

The Stability of Electron Orbital Shells based on a Model of the Riemann-Zeta Function

Michael Harney

841 North 700 West Pleasant Grove, Utah 84062, USA

E-mail: Michael.Harney@signaldisplay.com

It is shown that the atomic number Z is prime at the beginning of the each s^1 , p^1 , d^1 , and f^1 energy levels of electrons, with some fluctuation in the actinide and lanthanide series. The periodic prime number boundary of s^1 , p^1 , d^1 , and f^1 is postulated to occur because of stability of Schrodinger's wave equation due to a fundamental relationship with the Riemann-Zeta function.

1 Introduction

It has been known that random matrix theory, and in particular a Gaussian Unitary Ensemble (GUE), can be used to solve the eigenvalue states of high- Z nuclei which would otherwise be computationally impossible. In 1972, Freeman Dyson and Hugh Montgomery of the University of Michigan realized that the values in the GUE matrix used in predicting energy levels of high- Z nuclei where similar to the spacing of zeros in the Riemann-Zeta function [1]. Prior to these discoveries, the use of approximation in traditional quantum mechanical models was well known and used, such as the Born-Oppenheimer method [2]. These approaches experienced problems at high- Z levels where many interacting factors made approximation difficult. The remaining question as to why the periodicity of zeros from the Riemann-Zeta function would match the spacing of energy levels in high- Z nuclei still remains a mystery, however.

It is the goal of this paper to explain the spacing of energy levels in electron orbital shells s^1 , p^1 , d^1 , and f^1 , where these designations represent the first electron to occupy the s , p , d and f shells. The first electron in each of these shells is an important boundary where new electron orbital shells are created in the atomic structure. The newly created shell is dependent upon the interaction of many electrons in the previous orbital shells that are filled much like the many body problems of gravitational masses. The first electron in each of the s , p , d and f shells is therefore hypothesized to represent a prime stability area where a new shell can form within the many-electron atom without significant perturbation to previous shells. With enough computational power the interaction of electrons in any combination of orbital shells can be computed through multiple manipulations of a system of Schrödinger's equations, but even the present numerical methods for this approach will use rough approximations due to the complexity of several non-linear equations and their solutions.

Choudhury and Pitchers [3] have used a configuration-interaction method of computation for many electron atoms where Schrödinger's equation is reduced to a system of lin-

ear homogenous equations. They then argue that the energy eigenvalues obtained by truncating this linear set of equations will converge, in the limit, to those of the original system. They show that this approximation holds true for two-electron atoms, but they note that variations start occurring for the three or more electron atom. These approximation methods are difficult enough for two or three electron atoms but for many-electron atoms the approximation methods are uncertain and are likely to introduce errors.

It is therefore proposed that the final result of the many-electron atom be first evaluated from the standpoint of the Riemann-Zeta function so that a simplifying method of working back to a valid system of Schrödinger's equations can hopefully be obtained. To justify this approach, the atoms for each of the newly filled s^1 , p^1 , d^1 , and f^1 shells are examined to show a potential relation between the spacing of the non-trivial zero solutions of the Riemann-Zeta function, where the argument s in the Zeta function that produces the zero lies on the critical line of $\text{Re}[s] = \frac{1}{2}$.

2 The Riemann-Zeta function

The Riemann-Zeta function takes the form:

$$\zeta(s) = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \dots + \frac{1}{n^s} + \dots \quad (1)$$

Where $\zeta(s)$ is an alternating series function in powers of s as n terms go to infinity. The function $\zeta(s)$ is a single-valued, complex scalar function of s , much like the single complex variable of Schrödinger's wave equation. The addition of several Ψ solutions of Schrödinger's equation from many orbital electrons may be effectively modeled by (1), where additional $1/n^s$ terms in (1) contribute to the overall probability distribution of n interacting shells.

Hadamard and Vallée Poussin independently proved the prime number theorem in 1896 by showing that the Riemann-Zeta function $\zeta(s)$ has no zeros of the form $s = 1 + i\beta$, so that no deeper properties of $\zeta(s)$ are required for the proof of the prime number theorem. Thus the distribution of primes is intimately related to $\zeta(s)$.

Z number	Ln(Z number)	Z for S1 Shell	Ln (Z) from F	Number of S electrons at Z (x axis on graph)	Ln(Z) / (Number of S electrons) - y axis
1	0	1	0	0	undefined
3	1.098612289	3	1.098612289	1	1.098612289
5	1.609437912	11	2.397895273	2	1.198947636
11	2.397895273	19	2.944438979	3	0.98147966
13	2.564949357	37	3.610917913	4	0.902729478
19	2.944438979				
29	3.36729583				
31	3.433987204				
37	3.610917913				

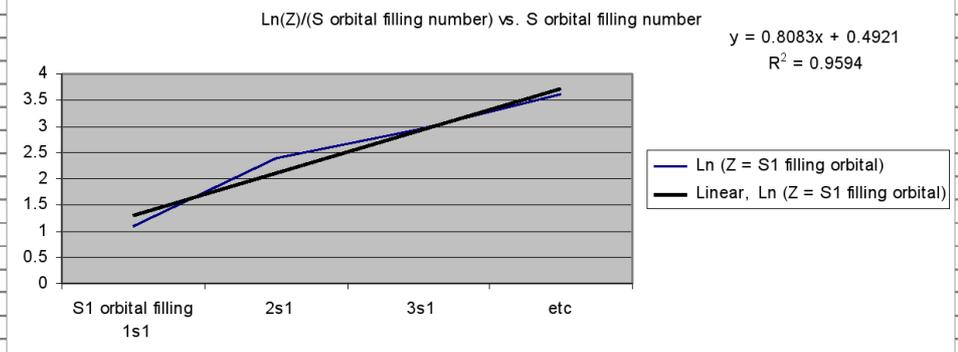


Table 2: $\ln(Z)$ for first s -orbital electron vs. Energy level (n).

3 The Periodic Table

From an analysis of the periodic table it is postulated that the stability of electronic shells s^1 , p^1 , d^1 , and f^1 follow a larger set of zeros which correlate to prime numbers from the Riemann-Zeta function.

If one examines the first and second periods of the periodic table as shown in Table 1, we find that the boundary of filling the first electron in the s , p , d and f shells of each quantum level designated as n is a stable zone that is indicated by a prime atomic number Z (the format in Table 1 is $Z: nLevel^1$).

Where (repeat) indicates a repeat of the shell from a previous Z number and where the use of the format $[Kr].4d^4.5s^1$ shows the previous electronic formula of Krypton with the additional filling of the d and s shells so as to show the repeated s shell with different d -filling electrons. From the above data, both $Z = 57$ and $Z = 89$ begin a sequence of f shells filling before d shells ($Z = 57$ is the beginning of the Lanthanide series and $Z = 89$ is beginning of the Actinide series). In both the Lanthanide and Actinide series, the d shells that fill after the f shells are primes, explaining why only these d shells (beginning with $Z = 71$ for Lanthanide and $Z = 103$ for Actinide) are filled with primes because they would normally be f shells in the sequence if we looked strictly at observed spectroscopic data.

Notice that the prime Z numbers — 1, 3, 5, 11, 13, 19, 29, 31, 37, 41, 43, 47, etc. shows one consecutive set of primes $\{Z = 3, 5\}$, skips a prime $\{Z = 7\}$ then has two more consecutive primes $\{Z = 11, 13\}$. Note that at $Z = 13$ where we have skipped a prime ($Z = 7$), the ratio of $13/\ln(13)$ is 5.0

Z:	Shell
1:	$1s^1$
3:	$2s^1$
5:	$2p^1$
11:	$3s^1$
13:	$3p^1$
19:	$4s^1$
31:	$4p^1$
37:	$5s^1$
41:	$[Kr].4d^4.5s^1$ (repeat)
43:	$[Kr].4d^6.5s^1$ (repeat)
47:	$[Kr].4d^{10}.5s^1$ (repeat)
57:	$5d^1$
71:	$5d^1$ (repeat)
87:	$7s^1$
89:	$6d^1$
91:	$15f^1$
103:	$7p^1$

Table 1: Prime Atomic Numbers with respect to s^1 , p^1 , d^1 , and f^1 orbitals.

and $Z = 13$ is the fifth prime Z number with a valid p^1 shell. The sequence then skips one prime $\{Z = 17\}$, then has a valid prime at $\{Z = 19\}$ and it then skips another prime $\{Z = 23\}$, which follows five consecutive primes $\{Z = 29, 31, 37, 41, 43\}$. At this point we have skipped $Z = 7, 17,$ and 23 but when we look at $Z = 43$, we take the ratio of $43/\ln(43) = 11.4$ and note that $Z = 43$ is the 11th valid Z prime (with three Z numbers skipped). There appears to be a similar relationship between this data and the prime number theorem of $n/\ln(n)$,

but unlike the traditional prime number theorem where all primes are included, this data considers only valid Z primes (where the first shell is filled, s^1, p^1, d^1, f^1) with other primes skipped if they don't fill the first $s, p, d,$ or f shell. From this consideration, the linearity of these values is significant to the periodic table alone. Table 2 shows the first five s -orbital shells filled (to $5s^1$) plotted against the $\text{Ln}(Z)$ where Z is the associated atomic number for the valid s^1 shell. The number of valid s^1 shells also corresponds to the energy level n ($n = 1$ through $n = 5$ for $1s^1 - 5s^1$). The slope in Table 2 for just the s -shell is good with a linear relationship to $R^2 = 0.95$.

This sequence is also hypothesized to be similar to the distribution pattern of primes produced by finding the zeros on the critical line of the Riemann-Zeta function of (1). Based on the results of linearity in Table 2 there may be a relationship between the difference between valid s -shell orbitals (the Z numbers of skipped shells) versus the total number of shells, a further indication that Riemann-Zeta function could explain the prime orbital filling. There is also a similar prime number correlation for the nuclear energy levels where s, p, d, f and g shells begin on prime boundaries [4].

4 Conclusions

It is found by examining the Z number related to the $s^1, p^1, d^1,$ and f^1 shells of the periodic table that Z is prime for the first filling of s, p, d and f orbitals. It is also found that for shell filling of ns^1 , the logarithm of the prime number associated with Z is linear with respect to energy level n . This relationship is believed to correlate with the Riemann-Zeta function, a complex scalar function similar to the complex-scalar wave function of Schrödinger. The atomic Z primes that correspond to the $s^1, p^1, d^1,$ and f^1 shells is predicted to follow the distribution of primes that result from the non-trivial zeros of the Riemann-Zeta function.

Acknowledgements

The author wishes to thank Kevin McBride for initially suggesting a connection between the Riemann-Zeta function and various aspects of nature and mathematics.

Submitted on October 15, 2007

Accepted on October 19, 2007

References

1. Dyson F. Statistical theory of the energy levels of complex systems. III. *J. Math. Phys.*, 1962, v. 3, 166–175.
2. Born M., Oppenheimer R. Zur Quantentheorie der Molekeln. *Annalen der Physik*, 1927, v. 84, 457–484.
3. Choudhury M.H. and Pitches D.G. Energy eigenvalues and eigenfunctions of many-electron atoms. *J. Phys. B: At. Mol. Phys.*, 1977, v. 10, 1209–1224.

4. Jiang Chun-xuan. On the limit for the Periodic Table of the elements. *Aperion*, 1998, v. 5, 21–24.