

# The Radial Electron Density in the Hydrogen Atom and the Model of Oscillations in a Chain System

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The radial electron distribution in the Hydrogen atom was analyzed for the ground state and low-lying excited states by means of a fractal scaling model originally published by Müller in this journal. It is shown that Müller's standard model is not fully adequate to fit these data and an additional phase shift must be introduced into its mathematical apparatus. With this extension, the radial expectation values could be expressed on the logarithmic number line by very short continued fractions where all numerators are Euler's number. Within the rounding accuracy, no numerical differences between the expectation values (calculated from the wavefunctions) and the corresponding modeled values exist, so the model matches these quantum mechanical data exactly. Besides that, Müller's concept of proton resonance states can be transferred to electron resonances and the radial expectation values can be interpreted as both, proton resonance lengths and electron resonance lengths. The analyzed data point to the fact that Müller's model of oscillations in a chain system is compatible with quantum mechanics.

## 1 Introduction

The radial electron probability density in the Hydrogen atom was analyzed by a new fractal scaling model, originally published by Müller [1–3] in this journal. This model is basing on four principal facts:

1. The proton is interpreted as an oscillator.
2. Most matter in the universe is provided by protons, therefore the proton is *the dominant oscillation state* in all the universe.
3. Space is not considered as completely empty, consequently all proton oscillators are somehow coupled to each other. A quite simple form to consider such a coupling is the formation of a chain of proton harmonic oscillators.
4. Provided that items 1–3 are correct, every process or state in the universe which is abundantly realized or allowed to exist over very long time scales, is consequently coupled to the proton oscillations, and should retain some properties that can be explained from the mathematical structure of a chain of proton harmonic oscillators.

Müller has shown that a chain of similar harmonic oscillators generates a spectrum of eigenfrequencies, that can be expressed by a continued fraction equation [2]

$$f = f_p \exp S, \quad (1)$$

where  $f$  is any natural oscillation frequency of the chain system,  $f_p$  the oscillation frequency of one proton and  $S$  the continued fraction corresponding to  $f$ .  $S$  was suggested to be in the canonical form with all partial numerators equal 1 and the

partial denominators are positive or negative integer values:

$$S = n_0 + \frac{1}{n_1 + \frac{1}{n_2 + \frac{1}{n_3 + \dots}}}. \quad (2)$$

Besides the canonical form, Müller proposed fractions with all numerators equal 2 and all denominators are divisible by 3. Such fractions divide the logarithmic scale in allowed values and empty gaps, i.e. ranges of numbers which cannot be expressed with this type of continued fractions.

In three previous articles [4–6] it was shown that the model works quite well when all the numerators were substituted by Euler's number, so that

$$S = n_0 + \frac{e}{n_1 + \frac{e}{n_2 + \frac{e}{n_3 + \dots}}}. \quad (3)$$

In this work, the attention has been focused to the spatial electron distribution in the Hydrogen atom, considering the ground state ( $n = 1$ ) and the first low-lying excited electronic states ( $n = 2-6$ ).

In the Hydrogen atom, the distance between the electron and the proton is always very small and quantum mechanics allows to calculate the exact spatial electron density distribution. If the proton is somehow oscillating and Müller's model applies, one can expect a characteristic signature in the set of radial expectation values.

Actually these values compose an extremely interesting data set to analyze, since the expectation values can be calculated by quantum mechanics from exact analytical wave-

functions and do not have any measurement error (errors in physical constants such as  $a_0$  and  $\hbar$  can be neglected).

Therefore, it can be requested that Müller's model must reproduce these expectation values *exactly*, which is indeed possible, but only when introducing a further modification to the model.

## 2 Data sources and computational details

When considering polar coordinates, the solutions of the non-relativistic Schrödinger equation  $\hat{H}\Psi = E\Psi$  for a spherical potential can be written in the form

$$\Psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi),$$

where  $R(r)$  is the so-called radial part of the wavefunction  $\Psi$ , and the functions  $\Theta(\theta)$  and  $\Phi(\phi)$  are the angular parts.

For every orbital or wavefunction, the probability to find the electron on a shell with inner radius  $r$  and outer radius  $r + dr$  is proportional to  $r^2 R^2 dr$  (note that the functions as given in Table 1 are not normalized). Following the formalism of quantum mechanics, the average or expectation value  $\langle r \rangle$  was calculated by numerical integration

$$\langle r \rangle = N \int_0^{\infty} r^3 R^2 dr, \quad (4)$$

where  $N$  is the normalization constant so that holds:

$$N \int_0^{\infty} r^2 R^2 dr = 1.$$

Table 1 displays the radial part  $R(Z, r)$  for the orbitals 1s to 6h of hydrogen-like atoms together with the corresponding radial expectation values (for  $Z = 1$ , wavefunctions taken from reference [7]). The expectation values are given in Å and were rounded to three significant digits after decimal point.

In a second step, these numerical values were expressed on the logarithmic number line by continued fractions. Numerical values of continued fractions were always calculated using the the Lenz algorithm as indicated in reference [8].

## 3 Results and discussion

### 3.1 The standard model is insufficient

In order to interpret the expectation values  $\langle r \rangle$  as proton resonance lengths, following strictly the formalism of previous articles, it must be written:

$$\ln \frac{\langle r \rangle}{\lambda_C} = p + S, \quad (5)$$

where  $S$  is the continued fraction as given in equation 3,  $\lambda_C = \frac{h}{2\pi mc}$  is the reduced Compton wavelength of the proton with

the numerical value  $2.103089086 \times 10^{-16}$  m. In the following tables,  $p + S$  is abbreviated as  $[p; n_0 | n_1, n_2, n_3, \dots]$ . The free link  $n_0$  and the partial denominators  $n_i$  are integers divisible by 3. For convergence reason, one has to include  $|e+1|$  as allowed partial denominator. This means the free link  $n_0$  is allowed to be  $0, \pm 3, \pm 6, \pm 9 \dots$  and all partial denominators  $n_i$  can take the values  $e+1, -e-1, \pm 6, \pm 9, \pm 12 \dots$

For consistency with previous publications, the following conventions hold: a data point is considered as an outlier (i.e. does not fit into Müller's model), when its continued fraction representation produces a numerical error higher than 1%. The numerical error is always understood as the absolute value of the difference between  $\langle r \rangle$  from quantum mechanics (given in Table 1), and the value obtained from the evaluation of the corresponding continued fraction.

It was found that the complete set of radial expectation values can be interpreted as proton resonance lengths without any outliers according to equation 5 (results not shown). However, small numerical errors were still present. Having in mind that this is a data set without measurement errors, this result is not satisfying.

From the obvious fact that the wavefunction is an electron property, it arouse the idea to interpret the data set as electron resonance lengths. Then, a fully analogous equation can be set up:

$$\ln \frac{\langle r \rangle}{\lambda_{C_{electron}}} = p + S, \quad (6)$$

where  $\lambda_{C_{electron}}$  is the reduced Compton wavelength of the electron with the numerical value  $3.861592680 \times 10^{-13}$  m.

Again the expectation values could be interpreted as electron resonance lengths according to equation 6 without the presence of outliers, but some numerical errors remained (results not shown).

Since the aforementioned equations do not reproduce the dataset exactly as proton or electron resonance lengths, possible changes of the numerator were investigated.

Müller had already proposed continued fractions with all numerators equal 2 in one of his publications [9]. As a first numerical trial, the number of outliers was determined when modeling the data set with numerators from 2.0 to 3.0 (step-size 0.05). Figure 1 displays the results for both, proton and electron resonances. It turned out that number 2 must be excluded from the list of possible numerators, as outliers are present. Moreover, the results suggest that the whole range from 2.55 to 2.85 can be used as numerator in equations 5 and 6 without producing outliers, thus, another criterium must be applied to determine the correct numerator.

Considering only the range of numerators which did not produce outliers, the sum of squared residuals (or squared numerical errors) was calculated. It strongly depends on the numerator (see Figure 2). Again the results are not satisfying. As can be seen, considering electron resonances, the "best numerator" is 2.70, while for proton resonances it is 2.78, de-

Table 1: Radial wavefunctions  $R(Z, r)$  of different orbitals for hydrogen-like atoms together with the corresponding radial expectation values according to equation 4 ( $Z = 1$  assumed).  $\rho = \frac{Zr}{na_0}$ ,  $n$  = main quantum number,  $a_0$  = Bohr radius,  $Z$  = atomic number.

Radial wavefunction $R(Z, r)$	$\langle r \rangle$ [Å]
$R_{1s} = (Z/a_0)^{\frac{3}{2}} 2e^{-\frac{\rho}{2}}$	0.794
$R_{2s} = \frac{(Z/a_0)^{\frac{3}{2}}}{2\sqrt{2}} (2 - \rho)e^{-\frac{\rho}{2}}$	3.175
$R_{2p} = \frac{(Z/a_0)^{\frac{3}{2}}}{2\sqrt{6}} \rho e^{-\frac{\rho}{2}}$	2.646
$R_{3s} = \frac{(Z/a_0)^{\frac{3}{2}}}{9\sqrt{3}} (6 - 6\rho + \rho^2) e^{-\frac{\rho}{2}}$	7.144
$R_{3p} = \frac{(Z/a_0)^{\frac{3}{2}}}{9\sqrt{6}} (4 - \rho) \rho e^{-\frac{\rho}{2}}$	6.615
$R_{3d} = \frac{(Z/a_0)^{\frac{3}{2}}}{9\sqrt{30}} \rho^2 e^{-\frac{\rho}{2}}$	5.556
$R_{4s} = \frac{(Z/a_0)^{\frac{3}{2}}}{96} (24 - 36\rho + 12\rho^2 - \rho^3) e^{-\frac{\rho}{2}}$	12.700
$R_{4p} = \frac{(Z/a_0)^{\frac{3}{2}}}{32\sqrt{15}} (20 - 10\rho + \rho^2) \rho e^{-\frac{\rho}{2}}$	12.171
$R_{4d} = \frac{(Z/a_0)^{\frac{3}{2}}}{96\sqrt{5}} (6 - \rho) \rho^2 e^{-\frac{\rho}{2}}$	11.113
$R_{4f} = \frac{(Z/a_0)^{\frac{3}{2}}}{96\sqrt{35}} \rho^3 e^{-\frac{\rho}{2}}$	9.525
$R_{5s} = \frac{(Z/a_0)^{\frac{3}{2}}}{300\sqrt{5}} (120 - 240\rho + 120\rho^2 + 20\rho^3 + \rho^4) e^{-\frac{\rho}{2}}$	19.844
$R_{5p} = \frac{(Z/a_0)^{\frac{3}{2}}}{150\sqrt{30}} (120 - 90\rho + 18\rho^2 - \rho^3) \rho e^{-\frac{\rho}{2}}$	19.315
$R_{5d} = \frac{(Z/a_0)^{\frac{3}{2}}}{150\sqrt{70}} (42 - 14\rho + \rho^2) \rho^2 e^{-\frac{\rho}{2}}$	18.257
$R_{5f} = \frac{(Z/a_0)^{\frac{3}{2}}}{300\sqrt{70}} (8 - \rho) \rho^3 e^{-\frac{\rho}{2}}$	16.669
$R_{5g} = \frac{(Z/a_0)^{\frac{3}{2}}}{900\sqrt{70}} \rho^4 e^{-\frac{\rho}{2}}$	14.552
$R_{6s} = \frac{(Z/a_0)^{\frac{3}{2}}}{2160\sqrt{6}} (720 - 1800\rho + 1200\rho^2 + 300\rho^3 + 30\rho^4 - \rho^5) e^{-\frac{\rho}{2}}$	28.576
$R_{6p} = \frac{(Z/a_0)^{\frac{3}{2}}}{432\sqrt{210}} (840 - 840\rho + 252\rho^2 - 28\rho^3 + \rho^4) \rho e^{-\frac{\rho}{2}}$	28.046
$R_{6d} = \frac{(Z/a_0)^{\frac{3}{2}}}{864\sqrt{105}} (336 - 168\rho + 24\rho^2 - \rho^3) \rho^2 e^{-\frac{\rho}{2}}$	26.988
$R_{6f} = \frac{(Z/a_0)^{\frac{3}{2}}}{2592\sqrt{35}} (72 - 18\rho + \rho^2) \rho^3 e^{-\frac{\rho}{2}}$	25.401
$R_{6g} = \frac{(Z/a_0)^{\frac{3}{2}}}{12960\sqrt{7}} (10 - \rho) \rho^4 e^{-\frac{\rho}{2}}$	23.284
$R_{6h} = \frac{(Z/a_0)^{\frac{3}{2}}}{12960\sqrt{77}} \rho^5 e^{-\frac{\rho}{2}}$	20.638

spite presenting a local minimum at 2.70 too. However, numerators different from  $e$  are inconsistent with previous publications. The fact that these “best numerators” are numerically very close to Euler’s number, suggests that the choice of  $e$  as numerator is probably correct and something else in the model must be changed for this particular dataset.

For any common experimental data set, the here found numerical inconsistencies could be explained with measurement errors. One could even think that Müller’s model is just too simple to reproduce nature’s full reality; then the numerical deviations could also be explained by the insufficiency of the model itself. Fortunately the high accuracy of the expect-

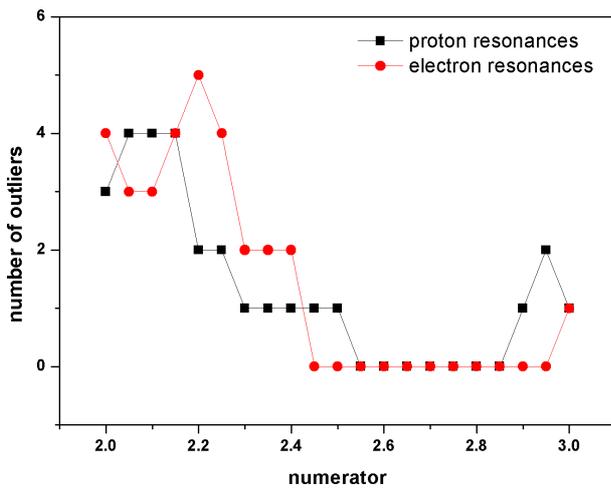


Fig. 1: Determination of the correct numerator for the dataset of expectation values (equations 5 and 6): the number of outliers as a function of the tested numerator.

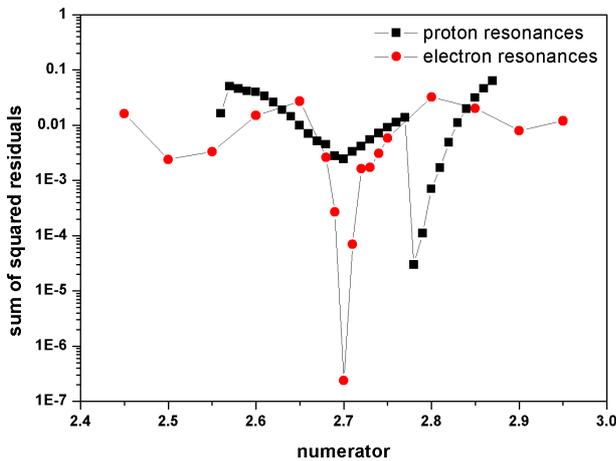


Fig. 2: Determination of the correct numerator for the dataset of expectation values (equations 5 and 6): the sum of squared residuals as a function of the tested numerator.

tation values creates the opportunity to test Müller's model very critically and to extend it.

### 3.2 Extending Müller's model

It is now shown that the following extension provides a solution, so that (i) Euler's number can be persist as numerator, and (ii) the whole dataset can be expressed by short continued fractions without any numerical errors, which means, this extended model reproduces the dataset *exactly*.

An additional phase shift  $\delta$  was introduced in equations 5 and 6. For proton resonances, it can then be written:

$$\ln \frac{\langle r \rangle}{\lambda_C} = \delta + p + S. \quad (7)$$

And analogously for electron resonances:

$$\ln \frac{\langle r \rangle}{\lambda_{C_{electron}}} = \delta + p + S. \quad (8)$$

As shown in previous articles, the phase shift  $p$  varies among the dataset, so that some data points take  $p=0$  and others  $p=3/2$ . Contrary to this, the phase shift  $\delta$  must be equal for all data points in the set. This means the fractal spectrum of resonances is shifted on the logarithmic number line and the principal nodes are not more at  $0, \pm 3, \pm 6, \pm 9 \dots$ , but now at  $0 + \delta, \pm 3 + \delta, \pm 6 + \delta, \pm 9 + \delta \dots$ .

The underlying physical idea is that  $\delta$  should be a small positive or negative number, characterizing a small deviation from Müller's standard model. To guarantee that the model does not become ambiguous, values of  $|\delta|$  must always be smaller than  $3/2$ .

For the here considered data set, the phase shift  $\delta$  could be determined as a *very small number*, with the consequence that all numerical errors vanished (were smaller than  $0.001 \text{ \AA}$ ). The numerical values were  $\delta = 0.017640$  when interpreting the data as proton resonances and  $\delta = 0.002212$  in case of electron resonances. Tables 2 and 3 show the continued fraction representations when interpreting the expectation values as proton and electron resonances, respectively.

### 3.3 Interpretation

As can be seen, when accepting a *small* phase shift  $\delta$ , the radial expectation values can be perfectly interpreted as both, proton and electron resonances. Besides that, the continued fraction representations are equal for proton and electron resonances, only the free link and the phase shift  $p$  differ. This is unavoidable due to the fact that different reference Compton wavelengths were used; so the logarithmic number line was calibrated differently.

The free link and the phase shift  $p$  are parameters which basically position the data point on the logarithmic number line, indicating the principal node. Then the first partial denominator determines whether the data point is located before or after this principal node. So the data point can be either in a compression or expansion zone, thus, now a specific property of its oscillation state is indicated. The equality of the set of partial denominators in the continued fraction representations is a necessary requirement for interpreting the expectation values as both, proton and electron resonances. Both oscillators must transmit at least qualitatively the same "oscillation property information" to the wavefunction.

However, when accepting the phase shift idea, it is always mathematically possible to interpret *any* set of proton resonances as a set of phase-shifted electron resonances. So what are the physical arguments for associating the expectation values to both oscillators?

- In an atom, electrons and the nucleus share a very small volume of space. The electron wavefunction is most

Table 2: Continued fraction representation of the radial expectation values of Hydrogen orbitals according to equation 7, considering proton resonances ( $\delta = 0.017640$ ).

Orbital	Continued fraction representation of $\langle r \rangle$
<b>1s</b>	[0; 12   e+1, -6, -6] [1.5; 12   -e-1, -9]
<b>2s</b>	[0; 15   -e-1, 9, e+1] [1.5; 12   e+1, 24, 6]
<b>2p</b>	[0; 15   -e-1, e+1, -e-1, 12, e+1] [1.5; 12   6, -e-1, 6, -e-1]
<b>3s</b>	[0; 15   132, -e-1]
<b>3p</b>	[0; 15   -48, -6]
<b>3d</b>	[0; 15   -12, 12, e+1]
<b>4s</b>	[0; 15   e+1, e+1, -6, 6] [1.5; 15   -e-1, e+1, 27, -e-1]
<b>4p</b>	[1.5; 15   -e-1, e+1, -6, e+1, e+1, e+1]
<b>4d</b>	[0; 15   6, -21, -e-1, e+1]
<b>4f</b>	[0; 15   9, -15, 9]
<b>5s</b>	[1.5; 15   -6, 45]
<b>5p</b>	[1.5; 15   -6, 6, e+1, -e-1, 6]
<b>5d</b>	[0; 15   e+1, -e-1, e+1, 6, -e-1, -12] [1.5; 15   -6, e+1, -e-1, e+1, -9]
<b>5f</b>	[0; 15   e+1, -e-1, -e-1, e+1, -33] [1.5; 15   -e-1, -e-1, -e-1, e+1, -6]
<b>5g</b>	[0; 15   e+1, -471] [1.5; 15   -e-1, 15, 9, e+1]
<b>6s</b>	[1.5; 15   -30, e+1, -18]
<b>6p</b>	[1.5; 15   -24, -9, e+1, -e-1]
<b>6d</b>	[1.5; 15   -18, -27]
<b>6f</b>	[1.5; 15   -12, -e-1, e+1, 12]
<b>6g</b>	[1.5; 15   -9, -21]
<b>6h</b>	[1.5; 15   -6, -6, 6, -e-1, 6]

Table 3: Continued fraction representation of the radial expectation values of Hydrogen orbitals according to equation 8, considering electron resonances ( $\delta = 0.002212$ ).

Orbital	Continued fraction representation of $\langle r \rangle$
<b>1s</b>	[0; 6   -e-1, -9] [1.5; 3   e+1, -6, -6]
<b>2s</b>	[0; 6   e+1, 24, 6] [1.5; 6   -e-1, 9, e+1]
<b>2p</b>	[0; 6   6, -e-1, 6, -e-1] [1.5; 6   -e-1, e+1, -e-1, 12, e+1]
<b>3s</b>	[1.5; 6   132, -e-1]
<b>3p</b>	[1.5; 6   -48, -6]
<b>3d</b>	[1.5; 6   -12, 12, e+1]
<b>4s</b>	[0; 9   -e-1, e+1, 27, -e-1] [1.5; 6   e+1, e+1, -6, 6]
<b>4p</b>	[0; 9   -e-1, e+1, -6, e+1, e+1, e+1]
<b>4d</b>	[1.5; 6   6, -21, -e-1, e+1]
<b>4f</b>	[1.5; 6   9, -15, 9]
<b>5s</b>	[0; 9   -6, 45]
<b>5p</b>	[0; 9   -6, 6, e+1, -e-1, 6]
<b>5d</b>	[0; 9   -6, e+1, -e-1, e+1, -9] [1.5; 6   e+1, -e-1, e+1, 6, -e-1, -12]
<b>5f</b>	[0; 9   -e-1, -e-1, -e-1, e+1, -6] [1.5; 6   e+1, -e-1, -e-1, e+1, -33]
<b>5g</b>	[0; 9   -e-1, 15, 9, e+1] [1.5; 6   e+1, -471]
<b>6s</b>	[0; 9   -30, e+1, -18]
<b>6p</b>	[0; 9   -24, -9, e+1, -e-1]
<b>6d</b>	[0; 9   -18, -27]
<b>6f</b>	[0; 9   -12, -e-1, e+1, 12]
<b>6g</b>	[0; 9   -9, -21]
<b>6h</b>	[0; 9   -6, -6, 6, -e-1, 6]

basically an electron property, always existing in close proximity to the nucleus (protons). From this it would not be a surprise that both oscillators contribute to the properties of the wavefunction. In general, one can now speculate that particularly physical parameters related to an atomic wavefunction are hot candidates to be interpretable as electron resonances.

- The phase shift was not invented to justify electron resonances, it is also required for an exact reproduction of the data set through proton resonances.
- When considering Müller's standard model (equations 5 and 6), the sum of squared residuals is much lower when interpreting the data as electron resonances. In this case the "best numerator" is also closer to Euler's

number (see Fig. 2). Therefore, the wavefunction is principally governed by the electron oscillations. Certainly the proton oscillations influence the system too, they can be interpreted as a perturbation. The system tends to adjust to both oscillators and this seems to be the cause of the observed phase shifts. Hopefully, similar data will confirm this in near future.

#### 4 Conclusions

Müller's model must be extended in two ways. First, it must be recognized that electron resonances exist in the universe as proton resonances do, and the same mathematical formalism for a chain of proton oscillators can be applied to a chain of electron oscillators. Second, an additional phase shift  $\delta$  is

proposed to provide a reasonable mathematical extension of the model.

Of course, much more data must be analyzed and the future will show if this extended model can stand and give useful results when applying to other data sets. Particularly interesting for analyses would be quite accurate data from quantum mechanics.

Now one has to ask regarding previously published papers on this topic [4–6]: are there any results that must be re-considered? The answer is definitively yes. In reference [4], masses of elementary particles were analyzed and only for 86% of the particles a continued fraction expression could be found. There is high probability that this exceptional high number of outliers (14%, nowhere else found) can be reduced considering a phase shift  $\delta$ ; or different phase shifts  $\delta$  can put the elementary particles into different groups. In another paper [6], half-lives of excited electronic states of atoms were found to be proton resonance periods, however, a possible interpretation as electron resonance periods has not been attempted yet. Possibly a small phase shift could here also reduce the number of outliers. This everything is now subject of future research.

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