Title: Lost Resonances in NIST Tables

It could be that perhaps I've found out a little about the structure of atoms,

Neils Bohr 1912

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Abstract:

This paper attempts to revise the classical approach to the analysis of hydrogen atom spectroscopic data, with particular emphasis on the reference datasets published by NIST. Orbital energy values were transformed into fractional, unrounded form, enabling precise identification of resonances between spectral lines. A number of simple (e.g., 3:1) and complex (e.g., 5:3) resonances were identified, indicating the existence of a deep harmonic structure in the hydrogen emission spectrum; for example, the H(5→4) wave is exactly the third harmonic of the H(20→10) wave, confirmed both analytically and within the NIST uncertainty range. The concept of subquantization was also introduced, postulating the existence of a fundamental energy unit $\varepsilon_0 \approx 7.71 \times 10^{-5}$ eV, multiples of which describe all electronic transitions in the hydrogen atom. Based on this, a lattice of resonances with modulus around 18.64 GHz was constructed, in which all identified emission waves are integer multiples of one fundamental wavelength λ_0 at that frequency. Taking these dependencies into account can significantly improve data precision, with potential applications in cosmology, high-resolution spectroscopy, and atomic structure studies, and the work invites further collaboration and the development of analytical tools based on resonance calibration of spectral data.

1. Introduction

The goal of this paper is to demonstrate that NIST ignores obvious resonance relationships that directly follow from the empirical data. Including them would result in an increase in data precision by several orders of magnitude, which is particularly useful in cosmology and materials science.

After more than a century of study, the hydrogen atom still presents challenges and opportunities to theoretical as well as to experimental physicists. [1]

1.1. Assumptions:

1. The amplitude of the photon emission wave (e.g. at different electron jumps) is a constant value.
2. The packet emission starts at a node of the sinusoid (from zero) and continues to the next node so that the number of periods in the packet is always an integer.
3. The research will focus on hydrogen emission waves originating from electron hopping between integer "s" orbits.

1.2. Critical Assessment of the NIST Methodology

When considering whether energy transfer within an atom occurs in a piecemeal or chaotic manner, we intuitively conclude that order is more likely than chaos. Although there are many possible mechanisms for exchanging orbital energy for photon emission energy, the dominance of Bohr's concept remains undisputed. [2]

Rydberg's 1890 analysis, which determined the relationship between spectral lines, was derived directly from empirical data, without prior theoretical justification. [3] This form of notation enables the precise search for interrelationships, especially resonances, between spectral waves of different frequencies. Only later was a physical foundation for this model found. [4]

Constructive interference of wave packets requires maintaining phase coherence throughout the packet. This means that the number of oscillation cycles must be finite and integer. Only then can the packets add constructively, creating stable resonances. This condition ensures phase coherence and eliminates destructive interference at packet boundaries. Laser device designers encounter this phenomenon daily. [5]

NIST specialists, however, do not assume resonances between spectral lines, treating each measurement as independent of the others, and do not even admit the possibility of the existence of resonances. As Sansonetti and Martin made explicit in the peer-reviewed J. Phys. Chem. Ref. Data (2004): "Each spectral line is treated as an independent datum; no assumptions are made regarding harmonic or resonance relationships between transitions." .[6]

As Bernath noted, the purpose of spectroscopy is not only to record data, but primarily to interpret them; in this context, my analysis of NIST tables (obs – ritz, unc) and the use of the harmonic raster (sQ) represents an attempt to move from the application of this application from table values to the disclosure of structure and correlation in the data.[7]

Former Soviet physicist, former employee of NIST, author of numerous studies on spectral lines, Dr. Alexander Kramida (Personal communication, 29 August 2025), when assessing my concept, stated that:

" *Regarding your findings, I believe they are largely numerological. There is no physical basis for assuming that the frequency ratios you propose are accurate. Approximate relationships can be found in the old Balmer formula. This*

formula, incidentally, was also initially strictly numerological in nature, but a physical basis was later found for it. (...) If your relationships do not agree with the reference data within their uncertainty limits, then they are incorrect .''

Using floating-point real numbers in analyses masks the simple proportions of energy values. [8] Therefore, in the paper ''The Key to Atomic Harmony,'' [9] a transformation was used that converts energy values to fractional values, without rounding.

2. Methods

To better assess the quality of NIST data, it will be necessary to introduce new concepts, but first a few sentences of introduction are necessary.

2.1 Energy Estimation E0 and Lossless Energy Recording

The starting point for the estimation was the energy value E0 for the first hydrogen orbit, which according to the encyclopedia is 13.6 eV, while the Bohr-Rydberg formulas indicate a value of 13.60569 eV as being closer to reality . In our analysis, we will assume that the exact value lies somewhere between these two values. In the paper ''The Key to the Harmony of the Atom,'' [9] the value of E0 was estimated as:

$$E0 = 2 * 2 * 2 * 5 * 5 * 5 / 3 * 7 * 7 = 2000/147 \text{ eV.}$$

2.2 Entering the value [Hn] – harmonic number

The dependencies of energy, frequency and wavelength of all lines from the Lyman, Balmer, Paschen and Brackett series were investigated for n ≤ 7 and m ≤ 4 (where n – higher orbit, m – lower orbit).
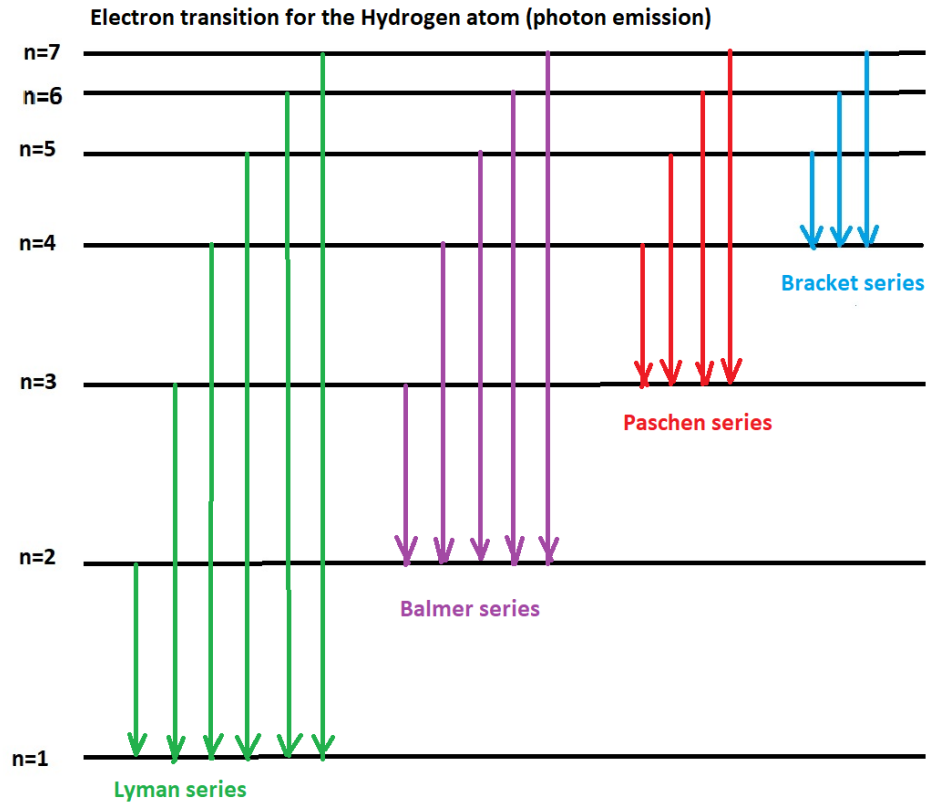
Figure 1. Electronic transition for the hydrogen atom

All tested lines were found to be integer harmonics of one main resonant wave **λ0** and their length was defined as:

λ0 = 3969 * Lambda Brackett-α (H 5->4)

Lambda wavelengths for resonance studies can be calculated using various methods, and the degree of rounding of physical constants is irrelevant – the result is always exactly the same. In this work, lambda values were calculated using the Rydberg formula: [10]

1/lambda = Difference of terms * Rydberg constant

*where =1.09677 * 10^7 m-1 (https://encyklopedia.pwn.pl/haslo/;3970382)*

The individual waves under study have N full wave periods [11] (N ∈ Natural) in one wave period λ0 and after a precisely defined number of periods (172800, 171500, 169344, 165375, 156800, 132300, 40500, 39200, 37044, 33075, 24500, 16000, 14700, 12544, 8575, 7425, 6125, 3969) they all meet in the same phase 0 from which the study started.

These values were described as "harmonic number" and the unit [Hn] was proposed for them, which works similarly to the wave unit [cm-1]. The phenomenon of resonance of all 18 Lyman, Balmer, Paschen, and Brackett lines simultaneously was called "superresonance."

2.2. Derivation of the conversion factor [Hn] → eV

For the emission of an electron from orbit 5 to 4 we write the energy equality:

E0 (1/4^2 – 1/5^2) eV = 3969 [Hn]

2000/147 (1/16 – 1/25) = 3*3*3*3*7*7 [Hn]

We get the conversion factor:

1 [Hn] = 2*2*2*2*5*5*5(9/16*25) / 3*7*7*3*3*3*3*7*7 = 5 /(3^3 * 7^4) [eV]

Example of lossless energy calculation (5→4)

We calculate the electron emission energy losslessly by substituting the value of the conversion factor:

In the case of emission of an electron from orbit 5 to 4, the energy is 3969 Je = (3969*(5/3^3 * 7^4) eV = 3^4 * 7^2 * 5 / *(3^3 * 7^4) = 5*3/7^2 = 15/49 eV – exact value without rounding.

The rounded value of this energy (loss) will be 0.306122449 eV

2.3. Unit [Hn] and frequency raster

Definition [Hn]: The [Hn] values in the table mean that the emission wave after the electron jumps between orbits has a frequency of Hn * 18.64 GHz, and the frequency separations between the emission waves of different orbits are (HnX – HnY) * 18.64 GHz.

The range of the transition table satisfying Bohr's P4 postulate

Covered transitions: Below is a table of some values of lossless emission of the hydrogen atom from a high to a low orbit: These are only orbits numbered 40, 35, 30, 28, 21, 20, 15, 14, 12, 10, 7, 6, 5, 4 and all their combinations preserve Bohr's P4 postulate.

Skipped transitions: The table does not show the transitions between orbits {1, 2, 3, 8, 9, 11, 13, 16, 17, 18, 19, 22, 23, 24, 25, 26, 27, 29, 31, 32, 33, 34, 36, 37, 38, 39} because they do not satisfy Bohr's P4 postulate, and the calculation of the energy balance requires two additional energy components, one of which is assigned exclusively to the higher orbital number and the other exclusively to the lower orbital number. A table of these energy values is available in the article " The Key to the Harmony of the Atom..."

3 Results

3.1 We discover regularities in the proportions between lines

Having a tool in the form of a fractional notation of energy values, we will try to discover regularities in the proportions of energy values between individual lines, the table below shows some values of emission energy from the higher to the lower orbit at the calculation stage, and as the final result in the form of a fraction of natural numbers (**we do not convert to real values so as not to lose accuracy**):

Initial orbit	Final orbit	Algorithm	Fractional form
5	4	3*5/(7^2)	15/49
6	5	2^2*11*5/(3^3*7^2)	220/1323
7	5	2^7*5/(7^4)	640/2401
7	6	2^2*5^3*13/(3^4*7^4)	6500/64827
10	6	2^6*5/(3^3*7^2)	320/1323
10	7	2^2*17*5/(7^4)	340/2401
12	6	5^3/(3^2*7^2)	125/441
12	7	5^4*19/(3^3*7^4)	11875/64827
12	10	11*5/(3^3*7^2)	55/1323
14	7	2^2*5^3/(7^4)	500/2401
14	10	2^5*5/(7^4)	160/2401
14	12	5^3*13/(3^3*7^4)	1625/64827
15	7	2^8*11*5/(3^3*7^4)	14080/64827
15	10	2^2*5^2/(3^3*7^2)	100/1323
15	12	5/(3*7^2)	5/147
15	14	2^4*29*5/(3^3*7^4)	580/64827
20	7	3^2*13*5/(7^4)	585/2401
20	10	5/(7^2)	5/49
20	12	2^4*5/(3^3*7^2)	80/1323
20	14	17*5/(7^4)	85/2401
20	15	5/(3^3*7)	5/189

Table 1. Lossless notation of the energy of atom emission in the form of fractions of powers of natural numbers .

For example, the 3rd harmonic resonance (3:1) occurs between the emission waves H(5->4), i.e. the hydrogen emission wave when an electron jumps from orbit 5 to 4, and H(20->10) – table below:

Initial orbit	Final orbit	Algorithm	Fractional form

5	4	3*5/(7^2)	15/49
20	10	5/(7^2)	5/49

Table 2. Example of resonance calculated from fractions of powers of natural numbers

The quotient is 15/5 = 3, which means that the emission wave H(5->4) is exactly the third harmonic of the emission wave H(20->10).

These The calculations themselves were made based on NIST data: [12]

Initial orbit	Final orbit	Algorithm	eV value
5	4	13 0545017 - 12 74854	0.3059624
20	10	13.56443886 - 13.46245155	0.10198731

Table 3. Example of lossy counting method according to NIST data

The quotient is 3.00000460841653, which means that the waves are not harmonic.

For the values to indicate a wave resonance, we would need to correct the energy of the 20th hydrogen orbit from 13.46245155 eV to 13.46245139 eV – the correction is 0.00000016 eV, which is a small fraction of *the Unc uncertainty value used by NIST,* and is within the range of values allowed as correct.

3.2 More complex resonances

The table below shows a larger number of resonances between spectral lines:

Initial orbit	Final orbit	Lambda	Initial orbit	Final orbit	Lambda	numerical harmonic resonance
5	4	4052.3	20	10	12156,826	3
7	5	4653.8	14	10	18615.14	4
10	6	5128.7	20	12	20514.64	4
10	7	8760.1	20	14	35040.27	4
5	4	4052.3	15	12	36470.46	9
20	10	12157	15	12	36470.46	3
7	6	12372	14	12	49487.6	4

6	5	7459.8	12	10	29839.49	4

Table 4. Example of a larger number of resonances between spectral lines

The remaining emission waves can also be in resonance, but in a fractional way, for example: after 8 full periods of the emission wave H(14>10) ~ 18615.14 nm and 17 full periods of the wave H(10>7) ~ 8760.068 nm, full synchronization occurs. In other words:

$$8760.068 \text{ nm} * 17 == 18615.14 \text{ nm} * 8$$

All of these resonances are from the NIST table, and the values discussed are within *the uncertainty range,* meaning they are accepted by NIST as correct and eligible for use.

3.3. The concept of superresonance and subquantization

Because [Hn] values are robust to changes in physical constants, I consider them more characteristic of atomic forces than conventional units, and I propose that the superresonant wave should serve as a natural unit of energy for describing atomic interactions. Therefore, I propose the following definitions:

- **Subquantization** – a postulated property of quanta, according to which the energy of particles (e.g. photons) is not only quantizable as integer multiples of $E = h \times f$, but can also be expressed as multiples of a more fundamental unit of energy $\varepsilon_0 =\sim 7.71 \times 10^{-5}$ eV.

- **Subquantum [sQ]** - this is the postulated smallest part of energy in photon processes, with the value $\varepsilon_0 = \sim 7.71 \times 10^{-5}$ eV*, which is an elementary unit of energy in quantum phenomena, defined as 1/3969 part of the energy of the hydrogen wave emitted when an electron transitions from orbit 5 to orbit 4 (1/3969 * H(5->4)).

- ***A wave with energy 1 [sQ]*** corresponds to the first superresonance in the electromagnetic spectrum – i.e. the fundamental wavelength λ_0, for which all 18 lowest electronic transitions in the hydrogen atom (Lyman, Balmer, Paschen series, etc. for n ≤ 7, m ≤ 4) show harmonic dependencies (they are integer multiples of frequency and energy).

It is legitimate to consider discrete energy steps smaller than ħω. In the cellular-automaton picture, the smallest allowed energy quantum can be much finer than the Planck-Einstein quantum $E = ħω$, provided the total energy is still an integer multiple of this super-fine unit. This opens the possibility of hidden harmonic sub-structures that are invisible to standard quantum field theory, yet perfectly legal in a deterministic, discrete theory. [13]

All the lines studied are arranged in a discrete raster with a modulus of approximately 18.64 GHz. The figure below illustrates some hydrogen transitions; it is limited only by the size of the figure.
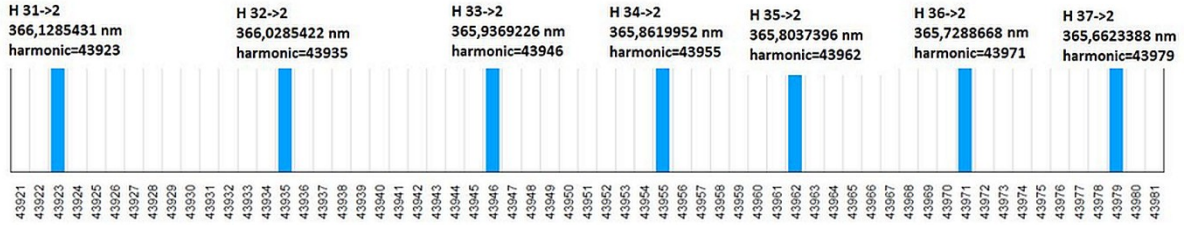

Figure 2 The known spectral lines on the horizontal axis of the [Hn] value occupy discrete positions that are integer multiples of 1 [sQ].

On the Hn axis, each subsequent wave has an energy greater by 1 [sQ] and a frequency higher by approximately 18.64 GHz than the previous one.

The model generates predictions of new transitions not seen in previous data sets. The free numbers Hn in the plot can be parameters for spectral lines discovered in the future. I attempted to predict the parameters of a previously undocumented line with the random number 43323. My calculations indicated a wave energy of 3.339 eV, corresponding to the transition from the 15th to the 2nd orbit of the hydrogen atom. At the time of this study, I had not yet used the NIST database. After analyzing the data, I discovered that the hydrogen line for this transition is marked with a measured wavelength of 371.19774 nm—which closely matches my prediction.

This predictive success echoes the historical role of Rydberg's 1890 analysis, which not only systematized known lines but also anticipated new ones later confirmed experimentally (Rydberg, 1890). In the same spirit, the resonance-grid approach provides a framework capable of forecasting spectral features beyond the scope of current tabulations. [3]

As Schiller and Karr point out, the accuracy of determining fundamental constants depends on how well we define the reference unit of energy. The constant E_0 and the units [Hn] I introduced are intended to provide precisely this purpose - to provide a consistent and algebraically transparent reference point. [14]

3.4. Examples of calculations using the [Hn] unit

From now on we can calculate wavelength ratios, e.g.:

wave energy H(6->4) / wave energy H(5->4) = 6125/3969

or

Lambda H(5->4) = Lambda H(6->4) * 6125/3969.

These calculations are free from rounding errors.

3.5 Comparison of the units [sQ] and [cm-1]

The concept of subquantization proposed here—in which quantum energy levels are structured as multiples of a deeper unit—extends the spirit of Bohm's exploration of determinism and structure beyond conventional quantum theory. [15]

The use of this unit is analogous to the use of the [cm^{-1}] unit, with the difference that [cm^{-1}] gives wave numbers in real numbers (because the base of counting, i.e. 1 cm, was arbitrarily set), while in the [sQ] units the harmonic numbers of subsequent waves are natural numbers, because they denote the multiple of the wave energy measured with respect to λ_0. They also determine the number of sinusoids in the packet (analogously to the unit [cm^{-1}]), because the basis for the calculations was the lambda0 wave of the first superresonance – i.e. approximately 1.60814 cm.

The unit 1 [sQ] is a measure of the energy of one complete sinusoidal period in any wave of any frequency).

4. Discussion

When analyzing the electromagnetic spectrum, we often notice that spectral lines—the characteristic wavelengths emitted by atoms—are not evenly distributed. This is particularly noticeable in the case of hydrogen, where:

1. In **the ultraviolet (UV) range,** the lines are **densely packed** — the differences between them in nanometers are tiny, on the order of thousandths of a nanometer.
2. In **the infrared (IR) range,** the lines are **dispersed** – the distances between them in nanometers are much larger, reaching even millions of nanometers.

This phenomenon results from **the non-linear relationship between wavelength and photon energy, and therefore also frequency** .

Shorter **wavelengths (lower λ)** mean **higher frequency.** Therefore, in the UV range, even a small change in wavelength causes a large change **in frequency** – spectral lines are "squeezed." In the infrared range, the situation is reversed: large differences in wavelength translate into small changes in energy – spectral lines are "stretched."
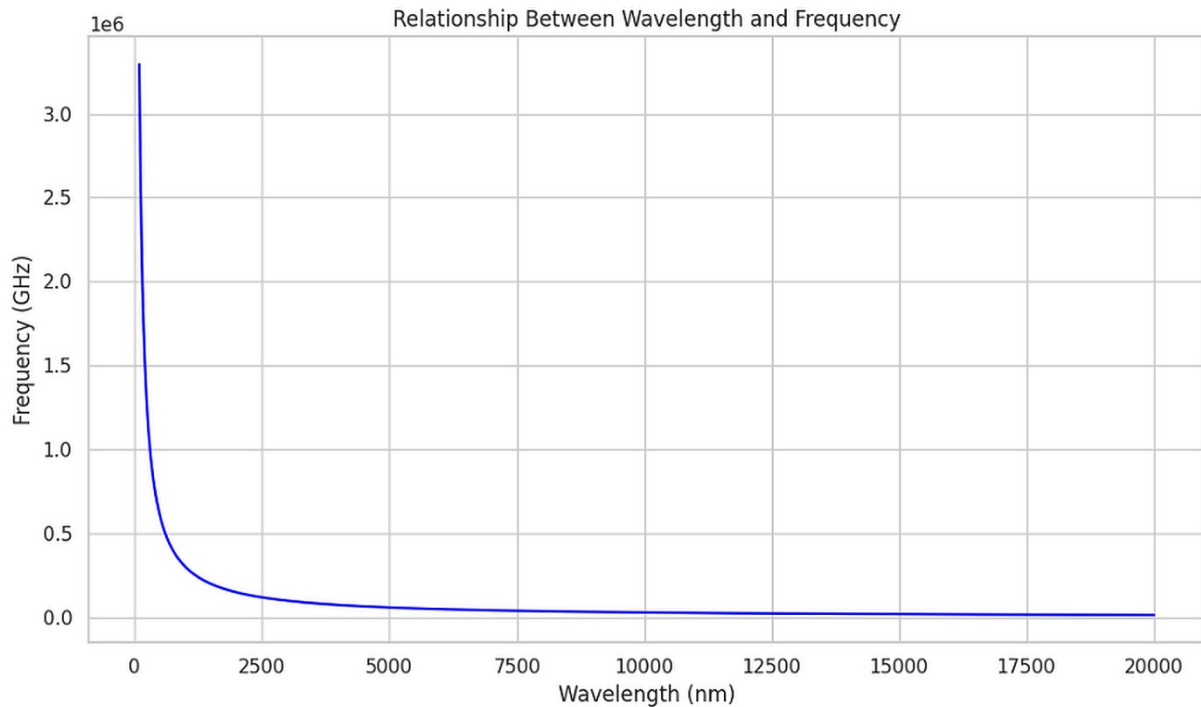
Figure 3. Relationship between wavelength and frequency

In the graph, we see that the frequency and energy increase rapidly with small changes in wavelength ranging from tens to hundreds of nanometers. If we assume that the spectral lines have discrete frequencies every 18.64 GHz, then in the energy range H 40->1 (91.232366 nm) and H 39->1 (91.2353295 nm) there will be room for 6 more lines between them.

A similar space, covering only a few lines, will be located between the lines 288225 nm and 337586 nm. As you can see, the wavelength range here is 16 million times wider to accommodate the same number of lines.   This phenomenon can lead to misinterpretations, especially in the UV range (91 nm), where the apparent proximity of the lines in nm does not reflect the actual energy density and small errors appear as insignificant "noise". [16]

Grinin et al. (Science, 2024) determined the 1S-3S transition frequency to be 102.50 nm with an accuracy of 10^-13 nm, while the NIST data (ASD, 2024) locates this line at 102.57 nm. In the [sQ] raster, this means that the NIST value corresponds to the 18sQ position, and Grinin's result is shifted by 6 discrete steps relative to it-a fact the authors are probably unaware of. Since the uncertainty interval reported in the NIST table is 0.0003 nm, the result effectively corresponds to two disjoint confidence intervals.

This raises the issue of how much certainty can, in fact, be assigned to the stated uncertainty interval, especially when the data originate from two independent research institutions.

While Brandt and colleagues (2021/22) presented an extremely precise measurement of the hydrogen transition, my harmonic raster (sQ) method reveals discrete differences in the NIST

and Grinin data, providing an alternative route to reducing uncertainty – not through increasingly sophisticated experiments, but through a new theoretical-analytical framework.[17]

4.1. Interpreting NIST Results in the Context of the New Unit [Hn]

Analyzing the NIST hydrogen tables, I found that the "obs–ritz" parameter for the H jump (10→1) can shift the line by 3 positions, and the ±"unc" parameter can shift the line by another 6 positions. When reading the data, we don't actually know which of the 9 consecutive lines we're talking about and to which the measurements refer. In fact, as Mohr, Taylor, and Newell (2021) point out, when the obs–ritz correction is comparable to the stated uncertainty, both contributions must be added linearly, and the effective wavelength window becomes a broad smear, not a single, clearly defined line.[2]

Observed Wavelength Vac (nm)	Unc. (nm)	Ritz Wavelength Vac (nm)	Unc. (nm)	Obs.-Ritz Wavelength (nm)	Transition Wavenumber (cm⁻¹)	Rel. Int.	Lower Level Conf., Term, J			Upper Level Conf., Term, J
92.0947	0.0014	92.096300	0.0000007	-0.0016	108 583.9	7400	1s	2S	1/2	10

Figure 4. Excerpt from the NIST hydrogen emission table .

Therefore, the description in cm-1 units, despite its systemic weakness, better reflects the distribution of spectral lines in the entire measurement range.[19] [20] The optimal representation of spectral lines will be units [sQ], which are a measure of the harmonic relative to lambda0, i.e. the number of multiples of the 18.64 GHz wave. And so:

Target orbit	Launch orbit	Lambda	photon energy [sQ]
1	40	91.2324	176269
1	39	91.2353	176264
1	38	91.2385	176257
1	37	91 242	176251
1	36	91.2458	176243
1	35	91.2498	176236
1	34	91.2543	176227
1	33	91.2591	176218
1	32	91.2645	176207
15	16	169411	95

16	17	204412	79
17	18	243925	66
18	19	288225	56
19	20	337586	48

Table 5. Comparison of data readability in the [nm] notation and in the [sQ] notation .

This notation accurately reflects the density of spectral lines in nature across the entire frequency band studied by NIST. I invite you to discuss the theses presented; time will tell whether the theory of energy harmony will gain greater cognitive value or whether the concept of randomness will persist.

5. Conclusion

Knowledge of atomic energy algebra allows us to improve NIST's results by reducing the uncertainty factor. Adopting this theory would allow for more accurate calibration of hydrogen emission line data.

Symmetry principles often reveal hidden structures in physical systems. [21] Based on fractional analysis, numerous simple 3:1 resonances have been identified, in which the sinusoidal node fully synchronizes with one period of the second wave after three periods of one wave. However, these cases are relatively rare; statistically, complex resonances, such as 5:3, where full synchronization occurs after five periods of one wave and three periods of the second, are observed more frequently. These relationships, one might assume, have remained unnoticed in physicists' research until now.

Rydberg's formulas, the values obtained in the most precise measurements and quantum theories should form a coherent system of mutually supporting references, and the aim of my work is to show this consistency and supplement it with a new algebraic-resonance perspective.[22]

Systematic correction of energy values - not only for individual lines, but simultaneously for the entire network, taking into account harmonic connections - could significantly increase the accuracy of the results. Improved calibration methods can reduce uncertainties by orders of magnitude in frequency measurements. [23]

5.1. Historical Contexts

At the turn of the 20th century, Marian Smoluchowski – a leading Polish theoretical physicist of the era and then a professor at the University of Lviv – turned his attention to the hydrogen spectrum. In 1900, he emphasized that understanding the relationships between individual spectral lines would provide crucial insight into the internal structure of the atoms responsible for the observed radiation.[24]

As early as 1912, Niels Bohr suggested that he might have discovered the first clues to the internal structure of atoms, and this sentence became the motto of this work.[25]

His intuition that spectral analysis can lead to conclusions about the structure of atoms is finding new development today. The algebra of atomic energy and the identification of harmonic resonances, presented in this paper, are an attempt to continue the same research program extracting atomic structure from the mathematics of spectra.

Additionally, the introduction of the Marker calculus, first presented in my earlier study entitled Systematic Deviations in Atomic Spectra: A New Analysis Method Based on the Harmonic Number Unit, opens the way to a further reduction of uncertainty - potentially by several orders of magnitude - thus indicating the possibility of a radical increase in the precision of spectroscopic data analysis.

Balmer worked with only four known lines, but his formula suggested there should be more. The humble teacher, who had no other scientific work to his credit, must have been pleased to learn of the discovery of further lines. All of them satisfied his formula. By the time of Balmer's death in 1898, a dozen were known.[26]

I hope that finding the resonance formula for the 18th line of hydrogen will contribute to the discovery of formulas for other elements, which will probably be an extension of the formula described in this publication.

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