What Gamble?

We normally consider physics and chemistry to be exact sciences, implying intuitively that the laws of science had been derived from first principles. This is not true. All the laws of natural science, such as those of thermodynamics, are empirical, based on experience, and true only in the sense that nobody has found convincing evidence of the contrary.

The area 100 ± 10 years ago represents two extremely important decades for physics and chemistry, indicated by the break-down of classical (Newtonian) mechanics and the foundation of quantum mechanics. It led to the recognition that the energies of low mass particles that are spatially confined by a force field are quantized and cannot adopt a smooth distribution of values, and that such systems are described adequately by wave equations. This is in analogy to the string of a guitar that is confined in its length and can vibrate only at certain frequencies.

So where is the gamble that the title of this book talks about? It comes in when we have a set of observations that we want to rationalise, and in order to do so we invent various models and analyse whether one of them can reproduce or predict the observations. The first example was the spectrum of emission lines of excited atomic hydrogen. The Swiss mathematics teacher Johann Jakob Balmer played around with the wavelengths of these lines and found a formula consisting of a set of two integers (quantum numbers) and a single adjustable parameter that was able to predict the spectral lines with high accuracy. Three decades later, Bohr developed a two-dimensional physical model that explains the Balmer formula. Today's accurate analytical three-dimensional solution for the atomic wave function is based on the Schrödinger equation.

Another example is the wave function of the hydrogen molecule for which still today there is no appropriate analytical solution. 1927, the so-called valence bond ansatz by Heitler and London suggested to use the product of two hydrogen atom wave functions. Shortly thereafter, Hund and Mulliken used the sum of two atomic wave functions in what is today known as the linear combination of atomic orbitals (LCAO) method. Both methods can basically explain the existence of a chemical bond, but can they both be correct? No, they are both wrong, they are merely initial guesses. These are then improved by introducing and optimising a multitude of parameters until a satisfactory approximate solution for wave function and energy is obtained.

For all of his life, Jan Boeyens questioned certain unjustified but creative guesses of quantum mechanics and searched for alternatives. He would have been a perfect member of the group of distinguished physicists 100 years ago.

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