.</i> [11]	Our result
5.77827	0.5853	0.584029	0.0001	0.0001	0.0001	0.0001249
4.87924	0.5656	0.565025	0.0009	0.0009	0.0009	0.000858
4.08889	0.5246	0.524712	0.0048	0.0048	0.0048	0.00477
3.45203	0.4712	0.466491	0.0196	0.0196	0.0196	0.019603
0.85089	3.7730	3.7695953	16.3192	16.3192	16.3192	16.3162
0.83155	6.0554	6.053087	15.9118	15.9118	15.9118	15.9087

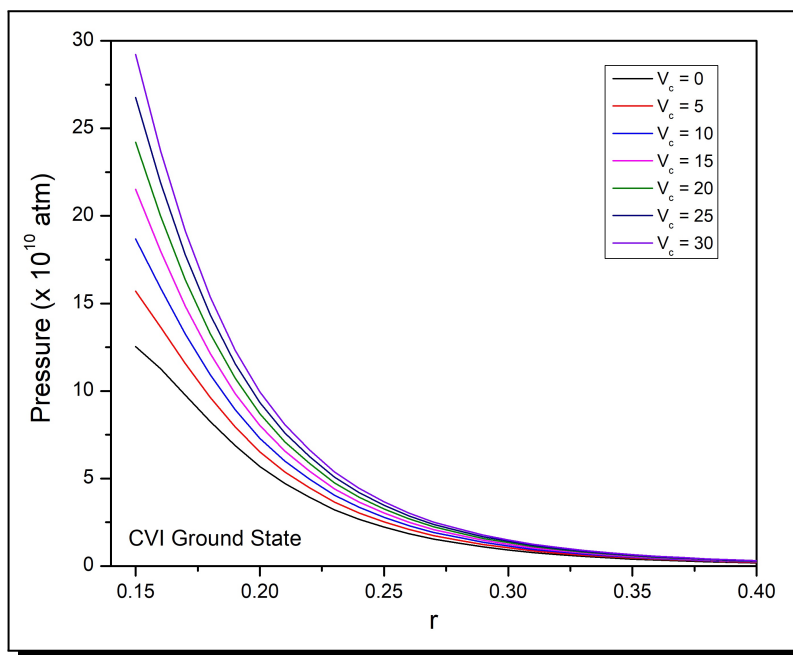


Figure 4. Variation of Pressure as a function of confinement radius for the ground state of CVI for different levels of penetrability

Figure 4 shows the change in the pressure due to the change in the confinement radius for CVI. The variation of pressure is investigated for seven different levels of penetrability. The pressure is found to increase with the decrease in confinement radius as well as with the decrease in the penetrability or increase in the height of penetrable wall.

As it is evident from the data for the energy eigenvalues, with the decrease in the confinement radius and the increase in the height of penetrable wall (i.e. as the confinement grows stronger) the electron does not remain bound. This can be attributed to the ionization due to effect of pressure on the atom as it is confined. The pressure results as a consequence of limiting the wavefunction after a finite radius. In the present study, pressure ionization is found to occur, for all the atoms and for all the energy levels. This kind of phenomena occurs in many astrophysical objects like in Sun, White Dwarf etc. Laser driven compression has opened the pathway for the study of properties of atoms in the stellar and planetary interiors. The dependence of evolution of dense stars on the pressure ionization of Hydrogen is well known [3, 13, 14].

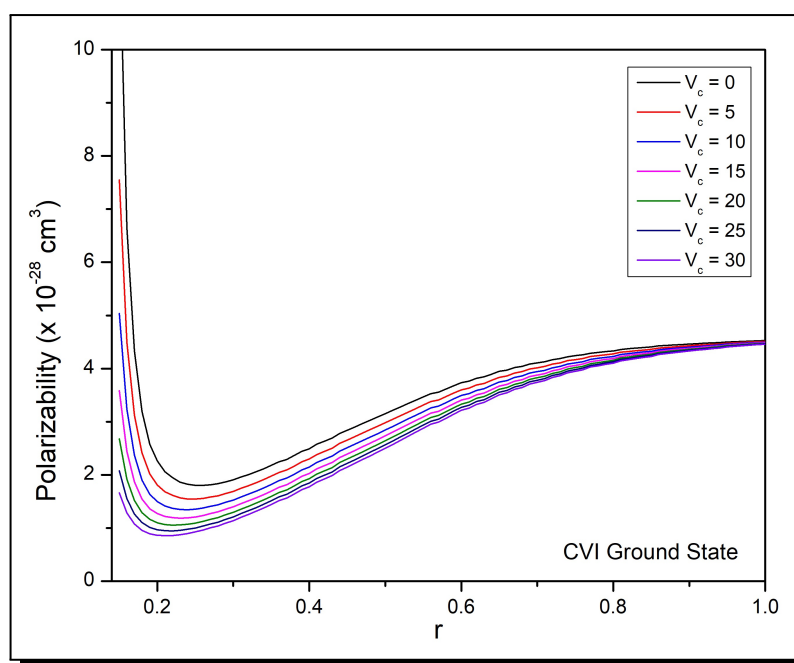


Figure 5. Variation of Polarizability as a function of confinement radius for the ground state of CVI for different levels of penetrability

Figure 5 shows the variation of polarizability with confinement radius for different levels of penetrability for CVI. The polarizability decreases as the confinement radius is reduced and then becomes minimum at a point and after that an increase is observed. As shown in the figure, and as the polarizability is proportional to the expectation value of r^2 , its value should decrease as the atom gets more confined.

Figure 6 shows the variation of diamagnetic screening constant with confinement radius for different levels of penetrability for CVI. It is seen that the values increase as the confinement radius is reduced and then becomes maximum at a point and after that a decrease in the values is observed. Since the diamagnetic screening constant is related to expectation value of $1/r$, the more the atom is confined larger will be the value of σ . The pattern observed in Figure confirms this prediction.

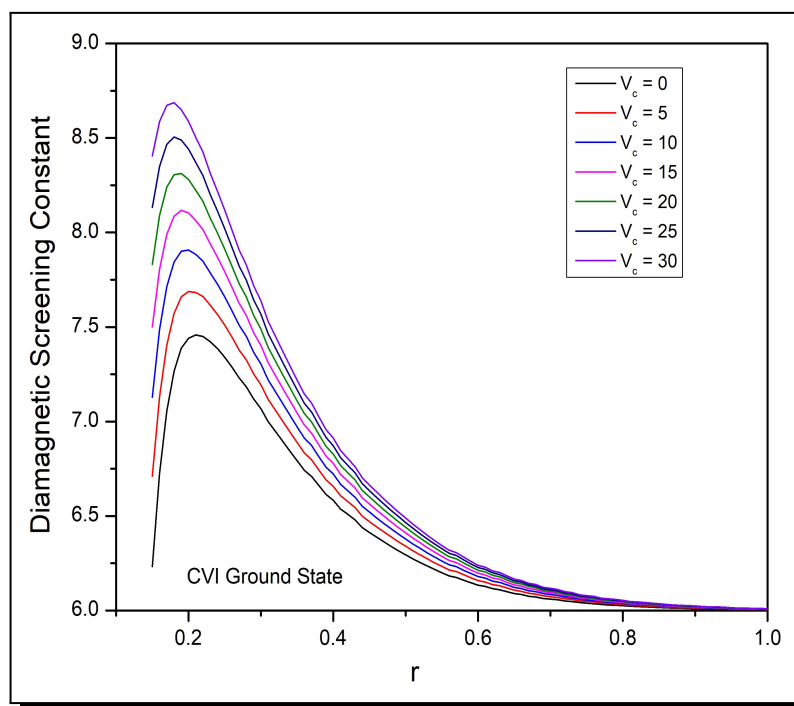


Figure 6. Variation of Diamagnetic screening constant as a function of confinement radius for the ground state of CVI for different levels of penetrability

4. Conclusions

We have investigated Carbon (CVI), Nitrogen (NVII) and Oxygen (OVIII)- a Hydrogen like one electron ions, compressed within the spherical penetrable box. Such environment seems to be viable at high density astrophysical sites. The confinement of elements is due to certain potential wall at the boundary of the confinement region, governed through the pressure from the surrounding. The analysis of such system has been carried out by solving time-independent Schrodinger Equation using Numerov method. Lower is the potential wall, energy is large which increases as the confinement radius increases. With decrease in confinement radius the bound state transformed to continuum state. This behavior is seen to start at relatively large radius for high potential wall (i.e. for high pressure) than the lower potential value. Ground state ions carry high energy than the $2s$ and $2p$ states, hence the penetration probability is more for $1s$ state ions. Furthermore, the tendency to cross the confinement region becomes less with the increase in the potential height which ultimately increases the pressure. The polarizability and Diamagnetic screening constant for the Carbon in ground state is seen to reach at extremum value (minimum for polarizability and maximum for diamagnetic screening constant) at a particular confinement radius corresponding to each potential wall, then at large radius they become constant and independent of the potential or pressure.

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Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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