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The Chemistry of Matter Waves

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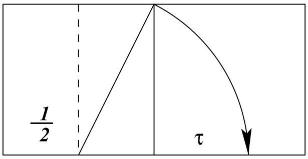
Preface

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

$$\mathrm{HCl} + \mathrm{NaOH} \rightarrow \mathrm{NaCl} + \mathrm{H_2O}.$$

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.

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Contents

Chapter 1
Of Electrons and Molecules

Abstract The discovery of X-ray diffraction promised to resolve the mystery of molecular structure, but a hundred years on it is fast receding into the fourth dimension. The contemporary development of quantum mechanics performed no better. It introduced, without explanation the notion of non-commuting dynamic variables, described by complex functions, failed to account for electron spin or optical activity and still appears to be at odds with special relativity. The confusion starts with Maxwell's formulation of the electromagnetic field, interpreted differently in quantum and relativity theories, and grows with the chemical practice of reducing complex quantum functions to real classical variables. This leaves the nature of a single molecule's structure undefined—neither classical nor non-classical.

1.1 Introduction

Chemical theory is based in the final analysis on two poorly understood concepts—*electron* and *molecule*. In principle both of these are wave-mechanically well defined, but in reality neither model reveals anything beyond the initial assumptions. The chemist's electron is a negatively charged particle and a molecule a set of atoms connected into a fairly rigid framework as dictated by classical valence forces.

The purpose of this introductory chapter is to review the theoretical problems with electrons and molecules in broad outline and to highlight important aspects to be discussed in subsequent chapters. It is necessary to recognize the problems, which are commonly ignored during unsuccessful computational simulations, in order to reformulate the wave-mechanical approach on a more fundamental basis.

1.2 Electrons in Chemistry

As the science that studies the transformations of matter, an understanding of chemistry depends on elucidating the behaviour of the electrons that mediate interaction between atomic cores. Elucidation in this sense is not to be confused with the simulation of intramolecular electron transfer, routinely performed by practising

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chemists, without appreciating the nature of electron spin, charge or mass. It is considered as sufficient common knowledge that an electron carries one unit of indivisible negative charge and half a unit of intrinsic spin, directed either up or down. The origin and meaning of these attributes are seldom contemplated and electron mass is no more than the natural property of an elementary point particle. The more surprising phenomenon of electron diffraction is considered adequately explained by the quantum-mechanical concept of wave-particle duality.

This amazing compliance can be traced back to the accepted infallibility of quantum theory, considered to underpin all of chemistry. Most theories are considered subordinate to experimental evidence, but occasionally some special theories acquire metaphysical importance by virtue of universal acclaim that results in dogmatic certainty. This recognition befell the peripatetic physics of Aristotle, Ptolemaic cosmology, the phlogiston theory of chemistry and the quantum theory according to von Neumann. Once a theory has been elevated to such a level, conflicting evidence is rationalized by the introduction of secondary concepts, not part of the seminal theory. Well-known examples include the epicycles of planetary motion and the negative mass of phlogiston. The accepted properties of the electron are immediately recognized as being of this nature.

Except for the quantum theory, all of the others had given way eventually under the pressure of experimental evidence. In the same way the prevailing theory of the electron needs replacement by another that accounts for its spin, charge and wave nature. Schrödinger's fundamental equation represents a modification of the general equation for wave motion according to de Broglie's postulate of a function $\psi = \exp(ip_x/\hbar)$ to describe matter waves.

The resulting wave-mechanical formulation of quantum theory has several defects. The most glaring is that, despite the evidence from special relativity, it is formulated as a theory in three-dimensional space. For this reason the spin function remains undefined. Solution of the resulting differential equation by further separation of the variables next reduces all electronic motion into the unrealistic classical one-dimensional vibrations of quantum chemistry.

As for all linear differential equations, superposition of any elementary solutions of Schrödinger's equation is another solution. The most general solution can hence be written as the Fourier sum of orthogonal functions

$$\psi(x) = \sum_k A(k)e^{ikx}.$$

For continuously varying k, the normalized solution

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)e^{ikx}\,dk$$

represents a wave packet, which is dispersive for de Broglie matter waves, *e.g.* an electron.

1.2.1 Wave-Particle Duality

Although the Schrödinger-de Broglie model failed to produce an acceptable wave description of an electron with spin, its confirmation of the Bohr-Sommerfeld hydrogen spectra instilled overwhelming confidence in the methodology. Instead of modifying the seminal equation to generate a non-dispersive electronic wave packet, the agreed remedy was to retain the equation without alteration, but supplemented by the addition of suitable *ad hoc* correction factors.

Without a stable wave packet to simulate the particle-like behaviour of an electron it was therefore redefined arbitrarily as a point particle with spin and wave properties. Of these stated attributes only the wave behaviour is consistent with the mathematical model. Spin could be introduced by the addition of a matrix operation to represent an extra two-level variability, not reflected in the seminal equation. However, the simulation of wave-like behaviour in terms of particle dynamics necessitated a drastically modified interpretation of the wave functions that characterize the eigenvalue solutions. The agreed innovation, sanctioned by neither de Broglie nor Schrödinger, was to interpret the square of the wave function $|\psi|^2 = P$, as a probability electron density. Not even this device could be argued to account for electron diffraction, which problem was overcome by the invention of the new term *wave-particle duality*. It has no operational meaning but is recommended to imply that an electron may behave as either a particle or a wave, as needed.

1.2.2 The Schrödinger Approximation

Quantum chemistry is based exclusively on the one-electron solutions of Schrödinger's equation. As a modification of Laplace's equation these solutions are modified spherical harmonics. Two-dimensional plane harmonics, better known as circular harmonics, underpin the original quantum theory of Bohr [1]. One-dimensional simple harmonics define the basis of de Broglie's postulate that relates linear momentum to wavelength.

The relationship between one-dimensional harmonic vibration and two-dimensional circular motion is demonstrated by the mechanical device known as a Scotch yoke, familiar to most as an automotive crankshaft. This device generates rotational motion about an axis perpendicular to two orthogonal vibrations that it locks into phase, as described by a complex function. In spherical rotation the phase relationship is described by a four-dimensional hypercomplex function. Mathematically the various modes of harmonic motion are all described by Laplace's equation. In one dimension it describes simple harmonic motion by a single real variable and circular harmonics by a complex function of two variables. Schrödinger's equation is obtained by separating the space and time variables of a three-dimensional wave equation [2].

Not only could this be the reason why quantum chemistry fails, but it also explains the notorious discrepancy between quantum mechanics and the theory of general relativity, which was developed as the common frame of reference for mechanical motion and the electromagnetic field. The equations of special relativity, known as the Lorentz transformation are formulated most generally as a complex rotation in four-dimensional space-time [3]. It is of the essence that this formulation does not allow the separation of space and time variables. The four-dimensional rotation operator is known as a *quaternion* and the argument as a *spinor*, which is a harmonic function in four-dimensional space-time.

There is a regular progression from one- to four-dimensional number systems. The familiar fields of *real* and of *complex* numbers are one- and two-dimensional respectively. A complex number has two real components. In the same way a four-dimensional *hypercomplex* number, known as a quaternion, has two complex components. Quaternions differ from complex numbers in not being *commutative* under multiplication. An *octonion* has two quaternion components and for it the distributative law does not hold.

Notably there is no normed division algebra in three dimensions [4]. Three-dimensional space is therefore described in terms of a complex plane, orthogonal to a linear polar direction. General, or spherical rotation, which defines a spinor is hence undefined in three-space. This explains why the important property of electron spin has to be added manually to the traditional quantum model. The standard model of quantum chemistry, which is based on three orthogonal orbital directions, is, for the same reason, undefined in Schrödinger space.

1.2.3 Four-Dimensional Waves

The appearance of an electron, as all other elementary forms of matter, cannot be reduced to a level lower than the physical vacuum, with geometrical shape defined by the space-time variables of general relativity. As a discrete object it must be seen as characteristic of a stable elementary distortion of space-time. While the nature of empty space-time remains unknown elementary objects, such as electrons, which appear in curved space-time, have been studied in detail.

To first approximation different elementary units have characteristic properties of mass, charge and spin, all of which relate to a specific mode of space-time distortion and the accumulated space-time density that results in the region of distortion.

If elliptic topology of space-time is assumed, the vacuum is represented by an equilibrium interface between material and anti-material regions and may be imagined to be in a state of gentle undulation. Space-time curvature generates interference patterns in this four-dimensional wave field with the formation of standing wave packets, recognized as electrons and other elementary entities.

To ascertain the characteristic mass (or energy) of such an entity, space-time density is multiplied by the volume in space, *i.e.* $m = \rho x^3$. In four-dimensional space-time the product of $\rho x^3 t = a$, corresponds to the more fundamental property known as *action*, $a \propto mt$. The elementary unit of action, given by Planck's constant,

$\hbar$, describes the spin, or the four-dimensional symmetry of the distortion. The three-dimensional symmetry (rotation) with respect to the local time axis, is observed as electric charge.

The more complex internal structure of hadrons is ascribed to extra symmetry (*e.g.* three-fold symmetry) of the internal wave field. It is suggested that such interactions could be described by octonions.

1.2.4 Nonlinear Schrödinger Equation

An obvious defect of wave mechanics is being based on linear differential equations. The computers to solve nonlinear equations simply did not exist in 1930 and, to a first approximation, solutions of the linear equations corresponded so well with experimentally known quantum effects that the model was generally accepted as adequate. Twenty years later when serious discrepancies started to emerge the paradigm was so firmly established that modification was considered heretical.

At the same time the theoretical analysis of chemical problems by the linear combination of atomic orbitals, which came into widespread use, was seen as the ultimate solution. A moment's sober reflection at the time should, arguably, have cautioned the numerous users of powerful new software that became widely accessible, that nonlinear effects in the handling of medium to large molecules cannot reasonably be ignored. The numerical simulation of ergodic effects at Los Alamos brutally exposed the inadequacy of linear statistical models and soon led to the recognition of soliton structures that could be of relevance in the simulation of elementary-particle models.

Computational chemists have been too slow to exploit the new techniques for the analysis of electron and molecular structures, while chemical and electrical engineers continue to make free use of nonlinear Schrödinger (NLS) and sine-Gordon equations.

It is of special importance to note that the NLS equation has the same structure as the so-called classical Schrödinger equation. This parallel identifies the quantum potential as the nonlinear term and defines a seamless transition between wave-mechanical and classical Hamilton–Jacobi systems. An exciting possibility arising from this is the recognition of a wave-mechanical basis of venerable classical concepts such as electronegativity, bond order, polarizability, valence state and molecular shape.

In order to fully appreciate the proposed modifications to the standard wave-mechanical model of chemistry it is necessary to examine the state of the art against the background of the historical developments over the previous two centuries.

1.3 Molecular Structure

The molecular-structure hypothesis originated during the 19th century in the work of Kekulé, van't Hoff and others [5]. It gained respectability as a reliable diagnostic of optical activity of molecules in solution and as the basis of the Lewis electron-pair model of chemical bonding. Final vindication of the three-dimensional structure of molecules in the crystalline state was provided by the pioneering work of J. Monteith Robertson who published a structure for anthracene as early as 1933 [6], with the significant comment that:

> It must be remembered, however, that the crystal molecule is far from being a free body in space.

On the other hand, the famous statement by Dirac [7] that:

> . . . the whole of chemistry are thus completely known. . .

signalled the prospect of deriving the molecular structure of any molecule by quantum-mechanical calculation.

The brave attempt [8] to formulate a quantum theory of chemistry during the period around the second world war, anticipating full development by powerful digital computing, has by now turned into an embarrassment. Despite the absolute confidence of quantum physicists in the enabling theory, the conviction of a few that it was incomplete must now be seriously re-examined.

1.3.1 Molecular Modelling

Despite the posturing of computational chemists the theory behind molecular modelling amounts to a computerized empirical generalization of the Lewis electron-pair model of a hundred years ago. This includes all quantum-chemical VB and LCAO-MO schemes, DFT and molecular mechanics.

Trying to understand what *Quantum Chemistry* is all about we may turn to one of its principal architects, C.A. Coulson. Two relevant passages from his monograph [9] put his vision and the ground rules of the pursuit into fair perspective:

> . . . the laws of quantum mechanics (of which wave mechanics is merely one particular formulation) allow us, in principle, to predict not only the electronic structure and the geometry of a molecule but indeed all of its properties.
>
> At the highest level, we attempt a highly accurate numerical solution of the Schrödinger equation; such calculations, which usually start from nothing more than a conjectured molecular geometry, are usually termed *ab initio*.

These two statements can, at best, be described as deliberate euphemisms to disguise the fact that quantum chemistry does not extend beyond a crude rationalization of the hydrogen atomic spectrum. The laws of quantum mechanics, whatever they are, do not, even in principle, allow the prediction of the electronic structure of a molecule and most certainly not the geometry and properties of any molecule, including H_2^+. This is confirmed by the second statement which admits the necessity of *assuming* a molecular structure in order to attempt a calculation at the highest level. It is fatally misleading to refer to such computations as *solution of Schrödinger's equation*. It is nothing of the kind.

The *solution* of any equation is exhaustive and excludes further alternatives. An *ab initio* 'solution' only demonstrates that a polynomial function can be constructed computationally to be apparently consistent with the assumed molecular Hamiltonian. For this to be considered a solution it would be necessary to repeat the exercise for the infinite number of alternative connectivities, permutations and configurations, consistent with the chemical formula of the 'molecule'.

The unspoken assumption that sanctifies the *ab initio* procedure is that once an acceptable level of agreement between the calculated electron distribution and the assumed Hamiltonian has been reached, the molecular structure has been confirmed quantum mechanically. This is utter nonsense, even in terms of the so-called laws of quantum mechanics. One of these, known as the uncertainty principle, forbids a fixed location for any quantum object, presumably including atoms and molecules.

Irrespective of the 'level of theory' no amount of hand waving or computing power can overcome this problem. A Hamiltonian based on a rigid, so-called Born-Oppenheimer, nuclear framework can never constitute a quantum-mechanical variable. The emperor simply has no clothes on.

Alternatively, a solution *ab initio* in terms of the Copenhagen laws of quantum mechanics must generate, not assume, the probability nuclear distribution, given the chemical composition of the target molecule.[1] Unless this can be achieved molecular quantum chemistry does not exist. Density-functional theory is refuted by the same argument.

Molecular mechanics has no such pretensions. Its only objective is to simulate a classical three-dimensional molecular structure according to the principles developed by Kekulé, van't Hoff, Lewis and others, using classical mechanics and Hooke's law. Within this formalism it serves the chemical community well, despite repeated efforts to belittle the technique for not being quantum based. In this respect it is no different from VB, MO and DFT methods, except for being honest about its theoretical background. In order to distinguish interactions of different order an unfortunate practice to label bonding types in orbital terminology, has developed, but this can be eradicated with little effort.

That orbital hybridization is a myth is now getting more widely accepted [10, 11]. It occurs most frequently to describe the interaction between first-period elements in terms of $s - p$ hybrid orbitals. According to Coulson [9]:

> …we describe each electron by an orbital, or 'personal wavefunction'…
>
> The p-functions occur in *sets of three*, each set describing three alternative states in which the electron has exactly the same energy; three such p-orbitals, which we denote by p_x, p_y, p_z are said to be *triply degenerate*.

What remains unsaid is that these p-orbitals are all **real** functions; therefore all with the same wave-mechanical quantum number of $m_l = 0$. At the same time we are reminded by Coulson [9] that

---

[1] Some science writers even claim that the molecular products of chemical reactions can be predicted quantum-chemically.

> Pauli's famous exclusion principle then takes a very simple form: *in the orbital description of an atom no two electrons can occupy the same spin-orbital.*

In any other branch of science such self-contradiction would be devastating. Quantum chemists respond that in this case quantum numbers are no longer needed, which, they forget to admit, therefore defines a classical system.

We conclude that a search for the quantum-mechanical basis of molecular mechanics is a *non sequitur*. It does not exist and there is no need for it. Still, it would be useful to have a non-empirical estimate of the variables, such as ideal bond lengths and angles, stretching and bending force constants and a measure of steric rigidity; that feature in MM force fields. Many of these are provided by the number-theory approach to covalent interaction. However, in practice there is little need of recalculating the force-field parameters which, in most applications, have been established empirically with care and suitable validation.

It does not mean that the search for a wave-mechanical model of molecular structure should be abandoned. New insight based on four-dimensional and nonlinear molecular models would be of tremendous advantage in the elucidation of chemical reactivity.

1.3.2 Atomic and Molecular Structure

The 4D equivalent of Schrödinger's equation remains to be solved. In the interim the number-theory simulation of atomic structure [12] confirms a spherical standing-wave structure of electron density as first indicated by golden logarithmic-spiral optimization [5]. The interaction between such wave structures depends on the interference of (hyper)spherical waves, which cannot be reconciled with the formation of rigid chemical bonds. The familiar structural formulae of molecules can only reflect connectivity patterns and not rigid three-dimensional structures.

We conjecture that curving of the space-time vacuum generates elementary four-dimensional distortions, which, for lack of better terminology, may be described as spherical wave packets of characteristic mass, charge and spin, summarized together by a quaternion wave function. As these elementary units coalesce into larger structures they appear as the classical objects familiar to three-dimensional observers in tangent space. Free molecules are not of this class, but molecular crystals are.

Free molecules only occur in empty intergalactic space-time. Radio astronomical analysis of Rydberg atomic spectra from interstellar space indicates electronic quantum numbers of up to 350, for atomic size of ∼6 micron and subject to strong polarization by weak electromagnetic fields [13]. Free molecules would be affected in the same way and are not likely to occur intergalactically. Stable small molecules of high symmetry are detected in dark interstellar clouds [14]. These molecules have no structure. As the concentration of matter in an environment increases, single molecules develop structure of lower symmetry, culminating in molecular crystals.

The shape of a single molecule therefore varies from a structureless 4D symmetry to a rigid 3D arrangement—from a non-classical to a classical molecule.

Intergalactic space-time is not a void, although depleted of matter in large enough concentration to cause further aggregation. The total uniformly distributed residual elementary wave structures constitute an enormous total mass which astrophysicists refer to as dark matter and energy. The mass density in interstellar space is sufficient for the condensation of clouds hot enough for the formation of primitive molecules.

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Chapter 2
The Classical Background

Abstract The development of physical science over the last two millenia is traced from the summary of Lucretius, through the early Christian era, to the transformation into critical science after Copernicus. This revolution saw the birth of physics and chemistry to replace Aristotelian authority and alchemy, guided by the principles formulated by Isaac Newton and John Dalton. The new awareness blossomed into the formulation of a comprehensive theoretical mechanics and the recognition of seventy well-characterized chemical elements to replace the four elements of antiquity.

2.1 Introduction

Modern theories of the physical sciences have developed through several refinements from ancient philosophical models and, not surprisingly, many an outdated concept has remained hidden in modern expositions. Most persistent are those that appear self-evident to the non-critical or casual observer and therefore quietly tolerated without further analysis. Some of the most debilitating inconsistencies in theoretical science are of this type and often the hardest to gainsay.

A useful strategy to weed out hidden fallacies is by historical scrutiny of the theoretical progress of science, starting from the classical roots. Most of the authentic ancient sources have been lost, but a reliable account of physical theories in Roman times (∼55 BCE) has been preserved in poetic form, as compiled by Lucretius [1]. The poem develops around six primary propositions:

(i) Nothing is ever created out of nothing
(ii) Nothing is ever annihilated
(iii) Matter exists in the form of invisible particles (atoms)
(iv) Besides matter, the universe contains empty space (vacuity)
(v) The universe consists of matter (with its properties and accidents) and of vacuity and of nothing else
(vi) The atoms are indestructible

These are augmented by two further propositions:

(vii) The universe is boundless
(viii) The universe has no centre

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The motion and shape of atoms are described by two sets of secondary propositions.

On atomic movement:

(i) The atoms are always on the move, either falling or rebounding
(ii) They move faster than light
(iii) The atoms normally curve downwards
(iv) Occasionally they swerve slightly from the vertical
(v) They were never either more or less congested than now
(vi) The apparent mobility of matter is an optical illusion

On atomic shape:

(i) The various properties of objects are due to the varieties in the size and shape of atoms
(ii) The number of atomic shapes is large but finite
(iii) The number of atoms of any one shape is infinite
(iv) All visible objects are compounds of different kinds of atoms
(v) Only certain compounds can exist
(vi) The atoms themselves are devoid of colour, heat, sound, taste, and smell, and sentience

These propositions are supported by three general corollaries:

(i) The world is one of an infinite number
(ii) Nature is self-regulating, without interference from the gods
(iii) The world had a beginning and will soon have an end

A number of important conclusions, drawn from appropriate analysis of the basic propositions, deserve special mention:

(i) The universe is not bounded in any direction. It stretches away in all directions without limit
(ii) Solid matter results from a closer union between atoms by the entanglement of their own interlocking shapes
(iii) Through undisturbed vacuum all bodies must travel at equal speed though impelled by unequal weights. The heavier will never be able to fall on the lighter from above
(iv) There is no visible object that consists of atoms of one kind only

Many of these propositions have a surprising modern ring to them, although based on a totally outdated cosmology of a flat earth in infinite space. The disturbing reality is that precisely these objectionable features again underpin the "standard cosmology" of the West. Despite the evidence from general relativity, space is still considered in the expanding universe cosmology as Euclidean (*i.e.* flat) and of infinite extent in all directions. Despite intimate experience with the electromagnetic field, the expanding universe is modelled exclusively in terms of matter moving through vacuity, precisely as presumed by Lucretius.

It would seem that apart from trivial refinement of the atomic model, the philosophical paradigm has not changed in two millenia. Where Lucretius ascribed chemical interaction to the entanglement of interlocking atomic shapes the modern quantum chemist achieves the same in terms of entangled hybrid orbitals, and with the same conviction as Lucretius.

The first millenium after Lucretius saw little change in the understanding of the physical world, except for an infusion of theological dogma and the revival of creation myths that have survived into the present as big-bang cosmology. Instead of progressing, theoretical physics regressed to the Aristotelian model, leaving it to Galileo to rediscover the Lucretian proposition of falling bodies. As the progenitor of chemistry the art of alchemy descended into mysticism and astrology.

By the end of the first millenium CE there was total consensus in the Western World over the workings of the cosmos and the odd heretic, who dared to challenge the revealed truth, could readily be disposed of. Only two problems, destined to disturb this tranquility, remained: how to make gold and where to find the universal remedy for all disease. In searching for the philosopher's stone and an elixir to end the quest, the variety of unexpected secondary products that turned up could no longer be understood within the standard model of alchemy. The emerging scepticism soon spread to other aspects of natural philosophy and it became feasible to challenge metaphysics with real physics; alchemy with chemistry. However, the development of a new scientific paradigm had to await the emergence of a new cosmology, which was initiated by Copernicus.

2.1.1 The Copernican Revolution

Mediaeval science was liberated from its paralysis, imposed by the canonized Aristotelian and Ptolemaic systems, by the new cosmology, inaugurated by acceptance of the heliocentric model proposed by Copernicus. The awkward questions that tortured Lucretius, such as the whereabouts and status of the sun at night, the cause of seasonal changes and the support structure of the earth in space, disappeared almost miraculously, although the new system was resisted by the establishment for more than a century.

The real hero of the revolution was Johannes Kepler, who supposedly [2, p. 178], murdered his superior, Tycho Brahe, in order to gain access to the data that eventually substantiated heliocentric planetary motion without epicycles. Although Kepler's three laws of planetary motion on elliptic, rather than circular, orbits[1] were, for ideological reasons, received with scepticism, they were embraced by a new generation of scientists and eventually inspired the long-awaited new paradigm. The idea of planetary orbits, stabilized by gravity, culminated in Newton's memorable work and it finally also invalidated the notion of astrological interaction between heaven and earth and its stranglehold on alchemy. The way was cleared for the development of modern physics and chemistry.

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[1] Only circles were assumed to reflect heavenly perfection.