# SOME COINCIDENCES CONCERNING THE ELECTRON OCCUPANCY NUMBERS OF ATOM SUBSHELLS

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Abstract. A minimum condition on a suitable function, built with the atom energy level values from Dirac's formula, produces coincidences involving the numbers, given by Pauli's principle, that describe the electron arrangement inside the atom shells.

As known, the electrón occupancy numbers of atom energy levels are given by the Pauli exclusion principle. There is no other independent reason that justifies or interpretes the electron distribution inside the atom shells, therefore some 'numerical coincidences' here presented, concerning these numbers, appear unforeseen. It will be shown that one can pose a suitable condition on a shell energy capacity, whence numbers coinciding with the Pauli occupancy numbers are obtained. This energy capacity will be computed from the Sommerfeld-Dirac formula that yields the energy levels of the hydrogen-like ions with distinct quantum numbers n (principal quantum number) and k ($k=j+1/2$, $j=l\pm 1/2$, $l=0,1,\ldots,n-1$; if $s=\pm 1/2$).

Let us first consider the following amount of energy

$$C_n(\underline{I}^{(n)}) = \sum_{k=1}^{n} I_k^{(n)} E_{Z_n,n,k} \qquad (1)$$

where $E_{Z_n,n,k}$ is the energy value (corresponding to a given n and k) for the hydrogen-like ion with atomic number

$$Z_n = \sum_{N=1}^{n} 2N^2 \quad ; \qquad (2)$$

and $\underline{I}^{(n)}$ is a vector whose n components $I_k^{(n)}$ are natural numbers satisfying the condition

$$\sum_{k=1}^{n} I_k^{(n)} = n^2 \quad . \qquad (3)$$

If, for a given n, the numbers $I_k^{(n)}$ are equal to the electron occupancy numbers of the various subshells identified by l, in the restricted case s=+1/2 (so that k=l+1), then eq.(1) gives an ideal energy capacity of the $n^{th}$ shell corresponding to $n^2$ bonds. The well known dependence of such occupancy numbers (for s=+1/2) on n, according to Pauli's principle, is reported in Table I. The computed energy capacity is called ideal because this calculation does not take into account the changes of binding energy due to the mutual interactions among electrons simultaneously present in an atom.

Let us then write the following quasi-equality, for $n \geqslant 2$,

$$\left[C_n(\underline{I}^{(n)})/(\tfrac{1}{2}\alpha^2 Z_n^2)\right] - \mu_{Z_n} c^2 \simeq \sum_{i=2}^{n} E_{Z_i,i} \qquad (4)$$

where $\alpha = 1/137.036$ is the fine structure constant; $\mu_{Z_n}$ is the electron-nucleus reduced mass for the atomic number $Z_n$; and $E_{Z_i,i}$ is a middle value of energy defined for each $i=2,\dots,n$ as

$$E_{Z_i,i} = (E_{Z_i,i,1} + E_{Z_i,i,i})/2 \quad . \tag{5}$$

It turns out that the n-tuples corresponding to the Pauli occupancy numbers of Table I minimize the relative error in eq.(4) for low n-values, and nearly minimize it for high n-values. The values of $I_k^{(n)}$ for which the first three minima of such an error are reached, under the constraint expressed by eq.(3), are shown in Table II. For n=2,3 the Pauli numbers correspond to the first minimum. In the last column the total number of the possible n-tuples is indicated. For n=4 the Pauli numbers give the second minimum over 455 possible n-tuples; and for n=5 the fifteenth minimum over 10626 n-tuples, or the first one over 192 if the further constraint $I_1^{(5)} \leqslant \dots \leqslant I_5^{(5)}$ is introduced. As it can be seen, such a new constraint would make also the set of four numbers from Pauli's principle correspond to the first minimum. However, without introducing this constraint, the Pauli numbers give the first minimum also for n=4 if the minimum search is averaged around $Z_4=60$. In such an average operation $Z_4$ in eq.(4) is substituted by Z varying, say, from 40 to 80, and the terms $E_{Z_i,i}$, for $i=2,\dots,n-1$, are multiplied by a suitable proportionality factor like $Z^2/Z_4^2$. Average operations for other values of n leave the results shown unchanged.

It seems then that eq.(4) contains some 'information' about the arrangement numbers of electrons in the subshells (according to 1) as such numbers are 'functional' in determining a strongly ordered dependence on n of the (above defined) ideal energy capacity of a shell for $s=+1/2$. Although I cannot justify theoretically the coincidences shown here, nevertheless they do not seem accidental to me.

## CAPTIONS TO TABLES

Table I. Electron occupancy numbers of the atom subshells (according to 1) for s=+1/2.

Table II. The n-tuples $I_k^{(n)}$ corresponding to the first three minima for eq.(4).

| n \ l | 0 | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| 2 | 1 | 3 | | | |
| 3 | 1 | 3 | 5 | | |
| 4 | 1 | 3 | 5 | 7 | |
| 5 | 1 | 3 | 5 | 7 | 9 |

TABLE I

| | $I_1^{(n)}$ | $I_2^{(n)}$ | $I_3^{(n)}$ | $I_4^{(n)}$ | | rel. error | total n-tuples |
|---|---|---|---|---|---|---|---|
| n=2 | 1 | 3 | | | | 0.001 | 3 |
| | 2 | 2 | | | | 0.5 | |
| | 3 | 1 | | | | 1. | |
| n=3 | 1 | 3 | 5 | | | 0.001 | 28 |
| | 1 | 4 | 4 | | | 0.09 | |
| | 1 | 2 | 6 | | | 0.09 | |
| n=4 | 1 | 4 | 2 | 9 | | 0.005 | 455 |
| | 1 | 3 | 5 | 7 | | 0.006 | |
| | 1 | 2 | 8 | 5 | | 0.007 | |
| | $I_1^{(5)} \leqslant I_2^{(5)} \leqslant I_3^{(5)} \leqslant I_4^{(5)} \leqslant I_5^{(5)}$ | | | | | | |
| (n=5) | 1 | 3 | 5 | 7 | 9 | 0.003 | 192 |
| | 1 | 2 | 7 | 7 | 8 | 0.009 | |
| | 1 | 3 | 5 | 6 | 10 | 0.009 | |

TABLE II