

QUANTUM STATES OF THE ‘ENIGMATIC’ 1-D HYDROGEN ATOM: DO THEY EXIST?

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Abstract: The quantum states of hydrogen atom in one dimension can be obtained by a careful application of the well-known Frobenius method. The exercise is highly educative and brings to focus the subtle aspects of quantum mechanics. The allowed states turn out to be only of odd parity and non-degenerate, having energy given by $E_n = -\frac{e^2}{2n^2a_0}$, $n = 1, 2, 3, \dots$, and a_0 being the first Bohr radius, in exact correspondence with energy levels of 3-D H-atom. In view of odd parity of all states the spectrum of 1-D H-atom is expected to be dominated by weak electric quadrupole transitions.

1. INTRODUCTION

In undergraduate courses of Chemistry, quantum mechanics of one-dimensional systems occupy a prominent position. Quantum states of a particle in a one-dimensional potential well, rigid rotator on a plane, harmonic oscillator, etc. are taught to demonstrate the techniques of arriving at solutions of the Schrodinger equation (SE) posed as a boundary value problem, emphasizing at the same time the importance of all mathematical conditions imposed on the wavefunctions. It is almost mandatory in all such courses to venture a little beyond and discuss quantum mechanics of the hydrogen atom in three dimensions. The bound energy levels and wave functions of the hydrogen atom are key to the development of general ideas and understanding of the level structures of heavier atoms. The (SE) for H-atom in 3D is not separable in Cartesian system of coordinates. The standard textbook recipe has been to transform the energy eigenvalue equation from Cartesian (x, y, z) to spherical polar coordinates (r, θ, ϕ) and separate the angular and the radial parts $R_{nl}(r)$ of the wave equation which are then analytically solved. The former turns out to be the spherical harmonics [$Y_l^m(\theta, \phi)$] while the latter takes the form of the associated Laguerre polynomials. The total wave function $\Psi_{nlm}(r, \theta, \phi)$ which is a product of the radial and angular parts of wave function [$\Psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$] has a well-defined parity eigenvalue equal to $(-1)^l$, l being the angular momentum quantum number in the n^{th} quantum state of the atom with l assuming values $0, 1, 2, \dots, n-1$, n being the principle quantum number. The Coulomb potential $V(\vec{r}) = -\frac{e^2}{|\vec{r}|}$ is

inversion symmetric. Its signature, the parity, is a ‘good’ quantum number and the hydrogenic levels alternately belong to even and odd parity. We note, however, that $V(\vec{r})$ is singular at the origin ($|\vec{r}| = 0$). *The role of the singularity, if any, in shaping the radial wavefunctions is usually bypassed or underemphasized at the introductory level of the undergraduate courses in Chemistry.* But several issues do come up and require careful handling while discussing the behavior of Ψ , in the neighborhood of $|\vec{r}| = 0$. Whatever be the ‘parity’, the allowed quantum states have $(2l + 1)$ fold degeneracy (the m -degeneracy, the magnetic quantum number ‘ m ’ taking integer values from $-l$ to l in steps of 1) arising from the rotational symmetry of the hydrogen atom. There is also an extra l -degeneracy (e.g., 2s, 2p) not connected with the rotational symmetry. It has been often called an accidental degeneracy, the origin of which is a dynamical symmetry.⁽¹²⁾ The hydrogenic energy levels turn out to be dependent only on the principal quantum number ($E_{nlm} = -\frac{R}{n^2}$, $n = 1, 2, 3, \dots$) revealing the l and m degeneracies referred to.

All these degeneracies and the separation problem of radial and angular motion disappear if the problem is reduced to one dimension, giving rise to the problem of finding the quantum states of the one-dimensional hydrogen atom. The Coulomb potential in one dimension is $V(\vec{x}) = -\frac{e^2}{|\vec{x}|}$. It has inversion symmetry just as $V(\vec{r})$ has in 3 dimensions. The singularity at the origin ($x = 0$), although reminiscent of the singularity at $r = 0$ in the 3-D hydrogen atom, is more problematic as it separates the available coordinate space into two regions ($x > 0$ and $x < 0$). The ‘enigma’ of the hydrogen atom in one dimension originates from this singularity at $x = 0$.

The following questions arise:

- (i) Is parity still a ‘good’ quantum number or does the singularity destroy parity?
- (ii) What is the energy level structure for the bound states, if any? Does the non-degeneracy theorem still hold? What are the energy eigenvalues like?
- (iii) What is the symmetry of the ground state, if it exists? What are the symmetries of excited state, if they occur?
- (iv) What kind of spectrum (vis-à-vis the 3-D hydrogen spectrum) can be anticipated?
- (v) What is the experimental status of the problem?

The one-dimensional hydrogen atom has been a controversial problem with a fairly long history, but its importance in understanding how the calculus of quantum mechanics operates in singular potentials, can hardly be overestimated. In this article, we briefly trace the history

of hydrogen atom in one dimension and elucidate how the standard Frobenius method (a generalized series expansion method) can be applied to this system vitiated as it is, by the singularity at the origin. As expected, the conditions that *the wave function $\Psi(x)$ must be single valued and continuous with continuous first derivative, Ψ remaining finite everywhere (including the singular point) and vanishing at the outer boundaries' ($x = \pm\infty$) play a key role in shaping the energy eigenfunctions and the corresponding energy eigenvalues.*

2. A BRIEF HISTORY OF 1-D HYDROGEN ATOM

The one-dimensional hydrogen atom has been at the center of controversies and debate ever since Loudon (1952)⁽¹⁾ published his theoretical work on the system. Since then, it has been debated if the system has an infinite or a finite energy ground state, whether there are energy degeneracies, violating the one-D non-degeneracy theorem, whether the states are localized (symmetry broken) on either side of the singularity ($x = 0$) or delocalized across the origin, and are parity eigenstates as well. There is no unequivocal or concrete experimental evidence on the existence of the hydrogen atom in one dimension and its spectral signatures; but there have been several attempts to define limiting experimental conditions (e.g., high magnetic field) which may lead to the realization of the one-dimensional H-atom and recording of its spectrum. Calculations of Landau & Lipshitz,⁽⁵⁾ which dealt with giving an estimate of the strength of such magnetic field, emphasize that the highest available magnetic fields in the laboratory is almost negligible compared to the range of the magnetic field strength required to approach the condition for the realization of the one-D H-atom.⁽⁶⁾ Some experiments on quasi-one-D polymer chains, which resembles the system of the one-D H-atom, reported optical absorption spectra with the dominance of the ground state.⁽⁷⁾ There are other such examples, such as semiconductor quantum wires⁽⁸⁾ and carbon nanotubes,^{(9),(10)} which reported various forms of the absorption spectra. However, these results are inadequate to characterize the exact experimental form of the absorption spectrum of one-D H-atom, as the conditions for its realization are still elusive. Thus, the one-D H-atom has largely remained a theoretical problem to test various theoretical techniques of handling quantum mechanical problems of the present kind. The result of all these investigations do not seem to have converged to a generally accepted conclusion about the nature of quantum states supported by the 1-D Coulomb potential, or their number. More significantly, the spectral signature of the 1-D H-atom, if it exists, is not yet known. Among the theoretical investigations, the series expansion method,⁽²⁾ Fourier transform method,⁽³⁾ Supersymmetric method⁽⁴⁾ and insertion of cut-off potential to the one-D potential function method^{(2),(6)} seem to suggest that the 1-D H-atom can exist in an

infinite number of discrete quantum states with exactly the same energy levels as found in the 3-D hydrogen atom, the reduction in the dimension (from 3 to 1) notwithstanding. However, these results are confined to research journals and reviews and are not easily accessible or comprehensible to chemists or students of chemistry, who could ultimately play a crucial role in the eventual experimental realization of the 1-D H-atom, if it exists. It is primarily this objective, that has guided us in exploring the problem and writing this article.

3. COULOMB SINGULARITY AND THE QUANTUM STATES OF H-ATOM IN 3-DIMENSION

We have already mentioned that the H-atom problem is separable in spherical polar coordinates (r, θ, ϕ) . The transformation of the energy eigenvalue equation $H\Psi(x, y, z) = E\Psi(x, y, z)$ to $H(r, \theta, \phi)\Psi(r, \theta, \phi) = E\Psi(r, \theta, \phi)$ begins by writing down the form of the ∇^2 in the (r, θ, ϕ) system:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{(r \sin \theta)^2} \frac{\partial^2}{\partial \phi^2} \quad 3.1$$

The eigenvalue equation for the quantum states of the H atom, then, becomes

$$-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial \Psi(r, \theta, \phi)}{\partial r} + \frac{L^2}{2mr^2} \Psi(r, \theta, \phi) - \frac{e^2}{r} \Psi(r, \theta, \phi) = E\Psi(r, \theta, \phi) \quad 3.2$$

where, L^2 represents the square of the angular momentum operator which appears naturally from the angular derivatives in the ∇^2 operator. Since the potential energy term $\left(-\frac{e^2}{r}\right)$ is spherically symmetric we can begin by writing $\Psi(r, \theta, \phi)$ as follows,

$$\Psi(r, \theta, \phi) = \chi(r)Y_l^m(\theta, \phi) \quad 3.3$$

where, $Y_l^m(\theta, \phi)$'s are the spherical harmonics – they are eigenfunctions of both L^2 and L_z operators which commutes with H. When (3.3) is introduced in (3.2) we get the following equation for the radial function $\chi(r)$:

$$-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d\chi(r)}{dr} + \frac{\hbar^2 l(l+1)}{2mr^2} \chi(r) - \frac{e^2}{r} \chi(r) = E\chi(r) \quad 3.4$$

(Note, that we switched over to total derivative in place of partial derivative in r as $\chi(r)$, free of angular dependence) Equation (3.4) can be reduced to a one-dimensional form by taking $\chi(r) = \frac{R}{r}$ whence,

$$-\frac{\hbar^2}{2m} \frac{d^2 R(r)}{dr^2} + \left(\frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e^2}{r} \right) R(r) = ER(r) \quad 3.5$$

The bracketed term in equation (3.5) can be considered as an effective one-dimensional potential $W_{\text{eff}}(r)$ in which the electron moves. The equation has singularities at $r = 0, \infty$ and the standard boundary condition requires us to set $\chi(r) = 0$ at both the singularities. Let us take

the case of $l \neq 0$ first. We note that at very small values of r , the $\frac{\hbar^2 l(l+1)}{2mr^2} R$ term will far outweigh the Coulomb term $\left(-\frac{e^2}{r}\right)$ in $W_{\text{eff}}(r)$ which can, therefore, be neglected along with the $ER(r)$ term in Equation (3.5) at very small values of r , i.e., close to the nucleus or the inner singular points. In the close neighborhood of the nucleus of equation (3.5) for the radial wave equation is reduced to the very simple form,

$$-\frac{\hbar^2}{2m} \frac{d^2 R(r)}{dr^2} = \frac{\hbar^2 l(l+1)}{2mr^2} R(r) \quad 3.6$$

Equation (3.6) can be solved by the substitution of $R(r) = r^\gamma$ which leads to the condition (3.7).

$$\gamma(\gamma - 1) = l(l + 1) \quad 3.7$$

That means γ can assume two values $\gamma = l + 1$ and $-l$, since

$$\chi(r) = \frac{R(r)}{r}$$

For $\gamma = -l$, $\chi(r)$ blows up to infinity for any value of l (including $l = 0$) as $r \rightarrow 0$ and fails to satisfy the condition that $\chi(r)$ vanishes or remains finite at the boundary ($r = 0$). The root $\gamma = -l$ is, therefore, rejected. The other root $\gamma = l + 1$ leads to

$$R(r) = A \cdot r^{l+1}, \quad 3.8$$

$$\chi(r) = \frac{R}{r} = A \cdot r^l \quad 3.8a$$

with $\chi(r)$ smoothly vanishing at the singular point $r = 0$ for any non-zero l -value.

The situation for $l = 0$ is different. In this case the centrifugal term disappears and we must retain the Coulomb term $\left(-\frac{e^2}{r} R\right)$ in equation (3.5). The resulting equation can be solved by making the substitution:

$$R(r) = a_1 r + a_2 r^2 + \dots \quad 3.9$$

The wave function for $l = 0$ assumes the form

$$\chi(r) = \frac{R}{r} = a_1 \equiv Ar^0 \quad (A = a_1) \quad 3.10$$

within a very small sphere around r . Equation (3.10) has the same form as equation (3.8a). Thus, at the coordinate origin (the inner singularity) the radial wavefunction vanishes in the form of a power law,

$$\text{i) } \chi_l(r) = Ar^l \quad (l > 0)$$

and,

$$\text{ii) } \chi_l(r) = a_1 \quad (\text{constant}) \quad (l = 0)$$

The difference in the behavior of $\chi_l(r)$ near $r = 0$ for $l = 0$, and $l > 0$ appears queer at the first sight, but can be physically understood in the following way.

The centrifugal force acting on the electron produces an effective repulsive potential $\frac{\hbar^2 l(l+1)}{2mr^2}$ which severely limits the classically accessible region around $r = 0$. This region around $r = 0$ is, however, accessible to a quantum particle via tunnelling. The wave function χ in this region however, decreases rapidly according to the power law ($\chi \sim r^{-1}$), the damping being stronger for higher l values. For $l = 0$ there is no centrifugal barrier and the electron (s electron) can therefore approach the nucleus infinitesimally closely.

The behavior of the radial function $R(r)$ infinitely away from the nucleus is determined by the equation (3.5) with both the centrifugal and the coulomb terms set to zero. The resulting equation is,

$$\frac{d^2 R}{dr^2} = -\frac{2mE}{\hbar^2} R \quad 3.11$$

For, $E < 0$, (or $E = |E|$) the only solution that vanishes as $r \rightarrow \infty$ is,

$$R = C \exp(-\sqrt{2m|E|} r) \quad 3.12$$

In the intermediate region ($0 < r < \infty$) one can model the wavefunction in the form,

$$R = \xi^{l+1} e^{-\xi(2\epsilon)^{1/2}} \{A_0 + A_1 \xi + A_2 \xi^2 + \dots\} = \xi^{l+1} e^{-\xi(2\epsilon)^{1/2}} \sum_{n=0}^{\infty} A_n \xi^n \quad 3.13$$

where, we have made the substitution $\xi = \frac{me^2}{\hbar^2} r$ and $\epsilon = \frac{\hbar^2}{me^2} |E|$ 3.14

The first term fixes the form of R as $\xi \rightarrow 0$, the second term determines how R behaves in the large ξ region and the power series in a way interpolates between the limiting forms taken by R in the interior and the exterior singularities. When 'R' of equation (3.13) is ploughed back in equation (3.8), and coefficients of the like powers of ξ are equated we arrive at the recursion formula for the coefficients of the power series.

$$A_{n+1} = \frac{2[1 - (n+1+1)(2\epsilon)^{1/2}]}{l(l+1) - (n+1+1)(n+1+2)}$$

The condition that the power series gets truncated into a polynomial is clearly,

$$1 - (n+1+1)(2\epsilon)^{1/2} = 0$$

which leads to the quantized energy levels of the H atom in 3 dimensions:

$$E_n = -\frac{me^4}{2\hbar^2(n+1+1)^2}$$

The 'parity' of the bound quantum states of the hydrogen atom is not, however, generated from the radial wave function – it is rooted in the angular wave function. It can be easily shown that the reflection through the origin of the coordinate system leads to^{(11),(12)}

$$Y_l^m(\theta, \phi) \xrightarrow{\text{Inversion}} Y_l^m(\pi - \theta, \phi + \pi) = (-1)^l Y_l^m(\theta, \phi)$$

The parity of an allowed quantum state of hydrogen atom is thus determined by its angular momentum quantum number. The determination of quantum states of the one-dimensional hydrogen atom can now be attempted in a similar manner. It turns out that the problem is more complicated and subtle in one-dimension.

4. THE SE FOR 1-D H-ATOM AND ITS SOLUTIONS

4.1 THE GROUND STATE

The Schrodinger equation for the stationary bound states of the one-dimensional hydrogen atom is

$$-\frac{\hbar^2}{2m_e} \frac{d^2\Psi_n(x)}{dx^2} - \frac{e^2}{|x|} \Psi_n(x) = E_n \Psi_n(x) \quad 4.1.1$$

where, $\Psi_n(x)$ is the wave function of the n^{th} stationary state with the discrete energy ($E < 0$), m_e being the mass of the electron.

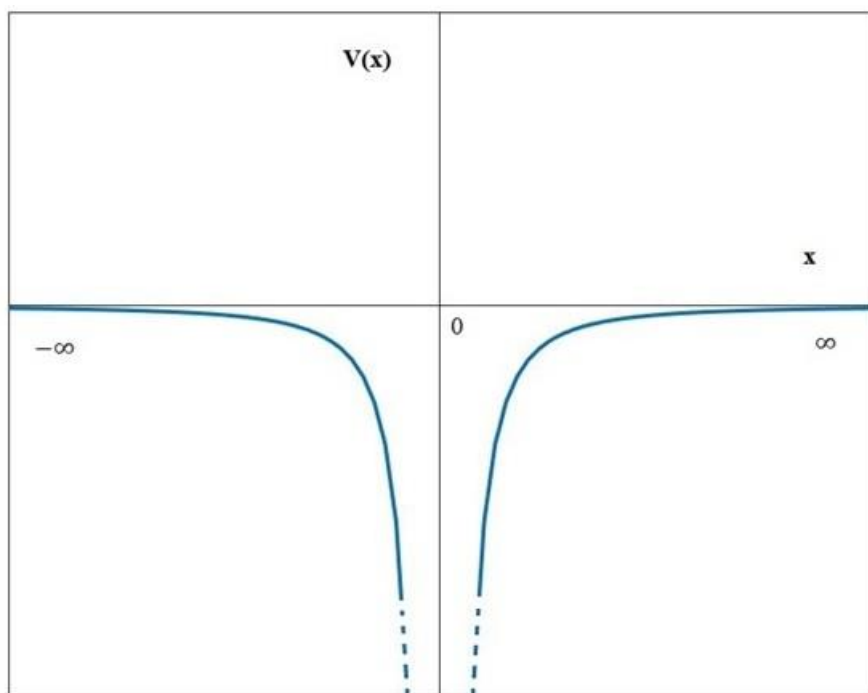


Figure 1: The one-D Coulomb potential

Due to the singularity in the potential energy $V(\vec{x}) = -\frac{e^2}{|\vec{x}|}$ (See figure 1 which displays $V(x)$ as a function of x) at $x = 0$, we will first look for solutions $\Psi(x)$ in the region $x > 0$, by invoking the standard Frobenius method⁽¹³⁾. It is convenient in this context to make few substitutions to transform equation (4.1.1) into a dimensionless form. With this end in view, let us first multiply both sides of equation (4.1.1) by $-\frac{2m_e}{\hbar^2}$, and set $\gamma^2 = -\frac{2m_e E_n}{\hbar^2}$, $\beta = \frac{m_e e^2}{\hbar^2 \gamma}$ and $\xi = 2\gamma x$, thus transforming equation (4.1.1) into the following form,

$$\frac{d^2\Psi(\xi)}{d\xi^2} - \left[\frac{1}{4} - \frac{\beta}{\xi} \right] \Psi(\xi) = 0, \quad (x > 0, \xi > 0) \quad 4.1.2$$

In the limit, $\xi \rightarrow \infty$ ($x \rightarrow \infty$), the asymptotic form of the wave equation (4.1.2) becomes:

$$\frac{d^2\Psi^\infty(\xi)}{d\xi^2} = \frac{1}{4} \Psi^\infty(\xi) \quad 4.1.3$$

and is solved by,

$$\Psi^\infty(\xi) \sim e^{-\frac{\xi}{2}} \quad 4.1.4$$

The general form of the solution in the region $\xi > 0$ ($x > 0$) can be written in the form

$$\Psi(\xi) = e^{-\frac{\xi}{2}} f(\xi) \quad 4.1.5$$

where, $f(\xi)$ is a function that needs to be determined. Substituting equation (4.1.5) in (4.1.2), we arrive at the differential equation that the targeted function $f(\xi)$ must satisfy, which is,

$$\xi \frac{d^2f}{d\xi^2} - \xi \frac{df}{d\xi} + \beta f = 0 \quad 4.1.6$$

Before proceeding with the task of solving equation (4.1.6), we must investigate how $\Psi(\xi)$ should behave in the neighborhood of $\xi = 0$ ($x = 0$). Let us note that equation (4.1.2) can be written in the form

$$\frac{d^2\Psi^0}{d\xi^2} = \frac{1}{4} \Psi^0 - \frac{\beta}{|\xi|} \Psi^0 \quad 4.1.7$$

where, Ψ^0 represents the form of Ψ at or near $\xi = 0$. Choosing $\Psi(\xi \sim 0) = \xi^\alpha$ (α being a real parameter) which is then substituted for Ψ^0 in equation (4.1.7), we arrive at following relation for determining α :

$$\alpha(\alpha - 1)\xi^{\alpha-2} = \frac{1}{4}\xi^\alpha - \beta\xi^{\alpha-1} \quad 4.1.8$$

Equating the coefficients of $\xi^{\alpha-2}$ (the lowest power of ξ) on both sides of equation (4.1.8) yields $\alpha = 0$ or 1 . Of these two values, $\alpha = 0$ can be rejected as it leads to $\frac{d^2\Psi^0}{d\xi^2}$ blowing up to an infinitely large value due to the third term on the right-hand side of equation (4.1.7), making Ψ^0 also infinite. The choice $\alpha = 1$, however, does not lead to a blow up. The correct form of $\Psi(\xi)$ from $\xi = 0$ to ∞ , that keeps $\Psi(\xi)$ *finite* at or near $\xi = 0$ and also makes it vanish at the right boundary ($\xi \sim \infty$) is therefore $\psi(\xi) = e^{-\frac{\xi}{2}} \xi g(\xi)$, where $g(\xi)$ may be chosen as a power series in ξ .

$$g(\xi) = \sum_{n=0}^{\infty} a_n \xi^n \quad 4.1.9$$

The form of $f(\xi)$ in equation (4.1.6) can therefore, be taken as

$$f(\xi) = \xi g(\xi) = \xi \sum_{n=0}^{\infty} a_n \xi^n = \sum_{n=1}^{\infty} a_n \xi^n \quad 4.1.10$$

Substituting $f(\xi)$ of equation (4.1.10) in (4.1.6) we get

$$\xi \sum_{n=1}^{\infty} a_n n(n-1) \xi^{n-2} - \xi \sum_{n=1}^{\infty} a_n n \xi^{n-1} + \beta \sum_{n=1}^{\infty} a_n \xi^n = 0 \quad 4.1.11$$

Equating the coefficients of ξ^n on both sides of (4.1.11) produces the following recursion relation for the coefficients a_n of the power series for $f(\xi)$:

$$a_{n+1} = \frac{n-\beta}{n(n+1)} a_n, \quad n = 1, 2, 3, \dots (\xi > 0) \quad 4.1.12$$

In order that the infinite series generated by the recursion relation (4.1.12) does not diverge but truncates at a finite number of terms converting it into a polynomial of degree 'n', the energy E of which β is a function must have such values that:

$$\beta = n \text{ or } \beta^2 = n^2 \quad 4.1.13$$

which immediately leads to the discrete energy levels,

$$E_n = -\frac{m_e e^4}{2n^2 \hbar^2}, \quad n = 1, 2, 3, \dots \quad 4.1.14$$

The quantum states supported by the one-dimensional Coulomb potential are linked to their energies. The corresponding wavefunctions $\Psi_n(\xi)$ ($n = 1, 2, 3$) are easily found to be:

$$\Psi_n(\xi) = N_n (e^{-\xi/2}) \xi \sum_{k=0}^{n-1} a_{k+1} \xi^k, \quad (\xi > 0) \quad 4.1.15$$

with the a_k 's generated from the recursion relation (4.1.12). It turns out now, that the right branch of the ground state wavefunction $\Psi_{1,R}(\xi)$ has the same energy eigenvalue as that of the hydrogen atom in the 3-dimension

$$E_1 = -\frac{m_e e^4}{2\hbar^2} = -\frac{e^2}{2a_0} \quad 4.1.16$$

with a_0 being the first Bohr radius; but unlike the 1s wavefunction Ψ_1 has a node, i.e., it has a value equal to zero at the centre of the potential ($x = 0$):

$$\psi_1(x) = N_1 e^{-\frac{x}{a_0}} \cdot \frac{2x}{a_0}, \quad (x \geq 0, n = 1) \quad 4.1.17$$

It needs to be stressed that $\Psi(\xi)$ or $\Psi(x)$ obtained so far, is localized on the right-hand side of the origin and as such lack symmetry. We can extend the calculation to the left-hand side of the configuration space by introducing only the change $\xi \leq 0$. (See Appendix I for further details)

The ground state wave function $\Psi_1(\xi)$ ($\xi < 0$) is found to be localized on the left of the origin and has the energy $E_1 = -\frac{e^2}{2a_0}$. We designate it as $\Psi_{1L}(\xi)$, where

$$\Psi_{1L}(\xi) = N_1 (\xi) e^{\frac{\xi}{2}} = N_1 \left(-\frac{2x}{a_0} \right) e^{-\frac{|x|}{a_0}}, \quad (\xi \leq 0, x \leq 0) \quad 4.1.18$$

Like $\Psi_{1R}(x)$, $\Psi_{1L}(x)$ too has a node at the origin and the two-degenerate and localized wavefunctions, Ψ_{1R} and Ψ_{1L} , together must describe the physical ground state of the hydrogen

atom in one dimension. The symmetric (+) combination $\Psi_1^{(+)}(x) = \frac{1}{\sqrt{2}} (\Psi_{1,R}(x) + \Psi_{1,L}(x))$ clearly vanishes everywhere, **so that the even parity ground state of the problem does not exist as a physical state**. The antisymmetric (-) combination of the two localized degenerate wavefunctions has the same energy ($-\frac{e^2}{2a_0}$) but has **odd parity** and describes the correct physical ground state that is an eigenstate of both the Hamiltonian and parity operator. This state designated as $\Psi_1^{(-)}(x)$ is,

$$\Psi_1^{(-)}(x) = 4N_1 e^{-\frac{|x|}{a_0}} \cdot \frac{x}{a_0} = N e^{-\frac{|x|}{a_0}} \left(\frac{x}{a_0}\right) \quad 4.1.18$$

N being the normalization constant. The profile of $\Psi_1^{(-)}(x)$ is displayed in figure 2. Thus, the 1-D H-atom has a finite energy bound ground state having odd parity as opposed to the ground state of H-atom in 3 dimensions, which is of even parity. It is not a nodeless ground state as expected in a 1-D system, **but is definitely non-degenerate**. The singularity at the origin has thus stamped its signature on the wave function for the ground state. Are there excited bound states as well with definite parity? Are they degenerate? We analyze these issues in the section that follows.

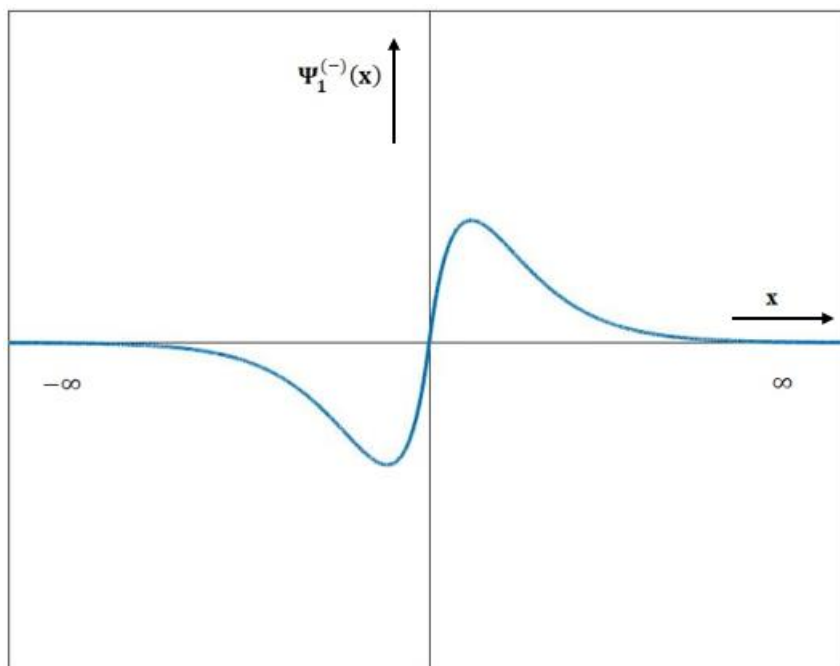


Figure 2: The ground state wave function $\Psi_1^{(-)}(x)$ of the H-atom in one dimension plotted as a function of x ($-\infty \leq x \leq \infty$). Note that the wave function has a zero value at $x = 0$, but a non-zero slope.

4.2 THE EXCITED STATES

The procedure adopted to calculate the ground state wave-function ($n = 1$) and energy (E_1) can be extended to higher values of n ($n = 2, 3, \dots$ etc) as well. The left ($x < 0$) and right ($x > 0$) localized components of the eigenfunctions of the energy operator for $n = 2$ and $n = 3$ (the first and the second excited states of the system) are reported in Table 1 along with their respective energy eigenvalues. Ψ_{nL} and Ψ_{nR} can be seen to have the same energy eigenvalue $E_n = -\frac{e^2}{2n^2a_0}$ for a particular value of n . They are *degenerate but lack parity and are therefore physically unacceptable as eigenfunctions in an inversion symmetric potential*. However, their symmetric and antisymmetric combinations ($\Psi_n^{(+)}$ and $\Psi_n^{(-)}$) have even and odd parity, respectively in each case. They are physically acceptable, although apparently degenerate in energy as displayed in Table 2.

TABLE 1: The left ($x < 0$) and the right ($x > 0$) components of $\Psi_n(x)$ ($n = 2, 3$) along with their energies E_n ($n = 2, 3$).

n	$\Psi_{nL}(x)$	$-E_n$	$\Psi_{nR}(x)$
2	$-N_2 e^{-\frac{ x }{2a_0}} \left[\frac{x}{a_0} + \frac{x^2}{a_0^2} \right]$	$\frac{e^2}{8a_0}$	$N_2 e^{-\frac{ x }{2a_0}} \left[\frac{x}{a_0} - \frac{x^2}{a_0^2} \right]$
3	$-N_3 e^{-\frac{ x }{3a_0}} \left[\frac{2x}{3a_0} + \frac{4x^2}{9a_0^2} + \frac{4x^3}{81a_0^3} \right]$	$\frac{e^2}{18a_0}$	$N_3 e^{-\frac{ x }{3a_0}} \left[\frac{2x}{3a_0} - \frac{4x^2}{9a_0^2} + \frac{4x^3}{81a_0^3} \right]$

TABLE 2: The symmetric and the antisymmetric combination of Ψ_{nL} and Ψ_{nR} producing the even ($\Psi_n^{(+)}$) and odd ($\Psi_n^{(-)}$) parity eigenfunction of the system for $n = 2, 3$.

n	$\Psi_n^{(-)}(x)$	$-E_n$	$\Psi_n^{(+)}(x)$
2	$2N_2 e^{-\frac{ x }{2a_0}} \cdot \frac{x}{a_0}$	$\frac{e^2}{8a_0}$	$-2N_2 e^{-\frac{ x }{2a_0}} \cdot \frac{x^2}{a_0^2}$
3	$2N_3 e^{-\frac{ x }{3a_0}} \left[\frac{2x}{3a_0} + \frac{4x^3}{81a_0^2} \right]$	$\frac{e^2}{18a_0}$	$-8N_3 e^{-\frac{ x }{3a_0}} \cdot \frac{x^2}{a_0^2}$

$\Psi_n^{(+)}$ and $\Psi_n^{(-)}$ ($n = 2, 3$) have clear parity labels, but other mathematical restrictions on the wavefunctions must now be considered. $\Psi_n^{(+)}$ and $\Psi_n^{(-)}$ ($n > 1$) clearly vanish at $x = \pm\infty$ and are finite at all the interior points. They are also continuous at all points including $x = 0$, and linearly independent. We may, however reject the even parity eigenfunctions ($\Psi_n^{(+)}$, $n > 1$) and accept only the odd parity eigenfunctions ($\Psi_n^{(-)}$, $n > 1$) on the mathematical ground that the

first derivative of $\Psi_n^{(-)}(x)$ is continuous at $x = 0$ (the singular point) while the first derivative of $\Psi_n^{(+)}(x)$ may not so be. This fact can be demonstrated in a slightly roundabout way. Let us consider the SE for the one-D H-atom for the quantum state $\Psi_n^{(-)}$ ($n > 1$):

$$\frac{d^2\Psi_n^{(-)}}{dx^2} = \left(E - \frac{e^2}{|x|}\right)\Psi_n^{(-)} \quad 4.2.1$$

Integrating both sides of equation (4.2.1) between the infinitesimal limits $\pm\epsilon$ we have,

$$\int_{-\epsilon}^{\epsilon} \left(\Psi_n^{(-)}\right)'' dx = \int_{-\epsilon}^{\epsilon} \left(E - \frac{e^2}{|x|}\right)\Psi_n^{(-)} dx \quad 4.2.2$$

The integral on the right-hand side vanishes as the integrand is odd with respect to inversion at $x = 0$. Accordingly, we can write,

$$\lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} \left(\Psi_n^{(-)}\right)''(x) dx = \lim_{\epsilon \rightarrow 0} \left(\Psi_n^{(-)'}(\epsilon) - \Psi_n^{(-)'}(-\epsilon)\right) = \lim_{\epsilon \rightarrow 0} \Psi_n^{(-)}(\epsilon) \quad 4.2.3$$

ensuring the continuity of $\Psi_n^{(-)'}$ at $x = 0$. Had we used the corresponding equation for $\Psi_n^{(+)''}$, the integrand on the right-hand side of equation (4.2.2) could not be equated to zero on the ground of symmetry. We are therefore, led to conclude that the discrete bound quantum states of the H-atom in one dimension exists for infinitely many integer values of n ($= 1, 2, 3, \dots$). They are all of odd parity and satisfy all the mathematical requirements that $\Psi(x)$ must satisfy. $\Psi_2^{(-)}(x)$ and $\Psi_3^{(-)}(x)$ are displayed in the figure 3(a) and 3(b). The still higher states can be calculated similarly.

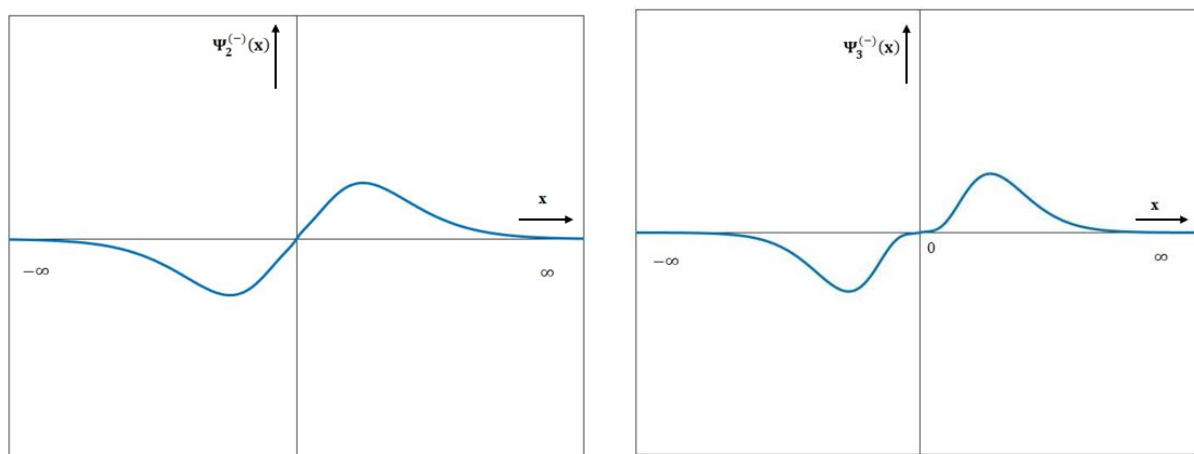


Figure 3(a, b): $\Psi_2^{(-)}(x)$ and $\Psi_3^{(-)}(x)$ respectively has been depicted

The odd parity of all the bound states suggests that the transition moment integral mediated by the electric dipole moment operator $d = ex$ vanishes in,

$$D_{nn'} = N_n N_{n'} \int_{-\infty}^{\infty} \Psi_n^{(-)}(ex) \Psi_{n'}^{(-)} dx = 0 \quad 4.2.4$$

The transition moment integrals mediated by the electric quadrupole moment operator ex^2 may, however, be nonzero (See Appendix II for further details). The spectrum of the one-D H-atom is, therefore expected to be dominated by electric quadrupole transitions while the spectrum of 3-D Hydrogen atom is essentially electric dipole driven spectrum. Experimental spectral data alone can confirm this prediction, which is unavailable at this moment.

5. CONCLUSION

The one-D hydrogen atom has infinite number of discrete bound states with energy $E_n = -\frac{m_e e^4}{2n^2 \hbar^2}$ ($n = 1, 2, 3, \dots$), which can be obtained by the judicious application of the Frobenius method, and the enforcement of all mathematical conditions on the wave function. The energy eigenfunctions have finite values everywhere, including the singular point ($x = 0$) vanishing at $x \rightarrow \pm\infty$, and are of the odd parity. The spectrum is thus expected to be shaped dominantly by the much weaker electric quadrupole transitions.

APPENDIX-I

The $\xi \leq 0$ counterpart of equation (4.1.2) becomes:

$$\frac{d^2 \Psi(\xi)}{d\xi^2} - \left[\frac{1}{4} + \frac{\beta}{\xi} \right] \Psi(\xi) = 0, \quad \xi \leq 0 \quad I.1$$

so that the asymptotic form of Ψ as $\xi \rightarrow -\infty$ becomes,

$$\Psi^\infty(\xi) \sim e^{\frac{\xi}{2}} \equiv e^{-\frac{|\xi|}{2}}, \quad (\xi \leq 0)$$

It is straight forward to find that $f(\xi)$ for $\xi < 0$ satisfies the differential equation:

$$\xi \frac{d^2 f}{d\xi^2} - \xi \frac{df}{d\xi} - \beta f = 0 \quad I.2$$

The power series solution for $f(\xi)$, then leads to the following recursion relation for the expansion coefficients,

$$a_{n+1} = \frac{n+\beta}{n(n+1)} a_n, \quad n = 1, 2, 3, \dots (\xi < 0) \quad I.3$$

The truncation condition for the power series expansion now becomes

$$\beta = -n \text{ or } \beta^2 = n^2 \quad I.4$$

so that, we get the same discrete energy levels for the $\xi < 0$ region as obtained for the $\xi > 0$ region: -

$$E_n = -\frac{m_e e^4}{2n^2 \hbar^2} = -\frac{e^2}{2n^2 a_0}, \quad n = 1, 2, 3, \dots \quad \text{I.5}$$

APPENDIX-II

The transition moment integral ($D_{nn'}$) mediated by the electric dipole moment operator (ex) can be shown to be zero, for the odd parity bound states, by considering the transition from $n = 1$ to $n' = 2$ state, for example, as

$$D_{nn'} = \int_{-\infty}^{\infty} \Psi_1^{(-)}(ex)\Psi_2^{(-)} dx = \int_{-\infty}^{\infty} \left\{ N_1 e^{-\frac{|x|}{a_0}} \left(\frac{x}{a_0} \right) \right\} (ex) \left\{ N_2 e^{-\frac{|x|}{2a_0}} \cdot \frac{x}{a_0} \right\} dx \quad \text{II.1}$$

which can further be written in a simplified form as,

$$D_{nn'} = N_1 N_2 e \int_{-\infty}^{\infty} e^{-\frac{3|x|}{2a_0}} \left(\frac{x^3}{a_0^2} \right) dx \quad \text{II.2}$$

The integral can be solved for the left side of the configuration space by considering only the changes for $x < 0$ in the above integral. The integral, thus results to zero as it is shown,

$$D_{nn'} = N_1 N_2 e \left[- \int_{\infty}^0 e^{-\frac{3|x|}{2a_0}} \left(\frac{x^3}{a_0^2} \right) dx + \int_0^{\infty} e^{-\frac{3|x|}{2a_0}} \left(\frac{x^3}{a_0^2} \right) dx \right] = 0 \quad \text{II.3}$$

At the same time, the transition moment integral ($Q_{nn'}$) mediated by the quadrupole operator moment (ex^2) can be shown to be non-zero, for the same set of odd parity bound states,

$$\begin{aligned} Q_{nn'} &= \int_{-\infty}^{\infty} \Psi_1^{(-)}(ex^2)\Psi_2^{(-)} dx = \int_{-\infty}^{\infty} \left\{ N_1 e^{-\frac{|x|}{a_0}} \left(\frac{x}{a_0} \right) \right\} (ex^2) \left\{ N_2 e^{-\frac{|x|}{2a_0}} \cdot \frac{x}{a_0} \right\} dx \\ &= N_1 N_2 e \int_{-\infty}^{\infty} e^{-\frac{3|x|}{2a_0}} \left(\frac{x^4}{a_0^2} \right) dx \end{aligned} \quad \text{II.4}$$

In the same way, as the case of the electric dipole operator, when we introduce the changes for $x < 0$ in the evaluated transition moment integral for the electric quadrupole operator, it does not vanish to zero as it can be shown as,

$$Q_{nn'} = N_1 N_2 e \left[\int_{\infty}^0 e^{-\frac{3|x|}{2a_0}} \left(\frac{x^4}{a_0^2} \right) dx + \int_0^{\infty} e^{-\frac{3|x|}{2a_0}} \left(\frac{x^4}{a_0^2} \right) dx \right] \neq 0 \quad \text{II.5}$$

which further justifies the expected domination of the spectrum by the electric quadrupole transitions.

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