The Importance of the Pauli Exclusion Principle

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In a provacative article published in *Science* (21 February 1975) with the title "Of Atoms, Mountains and Stars: A Study in Qualitative Physics," Victor Weisskopf illustrates the importance of quantum mechanics in understanding not only the nanoscopic world of atoms and molecules, and our macroworld of mountains, but also the cosmological world of stars and galaxies. Weisskopf's paper presents an analysis of material science in terms of two fundamental ideas: wave-particle duality for matter and light, and the Pauli exclusion principle for the basic building blocks of matter (electrons, protons and neutrons, all fermions).

Regarding the Pauli principle Weisskopf writes:

> If the Pauli principle did not hold, all electrons would be allowed to be in the lowest quantum state. That would mean that the ground states of all atoms would be similar: the atomic electrons would all assemble in the lowest and simplest quantum state. All atoms would exhibit essentially the same properties, a most uninteresting world. We owe the variety of nature largely to the exclusion principle.

The purpose of this tutorial is to illustrate what Weisskopf is saying in this paragraph. Using the following trial wave function, a general variational calculation will be carried out assuming all atomic electrons are resident in the ground 1s quantum level.

$$\Psi(\alpha) := \sqrt{\frac{\alpha^3}{\pi}}\cdot\exp(-\alpha\cdot r)$$

The calculation of the energy of the $1s^Z$ electronic configuration assuming this trial wave function yields.

$$E = Z\cdot\frac{\alpha^2}{2} - Z^2\cdot\alpha + \frac{Z\cdot(Z-1)}{2}\cdot\frac{5}{8}\cdot\alpha$$

Minimization of E with respect to α gives

$$\frac{d}{d\alpha}\left[Z\cdot\frac{\alpha^2}{2} - Z^2\cdot\alpha + \frac{Z\cdot(Z-1)}{2}\cdot\frac{5}{8}\cdot\alpha\right] = 0 \text{ solve}, \alpha \rightarrow \frac{11}{16}\cdot Z + \frac{5}{16}$$

Substitution of the optimum value for α into E yields the energy $1s^Z$ electronic configuration:

$$E(Z) := Z\cdot\frac{\alpha^2}{2} - Z^2\cdot\alpha + \frac{Z\cdot(Z-1)}{2}\cdot\frac{5}{8}\cdot\alpha \;\Bigg|\; \begin{array}{l}\text{substitute}, \alpha = \frac{11}{16}\cdot Z + \frac{5}{16} \\ \text{simplify}\end{array} \rightarrow \frac{-121}{512}\cdot Z^3 - \frac{55}{256}\cdot Z^2 - \frac{25}{512}\cdot Z$$

Comparing this result for the energy as a function of atomic number with the actual ground state energies of the elements confirms Weisskopf's statement. The energy result ignoring the Pauli principle presented here is lower than the experimental energies for elements beyond He.

Z	E(Z)	E(experimental)
1	−0.500	−0.500
2	−2.848	−2.903
3	−8.461	−7.478
4	−18.758	−14.668
5	−35.156	−24.658
6	−59.074	−37.855
7	−91.930	−54.609
8	−135.141	−75.106
9	−190.125	−99.801
10	−258.301	−129.044