Bulletin of the Chemists and Technologists of Macedonia, Vol. **25**, No. 1, pp. 61–63 (2006)
GHTMDD – 485
ISSN 0350 – 0136
Received: December 12, 2005
UDC: 546.11
Accepted: May 16, 2006

Education

THE FIRST EXCITED STATE OF THE HYDROGEN ATOM AND THE GOLDEN RATIO: A LINK OR A MERE COINCIDENCE?

Vladimir M. Petruševski

Institute of Chemistry, Faculty of Natural Sciences and Mathematics, Ss Cyril and Methodius University, Arhimedova 5, MK-1001 Skopje, Republic of Macedonia
vladop@iunona.pmf.ukim.edu.mk

The hydrogen atom is one of the systems for which (ignoring the electron spin) the Schrödinger equation can be solved exactly. The solutions of the radial part of the equation are usually given in terms of functions related to the associated Laguerre polynomials. Unexpectedly, the extremes (two maxima shared by a minimum) of the radial distribution function are related to the golden ratio (φ). It is quite possible that this finding is a mere coincidence, rather than a consequence of the 'eternal harmony of Nature' or 'the divine principle of beauty' etc., but still it is interesting to point to the existence of the above link.

Key words: science education; philosophy; hydrogen; quantum mechanics; golden mean

ПРВАТА ВОЗБУДЕНА СОСТОЈБА НА АТОМОТ НА ВОДОРОД И ЗЛАТНИОТ ПРЕСЕК: ЗАЕМНА ВРСКА ИЛИ ЧИСТА КОИНЦИДЕНЦИЈА?

Атомот на водород е еден од системите за кои (не земајќи го предвид спинот на електронот) е можно егзактно решавање на Шредингеровата равенка. Решенијата на радијалната бранова функција обично се прикажуваат преку функции што се во врска со придружените Laguerre-ови полиноми. Доста неочекувано, екстремите на кривата на радијална распределба се поврзани со златниот пресек (φ). Сосема е возможно дека овој наод е резултат на чиста коинциденција, а не, на пример, последица на „вечната хармонија на природата“ или „божествениот принцип на убавината“ итн. И покрај тоа, интересно е да се укаже на ваквата (макар и само случајна) врска.

Клучни зборови: образование; филозофија; водород; квантна механика; златен пресек

INTRODUCTION

Hydrogen, being the first element of the periodic table, has always attracted attention of both students and instructors by many of its unique properties. Let us mention few of them:

- it is the most abundant element in the universe;
- its atom is the simplest one, having a single electron in the shell;
- the molecular hydrogen is built of the simplest possible (neutral) molecules;
- the nucleus of the most common isotope (^1H) is, once again, the simplest one (it is the only stable nucleus containing no neutrons);
- compounds containing the heavier isotope ^2H (or D, deuterium) have different physical properties from those containing ^1H (although this is generally true for all isotopically labeled compounds, the differences for hydrogen isotopes are by far the most pronounced);
- it is the only element whose atomic spectra can be easily and precisely interpreted in terms of a simple algebraic equation;

- its atom (or, for that matter, any one-electron ion) is one of only a few systems for which the Schrödinger equation is exactly solvable;
- in gaseous state, it is the lightest of all gases;
- in gaseous state it has the highest rate for diffusion (and also for effusion);
- . . . .

All that has been mentioned above is well known and might be found in standard textbooks of general and inorganic chemistry [1, 2].

On the other hand, the problem of the golden ratio is known in mathematics for almost 3 millennia. The problem may be formulated in the following way: let us divide a segment into two parts, each having a length of x and 1, respectively (it is a common practice in mathematics that length, surface, volume etc. are dimensionless quantities). If the ratio of the larger and smaller part ($x : 1$) is the same as that of the segment and the larger part, i.e. if:

$$x : 1 = (1 + x) : x \tag{1}$$

then this ratio ($x : 1$, or simply x) is called *the golden ratio* or *golden mean* (also *divine proportion*) and is usually designated φ. The value of φ comes out as the positive root of the equation $x^2 - x - 1 = 0$ obtained by rearranging eq. 1, and equals

$$\varphi = \frac{1+\sqrt{5}}{2}. \tag{2}$$

The value of the other root is $-\varphi^{-1}$ (being negative it has no obvious geometrical meaning). Sometimes, due to a different convention adopted, it is $1/\varphi$ that is called the golden ratio. It is easy to prove that

$$\varphi^{-1} = \frac{-1+\sqrt{5}}{2}. \tag{2a}$$

The problem of the golden ratio is closely related to many other mathematical problems: the solutions of the equation $x^5 - 1 = 0$; the problem of existence of 5-fold symmetry axes/points; the Fibonacci numbers (defined recursively as $a_{n+1} = a_n + a_{n-1}$) etc. [3]. One finds it in Penrose (2D) and icosahedral (3D) quasicrystals [4, 5]. Many examples could be given where the number φ appears in nature: growth of shells (e.g. *Nautilus Pompilius*), various flowers, insects, and life forms in general [6]. It is often considered to be a criterion for 'beauty'. Indeed, when asked to pick a rectangle (from a set of many different rectangles) that they find to be aesthetically the most accomplished one, many people indeed choose the rectangle where the side lengths are such that $a/b \approx \varphi$. Mystical and deeply religious people are often inclined to believe that φ is definitely God's favorite number, a pure reflection of a harmony that may only have divine origin, offering lots of proofs (or 'proofs') for the above 'fingerprint of God' [7].

What possibly can the hydrogen atom and the golden ratio have in common? The answer will be offered in some detail, to complement the very brief letter just published [8].

Possible link: the First Excited State of the H-atom

As mentioned in the beginning, the Schrödinger equation for an electron in the Coulomb field of the nucleus (the electron been treated as spinless particle) is exactly analytically solvable [9]. The solutions (wave-functions), like in other cases where the potential is spherically symmetrical, can be factorized [10], i.e. the total wave-function may be presented as a product of two other functions:

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\cdot Y_{lm}(\theta, \phi) \tag{3}$$

where r, θ, ϕ are spherical coordinates, n, l, m are quantum numbers (for simplicity m has been written instead of m_l), ψ is the total wave-function, R is the radial part, and Y is the angular part of the wave-function. The solutions for the radial part are products of a decaying exponential function and a polynomial (the latter is closely related to the *associated Laguerre polynomials*), while the solutions of the angular part are known as spherical harmonics or spherical functions [10]. The square of the module of any wave-function (that is $|\psi_{nlm}(r, \theta, \phi)|^2$ which is always real and non-negative) is said to represent the *probability density* of the electron, at that particular point.

Since they are related to the probability of finding the electron, all these functions are normalized to 1, i.e.:

$$\int_0^{\infty} R_{nl}^2(r)\, r^2\, dr = 1 \tag{4}$$

$$\int_0^{2\pi}\int_0^{\pi} \left|Y_{lm}(\theta,\phi)\right|^2 \sin\theta \,\mathrm{d}\theta\,\mathrm{d}\phi = 1 \tag{5}$$

The function $R^2_{nl}(r)r^2$ appearing under the integral sign in eq. 4 is often called *radial distribution function*. Its square gives the probability density of the electron at a distance r from the nucleus.

Let us now consider the function $R_{20}(r)$ that corresponds to the first excited state of the hydrogen atom (actually, it is the radial part of the 2s orbital) defined as:

$$R_{20}(r) = \frac{1}{a_0^{3/2}}(1-\frac{r}{2a_0})\exp(-r/2a_0) \qquad (6)$$

Its radial distribution function is therefore $r^2R_{20}{}^2$ (sometimes designated as P_{20}, cf. Fig. 1):

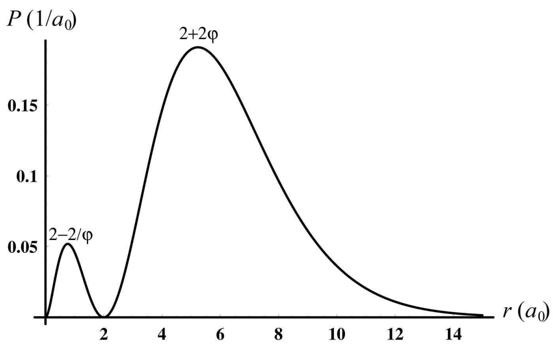

Fig. 1. The radial distribution function (P_{20}) for the first excited state of the hydrogen atom.

Now, it is easy to prove, either by using some elementary calculus to solve the equation

$$\frac{d}{dr}[R_{20}^2(r)r^2] = 0 \qquad (7)$$

or alternatively, using computer programs, that this radial distribution function has two minima (at r_1 = 0 and $r_2 = 2\ a_0$; a_0 is, of course, the Bohr radius of the hydrogen atom in its ground state), meaning that at these distances the probability of finding the electron is 0. There are also two maxima, that may conveniently be presented as $r_3 = 2(1 - 1/\varphi)\ a_0$ and $r_4 = 2(1 + \varphi)\ a_0$. Alternatively, one could say that an observer placed at the point $r = 2\ a_0$ where the radial distribution function is zero (or, in terms of the total wave-function, an observer sitting at any point of the nodal spherical shell where the probability of finding the electron is zero), sees maxima in the radial distribution function that are $-2/\varphi$ and 2φ (in the standard units of a_0) apart of him!

Thus, the criterion for beauty (i.e. φ or its inverse) quite unexpectedly appears in the problem regarding the electron density distribution in the simplest atom (and in the same time the atom of the most abundant element) of the Universe. Is this a mere coincidence or a part of a sophisticated (but unrevealed) plan? Having absolutely no indication that this is either 'a part of a Divine plan' or that it comes as a deep consequence of some principle, one is – the author believes – left only with the first (albeit much less spectacular) choice: it is a coincidence. Still, the result is an attractive one and deserves to be mentioned and added to the numerous problems in which the golden ratio suddenly appears. Perhaps a critical reexamination of all problems including the golden ratio might also show that few other links were, in fact, just 'links'.

CONCLUSION

The golden ratio unexpectedly appears in one more problem, this time in the microscopic world. The author (being truly agnostic) feels he has to say that this finding is most probably a mere coincidence. Still, he finds it interesting to be pointed out as a kind of curiosity. For some readers it could possibly be a thought-provoking stimulation.

REFERENCES

[1] J. D. Lee, *Concise Inorganic Chemistry* (4th edition), Chapman & Hall, London, 1991, pp. 240–271.

[2] J. E. Brady, *General Chemistry* (5th edition), John Wiley & Sons, New York, 1990, pp. 791–800.

[3] H. Walser, *The Golden Section*, The Mathematical Association of America (translation from German), 2001, pp. 1–142.

[4] V. M. Petruševski, S. M. Kalajdževski, M. Ž. Najdoski, Quasicrystals: Comparison with Crystals, Construction of 2D Lattices and Demonstrations Using a Laser Pointer, *Chem. Educator,* **8**, 358–363 (2003).

[5] M. V. Jarić, S. Lundqvist (eds), *Quasicrystals*, World Scientific, Singapoore, 1990.

[6] http://www.summum.us/philosophy/phi.shtml (accessed November 23rd, 2005.

[7] http://goldennumber.net/ (accessed November 23rd, 2005).

[8] V. M. Petruševski, The H-atom and the golden ratio: A possible link?, *J. Chem. Educ.* (in press).

[9] P. W. Atkins, *Physical Chemistry* (5th edition), Oxford University Press, Oxford, 1994, pp. 421–460.

[10] P. W. Atkins, P. W. *Molecular Quantum Mechanics* (2nd edition), Oxford University Press, Oxford, 1986, pp. 58–80.