

A Visualized Mathematical Model of Atomic Structure

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Abstract: A model of atomic structure is presented. Many questions that have baffled scientists for the past decades may be answered by this visualized mathematical model. In particular, the model mathematically relates the properties of the parabola to the atoms' shells and orbits. A series of parabolas represents the atom shells (vertical sections along paraboloids) from outer to inner part of the atom. A pair of electrons exists in a circular motion in each orbit. The orbits are contained in the parabolic shells. Orbits in a shell equal to the square of shell number. Furthermore, hydrogen atomic spectrum was simulated and a new relation was verified. The frequencies of the visible spectra of the hydrogen atom were found to be related to the change in the area enclosed by the first orbit in the second shell, 2s, when the electron is excited into the inner concentric orbits. A proportionality constant equals 0.238725 femto-sec has been found to satisfy that relation.

Keywords: Model, Atom Structure, Hydrogen Spectrum, Shell, Orbit

المستخلص: تعرض هذه الورقة نموذج لتركيب الذرة. في هذا النموذج الرياضي التصوري للذرة ترتبط الأغلفة والمدارات الذرية بخصائص القطع المكافئ. يفترض النموذج من خلال قطاع رأسي يوضح أغلفة الذرة أن يأخذ كل منها شكل قطع مكافئ وتبدأ من الخارج إلى الداخل. وأن كل غلاف يحوي مدارات دائرية يساوي عددها مربع رقم الغلاف. وفي كل مدار يدور زوج من الإلكترونات. تمت محاكاة لطيف ذرة الهيدروجين بواسطة النموذج وتم إستنتاج علاقة جديدة. فقد وجد أن الأطوال الموجية للأطياف المرئية لذرة الهيدروجين تتناسب مع مقدار التغير في مساحة المدار الأول في الغلاف الثاني، 2s، عندما ينبعث الإلكترون من أو الي مدار داخلي من نوع s في غلاف أعلى. مقدار ثابت التناسب يساوي 0.238725 femto-sec.

Introduction:

The simulation of atomic structure attempts to illustrate a more visually intuitive atomic model enabling a deeper understanding. This allows a much improved understanding of chemical bonding and the creation of molecules with minimal violation to the theory of quantum mechanics.

Thomson ⁽¹⁾ did a rigorous mathematical refinement to the atomic model advocated by Lord Kelvin. The atomic model proposed by Thomson ⁽¹⁾ was popularly known as the "plum pudding" model in which electrons and protons are assumed to be uniformly distributed throughout the atomic volume just like plums sitting in a pudding. Rutherford's thin gold-foil experiment provided a concrete evidence for the existence of a minute, positively charged atomic nucleus, from

which alpha particles could scatter in any direction,

Kleppner and Jackiw ⁽²⁾. These observations were not consistent with the predictions of Thomson's model. Thus, naturally Rutherford discarded the plum pudding model and argued that the only way the alpha particles could be deflected in backward direction was that, most of the atom mass is concentrated at the center called the nucleus.

Bohr developed his atomic model in 1911 and refined his atomic theory by applying quantum mechanics to explain the line spectrum of emitted radiations by atoms. Bohr ⁽³⁾ postulated that an atom may occupy only a certain number of stable states, each one associated with a certain amount of discrete energy, in which electrons would orbit the nucleus without emitting or absorbing electromagnetic radiation.

A new kind of mechanics with new formalisms was needed: quantum mechanics. This new mechanics started to develop in the early 1920s, with famous names like Schrödinger and Heisenberg. Schrödinger's ⁽⁴⁾ equation describes an electron as a wave function instead of as a point particle. This approach elegantly predicted many of the spectral phenomena that Bohr's model failed to explain. Although this concept was mathematically convenient, it was difficult to visualize, and faced opposition.

A consequence of describing electrons as waveforms is that, it is mathematically impossible to simultaneously derive the position and momentum of an electron; this became known as the Heisenberg uncertainty principle after the theoretical physicist Werner Heisenberg, who first described it in 1927. The modern model of the atom describes the positions of electrons in an atom in terms of probabilities. Recently, a variety of models and studies on atomic structure and related electron microscopy were developed and presented such as Ishida and Matsumoto ⁽⁵⁾, Matsumoto and Ishida ⁽⁶⁾, Jenner et al ⁽⁷⁾, Miyashita et al ⁽⁸⁾ and Rossmann et al ⁽⁹⁾.

This paper introduces a newly discovered model of the atomic structure. The model is derived by assuming simplified conceptual atomic shells. The shells are represented by a series of parabolic equations.

A Model of Atomic Structure:

A detailed study of the radiation from hydrogen gas, undertaken by Balmer as early as 1885, Bitter ⁽¹⁰⁾, showed that the emitted radiation had discrete frequencies. The spectral lines in the Balmer series of the hydrogen spectrum satisfy the formula. Balmer formula generalized by J.R. Rydberg in 1889:

$$f = 1/\lambda = R(1/2^2 - 1/n^2) \quad (1)$$

Where: f is the spectrum frequency, λ is the wavelength, R is the Rydberg constant.

Niels Bohr rescued the atom from radiating and collapsing by invoking the quantum theory and making two postulates that prevented the atom from radiating energy. Otherwise the atom should emit radiation resulting in its collapse. Bohr was able to derive a formula for the wave numbers of the lines of the spectrum of the hydrogen atom in exactly the same mathematical form as obtained by Balmer and generalized by Rydberg in 1889. Bohr's model gives $R = 1.097 \times 10^7$ per metre, in agreement with observation.

"It will be advantageous if, in the description of position, it should be possible by means of numerical measures to make ourselves independent of the existence of marked positions (possessing names) on the rigid body of reference. In the physics of measurement this is attained by the application of the Cartesian system of co-ordinates" Einstein ⁽¹¹⁾.

Assuming that the orbit in an atom is the probability density function of the electrons distribution in the space, the Cartesian coordinates are used, hereby, to represent the principal quantum energy levels (shells) of the atom. The vertex of these shells is assumed to be the origin, the nucleus. If the first shell, a vertical section along a paraboloid, is represented by a simple curve, an equation of a parabola.

$$y = x^2 \quad (2)$$

Axes are considered to be divided into units (atomic unit length, a.u.l.). At a distance of 1/4 a.u.l. from the origin, the focus of the paraboloid, a circle represents the unique orbit of a unity diameter in the first shell. The second derivative of the curve $y'' = 2$, indicates the number of electrons in the shell.

In the same manner, the equations of the parabolas;

$y = 4x^2$, $y = 9x^2$, $y = 16x^2$, etc. represent the second, third, fourth, inner shells respectively. The second derivative again determines the electrons capacity in each shell. In general, the shell equation is given by:

$$y = n^2 x^2 \quad (3)$$

Where n is the number of the shell.

Table (1) shows the properties of the shells.

Table (1): Properties of the Atom's Shells

Shell No.	Shell Equation	Focus a.u.l.	Electrons Capacity	No. of Orbits	Orbits in the Shell
1	$y = x^2$	1/4	2	1	1s
2	$y = 4x^2$	1	8	4	2s, 2p ₁₋₃
3	$y = 9x^2$	9/4	18	9	3s, 3p ₁₋₃ , 3d ₁₋₅
4	$y = 16x^2$	4	32	16	4s, 4p ₁₋₃ , 4d ₁₋₅ , 4f ₁₋₇
5	$y = 25x^2$	25/4	50	25	5s, 5p ₁₋₃ , 5d ₁₋₅ , 5f ₁₋₇ , 5g ₁₋₉

Figure (1) represents a simple visualized vertical section of the atom's shells containing the inside orbits. It can be clearly stated that, each parabolic shell contains an orbit of a unity diameter with its centre at the focus. Below that orbit, in a sequence of 1/4 a.u.l. along nucleus axis, the shell contains a number of concentric orbits of smaller diameters at 1/4 a.u.l. distant toward the nucleus. Consequently, at each level along the nucleus axis, there exists a series of

concentric orbits for which the diameter reduces towards the inner shells. For these concentric orbits, as the number of the shell increases the number of the orbits decreases. Each orbit contains a pair of electrons moving around the nucleus axis. Number of orbits in the shell is determined by n^2 . Thus, the number of electrons in each shell is given by $2n^2$.

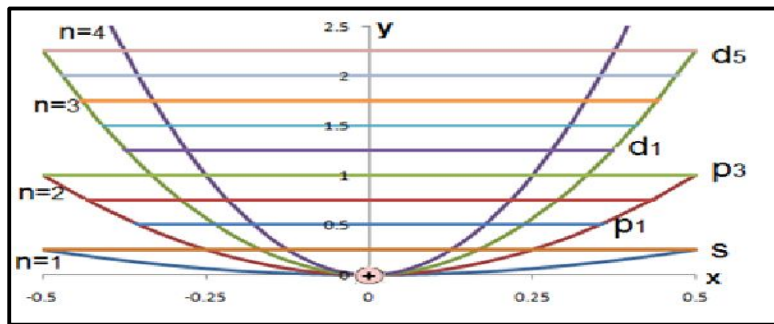


Figure (1): A Visualized Vertical Section of the Atom's Shells

Table (A-1) in Appendix A shows the orbit levels and the diameters according to the parabolic shell equations. The distribution of electrons is according to Aufbau principle, Pauli Exclusion Principle, Hund's rule. The s-elements,

p₁-elements, p₂-elements and p₃-elements in the orbits is shown in Table (B-1) in Appendix B.

Model Validation and Discussion:

By assuming that, an electron is excited, moves from or to an ns-orbit >

2s-orbit, the change in the area, δA , enclosed by the 2s-orbit is proportional to the frequency of the hydrogen spectrum f .

$$\delta A \propto f \tag{4}$$

$$\text{Or } \delta A = K \cdot c / \lambda \tag{5}$$

Where, K is the constant of proportionality, $\delta A = \pi /4[d^2(2s) - d^2(ns)]$ in square atomic units (s.a.u.), d (2s) and d (ns) are diameters of 2s-orbit

and ns-orbit respectively, note that d (2s) = 1/2 atomic unit length.

$f = c / \lambda$ where, λ is the wave length of the spectrum and $c = 3 \times 10^8$ m/sec, the speed of light.

Table (2) shows the value of the constant of proportionality K when applying the model for wave length values of the first five visible spectra of hydrogen.

Table (2): Values of the constant of proportionality

Shel l	S - Orbit	Dia. d(ns) (a.u.l.)	$d^2(2s)$ - $d^2(ns)$	λ (nm)	Constant (k) in femto-sec
3	3s	1/3	1/4 - 1/9	656.28	0.23872619
4	4s	1/4	1/4 - 1/16	486.13	0.23872455
5	5s	1/5	1/4 - 1/25	434.05	0.23872750
6	6s	1/6	1/4 - 1/36	410.17	0.23872328
7	7s	1/7	1/4 - 1/49	397.01	0.23872385

Change in area enclosed by the 2s-orbit, δA , for four spectra are shown in Figure (2). It is shown that, the enclosed area by 2s-orbit increases the wave length decreases, consequently the spectrum frequency increases.

It can be stated that, the constant of proportionality, K, explains the case of the radiated hydrogen atom spectra as interpreted by other previous models.

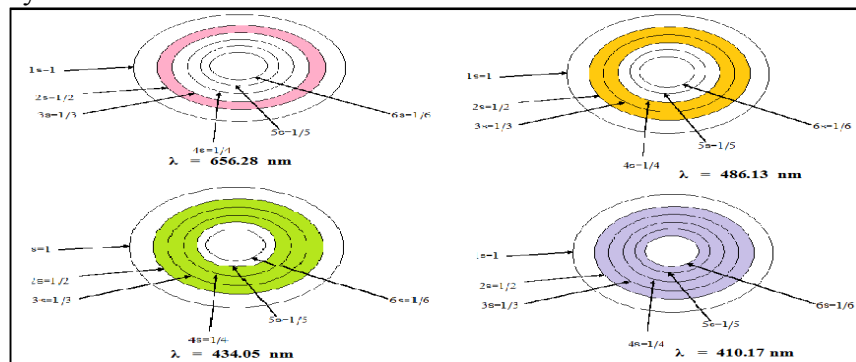


Figure (2): Changes in Area between 2s-orbit and Inner s-orbits

Applying the value of $K = 0.238725$ femto-sec, for the electron motion in the next 10 s-orbits, 8s to 16s, gives the

values of the corresponding wave length of radiated spectra. The results are presented in table (3).

Table (3): Wave length values of Radiated Hydrogen Spectra

Shell	S - Orbit	Dia. d(ns) (a.u.l.)	$d^2(2s)-d^2(ns)$	λ (nm)
8	8s	1/8	1/4 - 1/64	388.90
9	9s	1/9	1/4 - 1/81	383.54
10	10s	1/10	1/4 - 1/100	379.79
11	11s	1/11	1/4 - 1/121	377.06
12	12s	1/12	1/4 - 1/144	375.02
13	13s	1/13	1/4 - 1/169	373.44
14	14s	1/14	1/4 - 1/196	372.19
15	15s	1/15	1/4 - 1/225	371.20
16	16s	1/16	1/4 - 1/256	370.39

Conclusion:

A model which simulates the atom and electrons configuration was presented. The principal quantum energy numbers in the model were assumed to be in a form of parabolic shells (paraboloids) originating from the nucleus. A series of parabolas represents the shells in two dimensional cartesian coordinates. Each shell, parabola, contains an orbit of a unity diameter, in atomic unit length, at the focus level in which two electrons moving around the axis passing through the nucleus.

The outer shell is the first one and the order increases towards the nucleus axis. A sequence of smaller inner orbits exists in the lower levels below the unity diameter orbit in each shell. These orbits are at levels decreasing by 1/4 atomic unit length until the first shell. Thus, a series of concentric orbits are formed at each level, one for each inner shell.

The frequencies of Hydrogen spectra were simulated by the model. The wave lengths of hydrogen atom spectra are related to the change in the area of orbit 2s, the orbit exist in the first level and the second shell, when the electron moves to

or from an inner shell. A constant, $K = 0.238725$ femto-sec has been found to satisfy that relation.

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Appendix A: Table (A-1) Orbits Levels and Diameters (a.u.l.)

Orbit level	n=1	n=2	n=3	n=4	n=5	n=6	n=7	Type
0.25	1	1/2	1/3	1/4	1/5	1/6	1/7	s orbits
0.50		$\sqrt{2}/2$	$\sqrt{2}/3$	$\sqrt{2}/4$	$\sqrt{2}/5$	$\sqrt{2}/6$	$\sqrt{2}/7$	p1 orbits
0.75		$\sqrt{3}/2$	$\sqrt{3}/3$	$\sqrt{3}/4$	$\sqrt{3}/5$	$\sqrt{3}/6$	$\sqrt{3}/7$	p2 orbits
1.00		1	2/3	2/4	2/5	2/6	2/7	p3 orbits
1.25			$\sqrt{5}/3$	$\sqrt{5}/4$	$\sqrt{5}/5$	$\sqrt{5}/6$	$\sqrt{5}/7$	d1 orbits
1.50			$\sqrt{6}/3$	$\sqrt{6}/4$	$\sqrt{6}/5$	$\sqrt{6}/6$	$\sqrt{6}/7$	d2 orbits
1.75			$\sqrt{7}/3$	$\sqrt{7}/4$	$\sqrt{7}/5$	$\sqrt{7}/6$	$\sqrt{7}/7$	d3 orbits
2.00			$\sqrt{8}/3$	$\sqrt{8}/4$	$\sqrt{8}/5$	$\sqrt{8}/6$	$\sqrt{8}/7$	d4 orbits
2.25			1	3/4	3/5	3/6	3/7	d5 orbits
2.50				$\sqrt{10}/4$	$\sqrt{10}/5$	$\sqrt{10}/6$	$\sqrt{10}/7$	f1 orbits
2.75				$\sqrt{11}/4$	$\sqrt{11}/5$	$\sqrt{11}/6$	$\sqrt{11}/7$	f2 orbits
3.00				$\sqrt{12}/4$	$\sqrt{12}/5$	$\sqrt{12}/6$	$\sqrt{12}/7$	f3 orbits
3.25				$\sqrt{13}/4$	$\sqrt{13}/5$	$\sqrt{13}/6$	$\sqrt{13}/7$	f4 orbits
3.50				$\sqrt{14}/4$	$\sqrt{14}/5$	$\sqrt{14}/6$	$\sqrt{14}/7$	f5 orbits
3.75				$\sqrt{15}/4$	$\sqrt{15}/5$	$\sqrt{15}/6$	$\sqrt{15}/7$	f6 orbits
4.00				1	4/5	4/6	4/7	f7 orbits
4.25					$\sqrt{17}/5$	$\sqrt{17}/6$	$\sqrt{17}/7$	g1 orbits
4.50					$\sqrt{18}/5$	$\sqrt{18}/6$	$\sqrt{18}/7$	g2 orbits
4.75					$\sqrt{19}/5$	$\sqrt{19}/6$	$\sqrt{19}/7$	g3 orbits
5.00					$\sqrt{20}/5$	$\sqrt{20}/6$	$\sqrt{20}/7$	g4 orbits
5.25					$\sqrt{21}/5$	$\sqrt{21}/6$	$\sqrt{21}/7$	g5 orbits

5.50					$\sqrt{22/5}$	$\sqrt{22/6}$	$\sqrt{22/7}$	g6 orbits
5.75					$\sqrt{23/5}$	$\sqrt{23/6}$	$\sqrt{23/7}$	g7 orbits
6.00					$\sqrt{24/5}$	$\sqrt{24/6}$	$\sqrt{24/7}$	g8 orbits
6.25					1	5/6	5/7	g9 orbits

Appendix B: Table (B -1) Distribution of Electrons of *s*-elements, *p*₁-elements, *p*₂-elements and *p*₃-elements

Orbit & level	<i>n</i> =1	<i>n</i> =2	<i>n</i> =3	<i>n</i> =4	<i>n</i> =5	<i>n</i> =6	<i>n</i> =7
S 0.25	1 H	3 Li	11 Na	19 K	37 Rb	55 Cs	87 Fr
	1s ¹	2s ¹	[Ne]3s ¹	[Ar] 4s ¹	[Kr] 5s ¹	[Xe] 6s ¹	[Rn] 7s ¹
	2 He	4 Be	12 Mg	20 Ca	38 Sr	56 Ba	88 Ra
	1s ²	[He]2s ²	[Ne]3s ²	[Ar] 4s ²	[Kr] 5s ²	[Xe] 6s ²	[Rn] 7s ²
p ₁ 0.50		5 B	13 Al	31 Ga	49 In	81 Tl	<u>113</u>
		[He]2s ² 2p ₁ ¹	[Ne] 3s ² 3p ₁ ¹	[Ar] 4s ² 3d ¹⁰ 4p ₁ ¹	[Kr] 5s ² 4d ¹⁰ 5p ₁ ¹	[Xe] 6s ² 5d ¹⁰ 6p ₁ ¹	7p ₁ ¹
		8 O	16 S	34 Se	52 Te	84 Po	<u>116</u>
	[He] ----2p ₁ ²	[Ne] ----3p ₁ ²	[Ar] ----4 p ₁ ²	[Kr] ----5 p ₁ ²	[Xe] ----6 p ₁ ²	7p ₁ ²	
p ₂ 0.75		6 C	14 Si	32 Ge	50 Sn	82 Pb	<u>114</u>
		[He]2s ² 2p ₁ ¹ 2p ₂ ¹	[Ne]3s ² 3p ₁ ¹ 3p ₂ ¹	[Ar]4s ² 3d ¹⁰ 4p ₁ ¹ 4p ₂ ¹	[Kr]5s ² 4d ¹⁰ 5p ₁ ¹ 5p ₂ ¹	[Xe]6s ² 5d ¹⁰ 6p ₁ ¹ 6p ₂ ¹	7p ₂ ¹
		9 F	17 Cl	35 Br	53 I	85 At	<u>117</u>
	[He] ----2p ₂ ²	[Ne] ----3 p ₂ ²	[Ar] ----4 p ₂ ²	[Kr] ----5 p ₂ ²	[Xe] ----6 p ₂ ²	7p ₂ ²	
p ₃ 1.00		7 N	15 P	33 As	51 Sb	83 Bi	<u>115</u>
		[He] ----2p ₃ ¹	[Ne] ----3p ₃ ¹	[Ar] ----4p ₃ ¹	[Kr] ----5p ₃ ¹	[Xe] ----6p ₃ ¹	7p ₃ ¹
		10 Ne	18 Ar	36 Kr	54 Xe	86 Rn	<u>118</u>
	1s ² 2s ² 2p ⁶	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹⁰ 4p ⁶	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹⁰ 4p ⁶ 5s ² 4d ¹⁰ 5p ⁶	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹⁰ 4p ⁶ 5s ² 4d ¹⁰ 5p ⁶ 6s ² 4d ¹⁰ 4d ¹⁴ 6p ⁶	7p ₃ ²	