The Quantum Gamble

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Foreword



Quantum chemistry has developed to an extent that provides scientists with detailed information for understanding structures and properties of molecular compounds and assemblies, and software has been developed that allows to compute chemical systems and their properties in good agreement with experimental observations. Theoretical and computational chemistry has become an integral part of the education of scientists, and the computation of molecular and electronic structures, relative energies and pathways for transformations is an important tool for the interpretation of experimental data and the optimisation and even the 'rational design' of new systems in many areas of chemistry. Jan Boeyens' books discuss the fundamental basis of the physics of matter and quantum theory; their basis is a deep knowledge of the history of science, and they discuss features in quantum theory that are not much remembered and not directly included in modern computational chemistry—Jan's books and ideas are not mainstream; they are disputable and therefore are interesting and scientifically important. A computational model is

not necessarily related to truth; its quality derives from the accuracy with which it simulates or predicts experimental observations. One of Jan Boeyens' concepts was to relate simplistic models as well as current computational chemistry approaches to basic notions of quantum theory. The present book summarises many of the results and hypotheses discussed in Jan Boeyens' earlier texts, and it presents these and new thoughts with as little mathematical formalism as possible: a textbook that is as general and generally understandable as possible and still fundamental, highly scientific and thorough, different from many other books in this area and therefore needs to be studied carefully, with a critical and open mind. This book was not planned to be Jan Boeyens' last book but unfortunately is—Jan died at the age of 81 just after finishing this manuscript.

Jan Boeyens was a prominent scientist in the area of theoretical and structural chemistry, very influential for the sciences in the African continent, especially South Africa, and beyond. Besides the careful analysis of hundreds of single-crystal structures, he has been deeply involved in method development for X-ray crystallography. In the early 1990s, he funded the 'Centre of Molecular Design' at the University of the Witwatersrand, a think tank and internationally visible school for computational chemistry. Jan Boeyens has also made enormous contributions to professional societies. Most of all, Jan Boeyens constantly asked important questions and was on the relentless search for their answers.

Heidelberg, Germany June 2016

Peter Comba

Preface

More than a hundred years, ago a desperate manoeuvre by a German physicist resulted in a discovery that had the world of science in convulsion ever since. His name was Max Planck and he was of opinion that science was poised as a matter of course to find solutions to all but insignificant remnants of unsolved problems. His personal concern was to elucidate the conversion of heat into radiation, using the methods and laws of thermodynamics.

His initial subtle approach, based on appropriate mathematical models, produced nonsensical results such as the production of unlimited radiation energy from a modest input of heat. As an interim measure, he resorted to brute-force simulation to reproduce experimental data, with the intention that mature reflection would, in good time, eliminate the expedient but offensive enabling assumptions. This never happened.

Planck could never formulate a clear perception of the principle behind his successful simulation. The most puzzling aspect concerned the calculation of total energy as a discrete infinite sum, rather than by continuous integration, a procedure in conflict with the energy equipartition principle of thermodynamics.

Although Planck was not the only physicist who had a problem with the new discovery, he was one of the few who kept looking for a logical explanation. His more adventurous contemporaries recognised in it the emergence of a new nonclassical 'quantum' theory to replace classical physics.

The historical development and challenges of a new quantum paradigm during the early twentieth century are described in the first few chapters to follow.

The intransigence of, particularly, the particle lobby, in trying to obliterate the proposed wave model, led to the formulation of preposterous alternative concepts like probability waves, quantum uncertainty and subjective reality, developed into sensational philosophies by neophytes and eagerly endorsed by the masses. The difficulty of disputing this traditional consensus inspired by respect for authority rather than critical analysis is addressed. While many readers may be innocently unaware of the situation in quantum theory, some parallel, better publicised, scientific disputes are discussed for comparison.

The immediate objective was an understanding of spectroscopy and the nature of elementary matter. Both aspects are of immediate concern for chemistry and physics.

The major problem with quantum mechanics emerged in the theories of chemical matter, originating in a number of ill-conceived early assumptions and complicated by equally suspect subsequent embellishments. This is the big gamble that never paid off. The dilemma for chemistry arose from an uncritical acceptance of what appeared to be some harmless concepts from quantum physics. The most lethal are the assumption of wave-particle duality and the principle of linear superposition.

It is not only chemistry that suffered. As the perceived implications of quantum theory started to sink in, the philosophies of the Victorian era suffered an upheaval, over-reaction to which inaugurated a radically modified world view that persisted for the next century. This was a century of bitter dispute about issues, such as causality, non-Boolean logic, indeterminacy, free will, reductionism, non-locality and many other quasi-scientific concepts thought to be raised by the new physics. Only now has the pendulum slowly started to swing back. The time has come to reconsider the rigid interpretational models of twentieth-century physics and to eliminate obvious misconceptions that gained respectability through frequent uncritical repetition.

The new awareness behind the critical re-examination of quantum theory, in particular, stems from the recognition of nonlinearity as an important parameter in four-dimensional curved space-time. What complicates this exposition is that the implied theoretical modification is based on aspects of mathematics, which are largely ignored in modern curricula. A strictly non-mathematical account of essential concepts may hence become not only vague and unconvincing but, in some cases, practically impossible. Wherever words fail to communicate essential detail, mathematical formulation is provided in footnotes. On skipping these, unready readers, by accepting the conclusions on good faith, may hopefully be able to follow the main argument.

A sensible reassessment of quantum mechanics as a theory of chemistry for the uninitiated should start with a re-examination of the physical theories from which the new approach developed. This topic is addressed in Chap. 4.

A perceived anomaly of modern physics is the apparent inconsistency between its two major theories. Although the theories of relativity and the quantum developed in the hands of essentially the same group of scientists, a century's worth of refinement has failed to establish their common foundation. Quantum theory, which was the first to emerge as a nonclassical model of spectroscopic phenomena, soon developed into a search for an atomic model. The theory of special relativity, which established common ground between mechanical and electromagnetic motion, clearly addressed different aspects of the same phenomena that spawned the quantum theory. The conclusions reached by the two theories, however, could not be reconciled. The main disagreement centred around the speed which mechanical objects can attain and which the theory of relativity limits not to exceed the speed of light, whereas quantum phenomena appeared to be non-locally correlated. This philosophical dispute centred around the perceived probabilistic nature of quantum matter. Schrödinger's formulation of a quantum-wave equation that could account for the electronic energy levels in the hydrogen atom and explain atomic spectra without the unphysical idea of quantum jumps never gained acceptance over the orthodoxy of dimensionless subatomic point particles. The same fate befell Madelung's interpretation of quantum effects in hydrodynamic analogy, until the ideas of quantum waves were revived by Bohm.

Experimental study of electric and magnetic phenomena during the nineteenth century showed that the spread of such interactions depends characteristically on the nature of the conducting medium, including the vacuum. The product of electric permittivity and magnetic permeability in the vacuum was found to have the dimensions of an inverse velocity squared, $\epsilon_0\mu_0 = 1/c^2$. The functional relationship between electric and magnetic fields was formulated by Maxwell as a wave equation, according to which a combined electromagnetic disturbance, such as visible light, propagates through the vacuum at the same constant velocity, *c*. The spread of a disturbance, once initiated in the vacuum, depends exclusively on ϵ_0 and μ_0 and carries no momentum imparted by the source. The inference that the motion of a light source has no effect on *c* appears to contradict the time-honoured notion of relative velocity as dictated by classical mechanics.

In order to avoid the discrepancy between relative motion in mechanical and electromagnetic systems, it is necessary to modify the classical formulation of relative motion in a given direction into a transformation that also affects the measurement of time. According to this transformation law, space and time coordinates cannot be specified independently. The transformation has the same form as an orthogonal rotation through an imaginary angle. As this rotation mathematically interchanges time and space coordinates, it means that they are symmetry related and no longer separable in the usual way. It is therefore more appropriate to deal with fourdimensional space-time, rather than the traditional three-dimensional space and absolute time.

On rotation in four dimensions, the familiar vector \mathbf{r} , which remains invariant of length $r = \sqrt{x^2 + y^2 + z^2}$ in three-dimensional rotation, now appears, in projection, to contract as it moves into the fourth dimension. This so-called Fitzgerald contraction is compensated for by dilation in the fourth, i.e. time and dimension. For objects that travel at a speed of $v \ll c$, the relativistic formulae reduce to the familiar expressions of classical mechanics. Sensible physics requires the two theories to be compatible, but the link between quantum theory and the electromagnetic field has not been identified covariantly.

Special relativity excludes accelerated motion and the gravitational field. This defect led Einstein to the formulation of a theory of general relativity. The seminal argument depends on a simple thought experiment which relies on the result of special relativity that a body in high-speed linear motion contracts but only in the direction of motion. The circumferential length of a circular object accelerated in orbital motion therefore contracts, but the radius remains unaffected.

The only explanation of this result is that acceleration distorts the geometry that fixes the value of π . It means that the geometry of space-time is no longer Euclidean but positively curved. The experimental demonstration that inertial mass (linked to

the force generated by acceleration) and gravitational mass (linked to gravitational force) are equivalent resulted in the postulate of general relativity that matter is responsible for the curvature of space, which manifests as the gravitational field.

This action is modelled mathematically by Einstein's gravitational field equations. The important feature to note is the reciprocity between a curvature tensor and an energy-stress tensor. Curvature vanishes in Euclidean space. This observation confirms that space-time must be curved in order for matter to exist.

The development of physics is intimately connected with mathematics, in both content and structure. Too many quantum chemists appear to be blissfully unaware of the way in which physical models are strictly constrained by underlying mathematical number systems. This topic is briefly introduced and the relationship between major algebras, their characteristics and the link with linear number theory is outlined. The golden ratio of number theory is recognised as the single most important characteristic of space-time curvature, which is responsible for the ubiquity of self-similar spiral structures, from atoms to galaxies, and the periodicity of matter that underpins all of chemistry.

The geometrical requirement that any pair of straight lines intersect in a single point is at variance with the Euclidean axiom of parallel lines. The problem is overcome by adding an extra point at infinity that also contains negative infinity. The result is a straight line that turns back onto itself to define an involution and projective topology of space-time.

In Chaps. 6 and 7, the methods, results and abuse of traditional quantum theory and its relationship to the theory of relativity are examined more closely. It is a far cry from general relativity that predicts the appearance of matter in curved spacetime and the rival theories of wave and particle quantum mechanics, formulated to describe atomic matter in terms of linear equations. The gradual progress towards a reconciliation of the theories has been characterised by misunderstandings, personal hostilities, professional rivalry and downright bigotry. Maybe time has dulled the original bitterness sufficiently by now for a calm reassessment of the situation.

The non-local action ascribed to wave-function collapse represents the major discrepancy between quantum and relativity theories. According to quantum theory, the components of a spin vector are linearly independent and of random orientation until measured in a magnetic field. A previously correlated pair of spins are assumed to remain governed by a single wave function as they drift apart. Whenever a measurement creates a spin component for one individual, the collapsing wave function instantaneously creates a correlated spin component for the second remote partner. Such non-local communication is prohibited by the theory of relativity.

The fallacy of this argument is exposed on noting the four-dimensional nature of spin. Not only is it described by the same rotation that represents the Lorentz transformation of relativity, but it constitutes a variable with four inseparable quaternionic components. Spin remains well defined in all directions and does not depend on any measurement. A correlated pair remains correlated, and whatever is measured on one side must be automatically valid on the remote site.

The final chapters get to grips with the objective to purge physical theory of mystical reasoning and outdated misconceptions in searching for a new paradigm

based on appropriate mathematics, sound physics and sober philosophy. The major obstacle is the modern theory of particle physics, known as quantum chromodynamics (QCD). It is the most refined form of Newton's theory of matter, as composed of point particles which interact through the mediation of 'something else, which is not material.'

The particles of QCD are identified as unobservable objects, called quarks, with fractional electric charges, held together within mesons and nucleons by more unobservable agents, with well-defined properties, called gluons. The symmetry model that avoids all exclusion complications requires a total of 61 quarks and gauge bosons (gluons) with quantum numbers characteristic of isospin, strangeness, charm and colour eigenvalues. Mass is normalised empirically.

As an alternative working model, chiral matter is assumed to occur as wavelike nonlinear distortion of the four-dimensional aether in the double cover of closed projective space-time. The antipodal involuted domain is occupied by antimatter in dynamic equilibrium across the interface.

Electromagnetism is confined to the achiral interface in the form of bosonic waves, unimpeded by aether drag as recognised by special relativity. Neutrinos and cosmic rays that pervade the cosmos as pseudo-relativistic waves provide experimental evidence of residual elementary matter not incorporated into ponderable matter.

The four-dimensional harmonic modes of elementary waves define characteristic values of spin, charge and mass as observed for bosons, neutrinos, electrons and protons.

Confined to a limited region of space-time, the number of nodes of the resulting standing waves is traditionally interpreted as a quantum number. This is the number that baffled Planck and later interpreted in many fanciful ways.

In a highly nonlinear environment, the internodal segments separate into individual solitons, identified by Einstein as photons and as point particles by particle physicists.

The book is aimed at a general readership with high-school knowledge of science and especially also at the students and teachers of undergraduate chemistry and related sciences as a red flag. As a cautionary reminder, science should be practised with a critical open mind and with scant respect for authority. What the chemistry student has to glean from quantum theory is that elementary units of matter and radiation are best described as standing waves with intrinsic characteristic properties of spin, charge and mass in line with the harmonic modes of the wave. All of chemistry can be understood as the interaction between waves.

Pretoria, South Africa

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