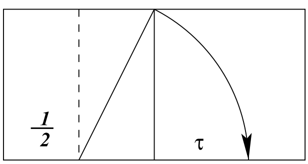
Preface

The spectacular successes such as the construction of lasers and magnetic resonance instruments, commonly credited to quantum physics and spectroscopy, make the expectation of a quantum theory of chemistry almost irresistable. Equally spectacular failures to account for high-temperature superconductivity, cold fusion, molecular diffraction, optical activity and molecular shape are conveniently ignored. Even the emergent concept of spin, correctly considered the most non-classical property of elementary matter, has never been explained in terms of first-principle quantum theory.

It is therefore not surprising to find that beyond the Bohr-Sommerfeld model of the atom quantum mechanics has caused more confusion than enlightenment in theoretical chemistry. However, to turn away from the fantasy of quantum chemistry, after a century of expectation, could be as traumatic as renouncing the prospects of alchemical transmutation.

Chemistry is the prodigy of alchemy as modified by the theories of modern physics. Even so, it still has not resolved the ancient enigma around the nature and origin of matter. Alchemy itself is the product of ancient hermenistic philosophies, traces of which have survived the metamorphosis into chemistry. Elements of the number-based Pythagorean cosmology are clearly discernible, even in the most modern theories of chemical affinity. Briefly [1]:

> The cosmic **unit** is polarized into **two** antagonistic halves (male and female) which interact through a **third** irrational diagonal component that contains the sum of the first male and female numbers (3 + 2) and divides the **four**-element (earth, water, fire, air) world in the divine proportion of $\tau = (\sqrt{5/4} - \frac{1}{2})$.



In Pythagorean parlance, any chemical interaction is essentially of the type

$$HCl + NaOH \rightarrow NaCl + H_2O.$$

It is facilitated by the affinity between opposites to produce a product that symbolizes the principle of substantiality, in harmonious equilibrium with the total environment.

All harmonic proportions and relationships are said to derive from the roots of 2, 3 and 5, the number of life. In modern terminology, the harmony that results from the interplay of integers and irrationals manifests at all levels of reality. It is colloquially referred to as self similarity, well known to be mediated by the golden ratio and golden logarithmic spirals. Modern theories perform little better in describing ponderable matter as resulting from the interaction between cold dark matter and a universal Higgs field. The mathematical model that underpins the theory is as mysterious as the divine proportion.

Chemistry distinguishes between space and time, and between matter and energy. The seminal theories of physics, independently developed by Newton and Huygens made the distinction between particles and waves. Hamilton's refinement of classical mechanics demonstrated some common ground between the two theories, but Maxwell's formulation of the electromagnetic field revealed a fundamental difference in their respective laws of motion. It was the unified transformation of Lorentz that finally established the four-dimensional nature of Minkowski space-time and the equivalence of mass and energy. The gravitational and electromagnetic fields remained poles apart. However, both of these could be shown, by Einstein's general relativity and the notion of gauge invariance as developed by Weyl and Schrödinger, to be products of Riemann's non-Euclidean geometry. Ultimate unification of the fields was achieved in terms of Veblen's projective relativity.

Analysis of the interaction between matter and radiation and the theories of chemistry were pursued in Euclidean space and remained at variance with the theory of relativity, culminating in the awkward compromise of wave-particle duality. It is only the recognition of spin as a strictly four-dimensional concept that holds the promise of wave structures, which behave like particles. Formulated as a quaternion structure it defines the common ground between relativity and quantum theories. The electron, defined as a nonlinear construct, known as a *soliton*, recognizes the importance of space-time curvature and represents final unification of its initially antagonistic attributes.

It is the theme of this book to show how refinement of the concepts matter and wave would lead to a consistent description of chemical systems without the confusion of probability densities and quantum jumps. The final model is that of Schrödinger, extended to four dimensions in nonlinear formulation.

The major effect of this more general proposed formulation is that the procedure of linear combination of atomic orbitals, at the basis of all "quantum chemistry" completely looses its validity and it needs to be replaced by entirely new modelling strategies. One alternative, already in place, is molecular mechanics, an empirical procedure based on classical mechanics and classical notions of molecular structure. It is encouraging to note that the same number-theoretic simulations, which are effective as a basis of elemental periodicity, are commensurate with molecular mechanics.

The number-theory simulation of chemical systems originated with the observation that the periodicity of atomic matter depends on the number ratio of atomic protons to neutrons that converges to τ as a function of either A, Z, $A - Z$ or $A - 2Z$. The same pattern is revealed by the golden proton excess $x = Z - \tau N$. By demonstrating that this convergence is a function of general space-time curvature the observed cosmic self-similarity is inferred to depend in equal measure on space-time curvature, the golden ratio and the shape of the golden logarithmic spiral.

To put the whole scheme into perspective it is noted that, because of curvature, the geometry of space time is non-Euclidean and different from the commonly perceived Euclidean geometry. Topologists distinguish between an underlying, globally curved space-time manifold and the local, approximately Euclidean, three-dimensional, tangent space and universal time. Any analysis performed in tangent space, using a model such as Newtonian mechanics or Schrödinger's linear equation, produces a good, but incomplete, approximation, compared to possibly more refined descriptions in four-dimensional detail.

To compensate for the neglect of curvature the golden parameter τ, or optimization in terms of golden logarithmic spirals, provides an immediate corrective, in the simulation of chemical systems by linear procedures. The very existence of matter is seen to depend on the nonlinear deformation of a hypothetical, Euclidean, four-dimensional energy field as described by the theory of general relativity. The product is a non-dispersive solitary wave packet, known as a *soliton*. Different modes of deformation lead to the formation of solitons of different symmetry, colloquially known as elementary particles. Dependent on mass, charge and spin these units are of different stability and in combination with those of complementary affinity develop into the different forms of ponderable matter—atoms, molecules, crystals, fluids and higher aggregates. The imprint of space-time curvature and the golden ratio remains with all matter, exhibiting a common self-similar symmetry.

The periodicity of matter arises as the product of a closed numerical system with a natural involution that relates matter to antimatter. In four dimensions such a function defines elliptic space in the form of projective space-time, as used by Veblen in the unification of the electromagnetic and gravitational fields.

The hard sell of convincing chemists that quantum mechanics in its present guise is too restrictive as a theory of chemistry necessarily involves unfamiliar mathematical arguments that may turn out to be counterproductive. To be convincing it is unavoidable to introduce various aspects of physics and applied mathematics traditionally considered to be way outside the chemistry paradigm. The bland alternative of starting from "well established" mathematical physics appears equally problematical. This is the exact strategy that created the present dilemma in the first place.

The most daunting prospect is to argue convincingly for the adoption of a four-dimensional world view, against the millions of three-dimensional molecular structures derived by sophisticated experimental techniques. To complicate matters by the introduction of nonlinear effects would surely be considered as meaningless, unless it can be supported with concrete examples. The anticipated response is difficult to predict.

The conservative respect for authority creates another problem. It comes naturally to reject, without thinking, dissident views that contradict the time-honoured ideas of respected pioneers. A prime example is in the handling of high-temperature superconductivity. The BCS theory, which ascribes superconduction to the formation of bosonic electron pairs, mediated by lattice phonons, offers no insight into the mechanism that operates in ceramic materials. Even the correlation of low-temperature metallic superconduction with normal-state properties remains an empirical observation without theoretical support. A reported room-temperature superconducting state is simply denied as theoretically impossible.

The credibility of the quantum-based BCS theory rests entirely on the reputation of its authors. Reluctance to abandon the model relates to the mistaken perception that it is supported by the mathematical simulation of a superconduction transition as the breakdown of gauge symmetry on cooling. However, the symmetry model applies to all forms of superconductivity whereas the phonon interaction is an empirical conjecture for one special case only.

The readily demonstrated dependence of superconductivity on the composition of atomic nuclei favours an alternative description of the phenomenon as a nuclear, rather than a strictly electronic, property. Special stability of the nuclear composition that corresponds to the Z/N ratio of τ implies a positively charged surface shell that correlates remarkably well with anomalous nuclear spin and superconduction. With this surface excess as a guide an alternative mechanism that effects all forms of superconductivity is recognized.

At a more speculative level the phenomenon of electrolytic “cold fusion”, appears to occur at cathodes, rich in high-spin isotopes of the same type. In this case the active process appears as neutron capture that converts symmetry-distorted nuclides to lower-energy forms.

These examples all point at the unpalatable conclusion that quantum theory, in its present form, falls far short of popular perceptions. It is not the all-embracing panacea that stretches beyond science and inspires the non-local metaphysics of fundamental acausality, probability and complementarity, which blossomed into multiverse cosmology. An “inner voice” told Einstein that something was amiss, but he lacked the data to support his intuition.

The central issue that defied comprehension was the apparent dual nature of both elementary matter and radiation. Efforts to account for this uncertainty resulted in concepts, universally accepted by now, such as an observer’s role in creating patterns from the conceptually unknown. This confusion between subject and object resonates with the musings of psychologists and philosophers, groping for an understanding of reality in terms of medieval mysticism through quantum theory [2].

The unfortunate conviction that inspires such pursuits, although hard to gainsay philosophically, has a simple resolution:

There is no such thing as an elementary point particle.

Matter, as the product of intrinsically nonlinear four-dimensionally curved space-time, or “condensation of the vacuum (æther)”, has a wave structure. Not in the form of dispersive wave packets, but as non-dispersive persistent solitary waves, or *solitons*, only known to occur in shallow water at the time when quantum theory was formulated.

Solitons are flexible and under certain circumstances may appear to behave like point particles. Futile efforts to account for a soliton's wave-like behaviour with a particle model result in the weird constructs, generally believed to reflect quantum effects. This statement is a concise summary of the argument to be developed in the following.

Acknowledgement

I thank Demi Levendis and Vimal Iccharam for their continued interest in this venture and Faan Naude for his friendly information retrieval service.

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Springer

http://www.springer.com/978-94-007-7577-0

The Chemistry of Matter Waves
Boeyens, J.C.A.
2013, XIV, 243 p., Hardcover
ISBN: 978-94-007-7577-0