Realism

a continuous, deterministic and chaotic wave theory of atoms based on Schrödinger self-adjoint operator.

by

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Dedicated to the memory of

José Crespin (1907-1988)
my father

and

Rodolfo Ricabarra (1925-1986)
teacher, friend, man of genius.

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Chapter 0

INTRODUCTION

This monograph proposes a continuous and deterministic wave theory of atoms. The new theory is called *realism* and owes much to the one originally introduced by the physicist Erwin Schrödinger in 1924. Physical intuition and mathematical skill led him to formulate the quantization phenomenon as an eigenvalue problem; his insatisfaction with the path taken by wave mechanics shortly after he made his contribution is well known. We belive he was right. Similarly unsatisfied were the previous founding contributors Max Plank, Albert Einstein and Louis de Broglie. Our labour will be more than rewarded if their coherent, logical, elegant, and commonsense attitude in physics regain the acceptance they merit. The initial parts of the analysis of atomic phenomena realized by Niels Bohr and leading to the concept of atomic transition is also relevant to us from the descriptive viewpoint.

The basic ideas discussed here can be of interest for Physics, Mathematics, Chemistry and Philosophy at levels ranging from college students to professionals. Additionally there is a large number of educated readers with a growing apetite for scientific developments. Mathematicians may understand projective spaces and physicists will be accustomed to the behaviour of electrons and atoms, but in some cases one may not be aquainted with the facts familiar to the other. Therefore the discussion starts at the most basic level and gradually builds up, providing as many details as neccesary for such diverse audience.

In Chapter 1 a discussion of wave theories in general is presented. This provides background and contrast to appreciate Schrödinger's theory, quantum Theory and real theory as particular cases of a general scheme. Some less standard material about rays (see section 1.1) will play a central role and is explained at this initial stage.

In Chapter 2 the original Schrödinger wave mechanics will be discussed as a particular case of wave theory. The usual presentations consider states as normalized wave functions but here states will be rays. Based on the ray formulation the accomplishments and limitations of Schrödinger theory will be examined in detail.

In Chapter 3 quantum mechanics will be presented as it was created, that is, as a modification of Schrödinger wave mechanics. The uncertainty principle, wave-particle duality and quantum jumps will be analyzed and their role in quantism interpreted. The main feats and, in our opinion, failures of quantism will be stated explicitly.

Chapter 4 is an introduction to realism. This alternative wave theory maintains continuity and determinism. Briefly, real wave dynamics consists of the states (given as rays) and observables of Schrödinger original theory together with a new non-linear evolution equation obtained in a natural manner from the standard Hamiltonian self-adjoint operator. As the reader will be able to verify, all the results of quantism that depend only on the calculation of eigenvalues can be automatically incorporated into realism.

In Chapter 5 the formalisms of both quantism and realism are presented at a more concise and technical level than in previous chapters.

The Appendix contains an example of a simple program that illustrates the sensitive dependency on initial conditions as it appears in realism. The basic insight that eventually led to realism was provided by the mathematical theories of Dynamical Systems and Global Analysis. A deep examination of quantism and the discovery of realism would have been extremely difficult without these tools. Therefore two studies previously elaborated by the author at a more technical mathematical level have been included as addenda (not included in the e-mail version). These are an edited version of a circulated but unpublished preprint called 'Stability of Dynamical Systems and Quantum Mechanics, I' and the paper 'Projective Spectral Theorems and Deterministic Atoms' published in *Acta Cientifica Venezolana*, 38, pp 570-574, 1987. The last one contains, from the physical viewpoint, a basic study of symmetry breakdown in a magnetic field. Both addenda contain also results of independent mathematical interest.

Besides the already mentioned founders of modern atomism there are numerous contributors to the topics here discussed. Instead of attempting the colossal work of compiling a complete bibliography it is more practical to refer the reader to the on-line electronic versions of the Science Citation Index and Mathematical Reviews under the heading 'Foundations of Quantum Mechanics' or similars. It will be enough to quote here the following minimal list of

References

An elementary introduction to quantum physics is Bohm, D. *Quantum Theory*, Prentice Hall INC. New York, 1951.

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Some key historical remarks can be found in Jammer, M. *The Philosophy of Quantum Mechanics*, John Wiley & Sons. New York, 1974.

Possibly the best technical exposition of quantism is Mackey, G.W. *The Mathematical Foundations of Quantum Mechanics*, W. A. Benjamin. New York, 1963.

An already classical source for Dynamical Systems and Global Analysis is Abraham, R. and Marsden, J. *Foundations of Mechanics*, 2nd edition, Benjamin. New York, 1978.

To place the mathematical results of the addenda in perspective see Problem 10 of Smale, S. *Dynamics Retrospective- Great Problems, Attempts that Failed*, Physica D, 1991, vol 51, No. 1-3, pp 267-273.

An enjoyable attempt to understand how some scientific theories are rejected and others, say quantism, become mainstream science, see Kuhn, T. S. *The Structure of Scientific Revolutions*, University of Chicago Press. Chicago, 1962.

A less romantic but extremely refreshing viewpoint on the philosophy of science is Feyerabend, P. *Against Method*, New Left Books. London, 1975.

The reader interested in the philosophical viewpoints that inspired the author of this monograph should consult *El Cantar de Ashtavakra*, specially the last few chapters; Spanish translation by Ana D'Elia, Editorial Dédalo, Buenos Aires, 1979. There is an English version, *Ashtavakra Gita*, translation by H. P. Shastri, Shanti Sadan, London, 1961.

Chapter 1

WAVE THEORIES

1.1.-Definition of wave. Traditionally, a *wave* is any unhomogeneity or deformation of a continuous medium. When deformations have a regular shape or repetitive qualities they are generally called oscillations or vibrations, but the concept of wave is not restricted to that case. A deformation can be localized in a small region and have a rather irregular shape. The following are typical illustrative examples.

Deformations of a stretched string can be represented by numerical valued functions defined over an interval. The interval represents the string (continuous medium) and the numeric values of the function represent displacements from the resting position (physical magnitude).

The electromagnetic field is a wave in ordinary space and at each point it is defined by a pair of vectors: The electric field density vector, that measures the force exerted by the field on a charge at rest, and the magnetic density that measures the additional force exerted by the field on a moving charge. Here three dimensional vectors represent ordinary space (continuous medium) and an additional pair of vectors represent the electric and magnetic forces (physical magnitude).

The electron can be represented by means of a wave. One possible meaning of this assumption is that the electron is an extended object that occupies a volume and has a certain structure. This structure would give rise to the wavelenght and other properties of the elecron.

In order to physically define a wave the homogeneous medium and the physical magnitude of interest have to be first identified. These depend on the physical phenomena under study. The homogeneous medium can be space

or space-time, a gas, a liquid, a solid, etc. The physical magnitude can be gravitational or electromagnetic force, pressure, velocity, displacements, etc. The particular formalism used to describe the waves is the *kinematics* of the theory under study. Two classes of theories will be relevant for us, depending on the kinematics.

The first class is related to the need for standard units of measurement in applied science and engineering. This is the class of theories with a *linear kinematics* or *wave function kinematics.* Consider a scalar physical magnitude, that is, a magnitude whose values have one degree of freedom. A unit of measurement is chosen and the wave is then specified indicating, at each point of the medium, the ratio of the magnitude to the unit. The result is a *(scalar) wave function.* Note that this wave represents a physical object or situation only when the chosen unit is specified. On the other hand, physical phenomena are intrinsically independent of choice of units. Units are conventional technological objects.

In the more general situation of vector or tensor magnitudes (the values of the magnitude have several degrees of freedom) a set of numbers instead of a single number is required. The result is a *vector wave function* or a *tensor wave function,* as the case may be. These scalar, vector and tensor wave functions can be added and multiplied by scalars, that is, they form *linear spaces* (also called *vector spaces*) which is the reason for the term 'linear kinematics'.

Since ratios have been mentioned above, the following comment is in order: usually a ratio is a real number. It is the case, however, that sometimes complex numbers are considered, as with the impedance of an electrical circuit. Therefore ratios have to be understood as either real *or* complex numbers. See the end of this section.

The second class of theories can perhaps claim older historical roots, arising more directly from the classical ideas of proportionality. These are the theories with a *projective kinematics.* A projective theory specifies waves independently of the choice of units. After the continuous medium of interest is singled out, rather than the ratio to a chosen unit one considers the *relative ratios* of the physical magnitude at pairs of points in the medium; these

relative ratios are independent of particular units. The result is a *scalar ray* or simply *ray.* Rays are collections of wave functions. Wave functions and rays are related as follows: Any wave function that is not identically zero defines a ray. Two wave functions define the same ray if they differ by a constant factor. Finally, all rays are obtained in this way. A wave function and the ray it defines are *associated* to each other.

In standard mathematical notation, if ψ is a wave function then the associated ray is denoted $[\psi]$ with

$$[\psi] = \{\lambda\psi | \lambda \in scalars\}$$

The term 'projective' comes from certain relations to Projective Geometry. A projective space is a classical mathematical object constructed as the set of lines through the origin in a linear space. But two points in the linear space lie in the same line through the origin whenever one is a scalar multiple of the other. Therefore the rays defined above are the elements of the projective space associated to the linear space of wave functions. Furthermore, lines through the origin can also be portrayed arrows emanating from the origin, and this is the reason for calling $[\psi]$ a ray.

Since rays are ratios of values of a physical magnitude, the magnitude cancels out and only the numerical ratio remains. Hence, rays are *physically dimensionless.* They will play a central role in the critique and proposals below.

Rays can also be considered for physical magnitudes with more than one degree of freedom; in this way *vectorial rays* and *tensorial rays* are obtained. However, only the case of one degree of freedom will be necessary; the vectorial and tensorial rays will not appear in our discussion.

On the other hand, two classes of scalars will be used: Real scalars (real numbers) and complex scalars (complex numbers). Complex scalars appear in Schrödinger theory and in quantism; note that there is no clear or simple physical justification for their introduction. But the previous considerations about wave functions and rays are valid both for real scalars and for complex scalars.

1.2.-Continuity of waves. Continuous waves occur in continuous, extended media. Continuous media are built from infinitely many points arranged in such a way that if one point is singled out then, arbitrarily close to this one, other points can be found. This description does not categorically determine the continuous media generally used in physics, but a detailed discussion requires mathematical concepts like topological spaces and differential manifolds, which are beyond our present limits. For our purposes it suffices to state that intervals, curves, surfaces and regions in ordinary three dimensional space are continuous media.

Consider now a wave or unhomogeneity on a continuous medium. In linear kinematics this wave consists, once a unit is chosen, of values of a physical magnitude associated to points of the medium. The values vary according to the point being considered. The wave is continuous if the following holds: Whenever two points approach becoming close to each other then the values of the magnitude at these points become close as well, and as the two points merge into a single one the corresponding values become equal.

In projective kinematics a wave is continuous if one of the wave functions associated with the ray is continuous.

1.3.-Spaces of states. The mathematical description of a particular wave or unhomogeneity is called a *state* and all states taken together form the *space of states.* Therefore the space of states is the collection of all conceivable configurations the deformable medium can adopt.

Recall that in linear theories the space of states is the collection of all wave functions, and this is provided with the operations of sum of wave functions and multiplication of wave functions by scalars. Also, these algebraic operations give to the space of states of a linear wave theory the structure of a linear space.

In projective kinematics the space of states is the collection of all rays. Note that the operation of sum of rays *cannot* be defined in a consistent manner. Therefore the space of states of a projective theory is a non-linear space. This non-linear space is a projective space as explained in section 1.1. Mathematically, the non-linearity of projective spaces is an unavoidable consequence of

their global topological properties.

Note that since scalars can be real numbers or complex numbers, there are so far in our discussion four possible types of spaces of states: Real linear, real projective, complex linear and complex projective.

1.4.-Observables. The second ingredient of a wave theory are the various scalar magnitudes that can be associated to states. Recall that a wave can present diverse peaks, wells and anfractuosities, being in general a complicated structure. It is therefore convenient to make abstraction of details and consider simple numerical magnitudes that nevertheless give relevant information on the wave. An *observable* is a function of state, that is, a rule that assigns a number to each wave.

1.5.-Energy. In this discussion the most important observable is energy. The following simple physical definition will be adopted here: The *energy* of a wave is its capability to produce movement. Since all forms of energy are assumed interconvertible and equivalent other definitions are possible, but the above seems well suited to our ilustrative purposes.

The *kinetic energy* is the energy the wave directly posseses by virtue of its translational velocity. It depends on the reference system used to measure the velocity.

The *inner energy* of a wave is the energy the wave has due to its particular form. The following example clarifies the concept. A motionless spring can be compressed, distended or flaccid; in the last case the inner energy is less than in the others. This form of energy is intrinsic to the configuration of the object.

The *potential energy* is the one attributable to an interaction between the wave and other entities. It happens that this interaction implies a possibility of movement and the potential energy is the energy the wave would gain if the possible movement actually happened. Thus, a rock at the top of a hill has potential energy due to its interaction with the Earth. If the rock falls the potential energy effectively becomes movement.

The *total energy* is the sum of the various energies under consideration. For example, if only the internal and potential energies are relevant then the total energy is their sum.

1.6.-Conservation of energy. As waves change in time their energy may change, but the process is always subject to the *Principle of Conservation of Energy.* This principle says that if the energy of a given physical system decreases then the energy of some other system increases by an equal amount. Conversely, if the energy of a system increases then in some other system the energy decreases. This applies in particular to wave systems. For example, a vibrating string in a violin has energy and as the vibration decreases the string energy becomes less. However, the energy has not dissapeared; some was transmitted to the air as sound vibrations, some became heat and produced a temperature increase in the string, etc.

In the last analysis the principle of conservation of energy does not apply to partial systems but rather to the Universe as a whole. The reason is that any known portion of the Universe interacts with its exterior and the interaction implies energy exchange. If some strictly closed and isolated system exists then it is not accessible to our physical knowledge.

Many systems can be studied theoretically assuming that they are isolated; in this way useful approximated descriptions of their behaviour can be found. An important advantage of these idealized treatments is their relative simplicity.

1.7.-Wave movement. Movement of a wave means its change as time goes on. Hence, a wave that occurs in three dimensional space can stay motionless, can move in a rectilinear path with uniform speed, rotate, modify its shape, etc. or can simultaneously undergo several of these transformations.

1.8.-Continuity of movement. The continuity of wave movements will be considered now. The continuity of a wave was explained in section 1.2. Continuity reappears now but in a different context. While formerly the continuity properties of waves themselves were discussed, now the discussion refers to the continuity of the process of wave movement.

Consider a moving wave and the pair of configurations adopted by the medium at two instants. The movement is *continuous* if whenever the two instants are close enough in time then the configurations are more similar and close to each other, becoming the same as the two instants merge into a single one. This property must hold all along the process. If at some instant it fails then the wave takes at that instant a shape that cannot be approximated by shapes adopted at nearby instants.

The continuity of the process is important because it establishes a relationship between cause and effect. If the wave is modified in a sudden and discontinuous way it could not be said that the final wave comes from the initial one, the connection between them is broken and it does not make sense to say that the initial wave produced the final one. Therefore, in a hypothetically discontinuous movement the connection between cause and effect is broken. The initial wave (cause) is just an antecedent in time to the final one (effect) without a causal relation in between.

Furthermore, the hypothetical existence of strictly discontinuous changes in the configurations adopted by a supposedly continuous medium creates problems about the nature of the continuity of the medium.

Within the same circle of ideas, a finite physical wave that transforms itself by means of continuous movements cannot suddenly cease to be an extended wave and become a particle, that is, a point-like infinitely small object.

1.9.-Continuity as a doctrine. It is possible to raise physical continuity to the level of a doctrine. This continuistic doctrine states that if in the study of an object or phenomenon discontinuities appear, these are due to simplifications (no doubt useful) that allow to ignore finer details or deeper levels in the problem at hand. Therefore, doctrinary continuity assumes that it is always possible to find an appropiate level where the object or phenomenon will show its continuous character. For example, the initial idea of action at distance leaves an empty gap (discontinuity) between gravitationally interacting bodies. Curved space-time postulated by general relativity provides a continuous medium (space-time itself) whose continuous unhomogeneity (curvature) fills the gap and provides a physical model more acceptable to continuism.

Similarly, it would be more satisfactory if some continuous medium could be clearly defined whose unhomogeneities constitute electromagnetic radiation. This hypothetical medium is known as 'luminiferous ether' and is still an open problem.

From the previous section it follows that doctrinary continuity is related to a general conception of the way in which causes relate to effects: The cause has to actually become the effect and this should happen in a continuous way.

The ultimate foundation of the continuistic doctrine is the belief that the physical universe has an everywhere continuous structure. This belief, as well as its opposite (that the universe is essentially discontinuous) or any other equally general doctrine, cannot be disproved. This type of doctrine, unavoidable inside and outside science (scientific paradigms, religions, political or economical creeds, etc.) cannot be rigurously demonstrated nor refuted. Their acceptance is always a convenience or an act of faith.

1.10.-Determinism of wave movement. When a given initial wave moves, it modifies its shape and a continuous succession of new waves is seen to arise. The waves in the succession are the new shapes successively assumed by the initial wave. Suppose that the medium can be reset to the initial wave whenever necessary. The movement is *deterministic* if each time the medium is reset to the same initial wave then the same continuous succession of configurations is generated. Therefore, if the succession is not the same then the initial wave could not have been the same.

To make these considerations valid in general it may be necessary to extend the concept of state to include the speed of the wave, its acceleration or other relevant factors, as in classical mechanics the state of a material point includes not only its position but also its velocity or momentum.

If a coin is thrown several times with exact repetition of the initial setting then the same side turns up in all instances: Adequate control of relevant conditions transform an apparently random phenomenon in a deterministic one. This can be extrapolated to the following hypothetical situation: If the Universe is reset to some past moment with all its parts occupying exactly

the same relative states then, physical laws being equal, exactly the same events and history would repeat themselves again.

Metaphorically, according to determinism, the same way of playing the violin should produce the same music. If the music is not the same then the string, the fiddling, the air, the listener or something else should have changed.

1.11.-Determinism as a doctrine. The deterministic doctrine centers on the general belief that past states of the whole Universe determine the present one and that the present state determines the future ones. The relevant point is that the succession of states unfolds in a way that is, in principle, unique and necessary consequence of the initial state. In other words, and repeating the extrapolation of last section, future states of the Universe will be necessary consequences of the present state as well as the present is an unavoidable outcome of past states. A remarkably lucid and famous metaphor of determinism is due to P. S. Laplace from which the term 'Laplacian determinism' arose.

A wave mechanical formulation of determinism considers the Universe as an immense unhomogeneity with extremely varied structure. The states of the Universe are then configurations of this hypothetical universal wave and what was said in the previous paragraph about states of the universe applies to this wave.

When referred to a limited system or portion of the Universe determinism can often show partial validity only. But ample historical experience supports the viewpoint that whenever determinism apparently fails it is in general possible to extend the system under consideration and find contingencies responsible for two seemingly identical initial configurations to produce disparing results.

For example, certain standard routine initial conditions are always assumed at takeoff time for airplanes. The airplane is then expected to reach its destination. But if a crash happens, the assumed routine initial flight conditions have produced an unexpected result. A search is then launched to find the cause, that is, to find the relevant initial differences responsible for the accident. Various possibilities are considered. Mechanical or structural failure, human error, insufficient fuel and similars could be causes localizable in the

immediate vicinity of the airplane at takeoff time. A storm near the destination point, a colliding object and other contingencies could be far away from the airplane at takeoff time, hence in this case the explanation requires an extension of the initially considered system (airplane) to a larger one (airplane and atmospheric conditions or objects at far away places). Even if experts disagree about the possible cause of the accident they share a deeply rooted belief that the cause exists. This sought cause is the difference in initial conditions that produced the unexpected outcome.

Determinism is still the foundation stone of scientific theories. The reproducibility of phenomena is an essential requisite to establish the so called scientific truths. Since the advent of quantism this important principle has been partially neglected.

1.12.-Evolution laws. As a third and last component of a wave theory, a *dynamics* or *evolution law* is required, that is, a rule that tells exactly *how waves move.*

It is possible to theoretically conceive many different continuous and deterministic evolution laws. In principle there are countless evolution equations. Continuity and determinism are not enough to specify a process. In a wave theory the specification of the dynamical law or precise way in which waves move is made mathematically, in most cases, by means of partial differential equations. If the equation can be solved it then provides an explicit formula which specifies the continuous sequence that unfolds from each initial wave; this formula is called a *flow.* In the wave theories relevant to our discussion this continuous wave sequence contains also all waves that preceded the given initial wave. This manner of specifying the process is explicit and exhaustive. The posterior future and the previous history of each configuration are completely known in the style of Laplacian determinism.

In linear kinematics the symbolism of wave dynamics is as follows. If ψ is a wave function at a given instant and t indicates a time interval then $\psi^{(t)}$ or $U_t\psi$ symbolizes the wave function that (according to the equations) arises from ψ after time t has elapsed. So, if ψ and t are given data, the explicit formula mentioned above allows the calculation of $U_t\psi = \psi^{(t)}$.

The evolution laws of theories with projective kinematics can in general be obtained from the evolution laws of theories with linear kinematics. So, when dealing with projective dynamics it will be assumed that it comes from an evolution law U_t given for the corresponding linear kinematics. In formal notation, if $[\psi]$ is a ray at a given instant and t indicates a time interval then the new ray after time t will be $[U_t\psi] = [\psi^{(t)}]$.

1.13.-Interpretation of theories. A wave theory is made up of methods to study a more or less wide class of wavelike phenomena by means of the mathematical construction of spaces of states, observables and evolution laws. These correspond roughly to possible shapes or configurations of the objects under study, properties of these objects that can be associated to numbers and behavior or way the objects move, respectively. The states-observables-evolution scheme has a general character and applies to other physical theories, not necessarily wavelike, as is the case with Newtonian classical mechanics or Hamiltonian classical mechanics.

But for one of these mathematical constructions to be understood as a physical theory it has to be linked to the 'physical world' by means of a semantic element: An interpretation is conventionally required in order to provide some of the mathematical entities with a 'physical meaning'.

The interpretation seems necessary because the same mathematical object can represent different physical situations. For example, if a vector (mathematical entity) is associated to each point in three dimensional space, a wave is defined; the wave can represent displacement, speed, acceleration, electric force, etc., depending on how it is interpreted.

The interpretation gives a specific physical meaning to one or more mathematical objects of the theory and is the link that binds the precise abstractions of mathematics with the less precise abstractions of physics and eventually with objects in the 'real' world. The ultimate nature of these objects is neither physical nor mathematical and seems unsolvable or inaccessible under these schemes.

However, not all the mathematical componenets of a physical theory have an obvious interpretation. In the case of theories with a projective kinematics

the rays are physically dimensionless quantities and therefore any possible physical interpretation of the wave function will cancel out at the level of rays and will not appear explicitly in the theory. Thus, for projective theories, interpretation of the rays $[\psi]$ is not possible and interpretation of the wave function ψ seems unnecessary or useless (and also harmless) since it will affect neither the kinematics nor the dynamics. But some component of the theory must have a physical interpretation. If there is no link with the 'real' world the theory is only mathematical and not physical. Some connection with physical magnitudes is always necessary. For example, time t is a physical magnitude that appears in all theories with a dynamics. Also, the quantity defined by equation 16 below is interpreted as energy and this makes the theory of Chapter 4 a physical theory.

1.14.-Diversity of wave theories. Many wave theories exist. They are used to study sound, heat, fluids, electromagnetism, etc. The theories differ according to their various spaces of states, observables, dynamical laws and interpretations.

1.15.-Validity criteria. No physical theory so far known is universally valid. Each applies to a restricted or particular universe of discourse.

A wave theory is considered more or less correct depending on the degree of concordance between the physical wave (that exists and changes as an object in the physical world) and its behavior predicted theoretically by means of the mathematical constructions and equations.

The case can arise of two theories with more or less similar predictions. If the theories are not equivalent it is necessary to elaborate their differences up to a point where distinct and experimentally verifiable predictions are obtained. Once that level is reached the realization of experiments should decide in favour of one. If the predictions are identical or the experiments cannot resolve the matter then the simplest theory should prevail.

Theories are also expected to be free from contradictions. This means that within the realm where the theory applies an object will not posses incompatible qualities.

Of extreme importance and far above other aesthetic considerations, is the simplicity of the theory. Regardless of being a seemingly subjective criterion, it has had, and can be expected to keep having, great importance in the elaboration and acceptance of models of the world.

CHAPTER 2

SCHRÖDINGER WAVE MECHANICS

2.1.-Schrödinger waves. Schrödinger wave theory studies atoms considering the electrons as waves. These waves happen in three dimensional physical space. They are mathematically specified assigning to each point a complex number, that is, the wave is specified by a *complex valued wave function* or *Schrödinger wave function*

$$\psi : \mathbf{R}^3 \to \mathbf{C} \tag{1}$$

The space of states is then a complex linear space. But, as will be shown below, it is possible and convenient to modify Schrödinger theory to represent the electron as a ray in the sense explained in section 1.1. See section 2.4 below.

2.2.-Interpretation of Schrödinger of wave functions. A Schrödinger wave function specifies for each point in three dimensional space a complex number. A complex number is also a plane vector; a new wave function can be defined assigning to each point the square of the length of this vector. The new wave function, denoted $|\psi|^2$, is the *amplitude* of the original wave; the values of the amplitude are not arbitrary complex numbers but rather they are positive or zero real numbers.

The amplitude was interpreted by Schrödinger as an *electric charge density*; see Jammer, M. *The Philosophy of Quantum Mechanics*, John Wiley & Sons. New York, 1974., page 24. This means that the electron is considered as a charge continuously distributed over space in such way that at points where the amplitude takes larger values the charge is more intense and concentrated. Similarly, at points with lesser values the charge concentration is more tenuous and diluted. This interpretation can be justified appealing to formulas from Electrostatics.

The wave function itself, as distinct from its amplitude, was not interpreted

by Schrödinger. Neither has quantism solved the problem of interpreting the wave function (there is however a quantum interpretation of the amplitude; see section 3.2).

Summing up, the amplitude of a wave function represents in Schrödinger theory an electric charge continuously distributed in space: The 'electronic configuration' or 'electronic cloud'.

2.3.-Waves vs. particles. The wave function ψ and its amplitude $|\psi|^2$ are entities that occupy a volume in space; in fact they usually occupy the whole space (have non-zero values almost everywhere). Therefore there is an extreme disparity between these extended objects and the material points of classical mechanics or the point charges in electrostatics (infinitely small particles). However, waves that represent microscopic particles are usually localized in a relatively reduced region of space. This means that although both the wave function and its amplitude extend theoretically everywhere, its values outside the region are extremely small relative to the values inside the region.

The question arises of the advantages gained studying a microscopic particle by means of waves, when it could be more practical to simplify the problem and consider instead the physical particle as an infinitely small point. The answer is, first, that knowledge expects a representation as exact as possible of its objects and if the electron, an ever present component of matter, is in fact an extended object with structure, we want to know it as such. Second, the detailed structure of Schrödinger waves is crucial to understand basic facts like the periodic table, crystal structure, chemical afinity, etc.

2.4.-Schrödinger rays. Schrödinger theory will be now formulated in terms of rays. As a preliminary step, passage from wave functions to rays can be justified with a physical argument. The total charge is assumed constant and the same for all electrons and, if taken as unit, the sum of the wave function amplitude, or more precisely the integral over three-space of the wave function apmitude, should be equal to 1. This is the *normalization condition.* Furthermore, if the charge distribution is the physical state, two waves differing in a phase, that is, in a complex factor of unit modulus, correspond to the same physical state. This means that when states are

represented by linear waves a redundancy is present.

It is possible both to normalize and to eliminate the phase redundancy in a single step if wave functions that differ in a non-zero complex factor are considered equivalent. Hence the states should not be wave functions ψ but rather classes of wave functions; each class $[\psi]$ is made up from the wave function ψ and all its non-zero multiples. These classes are precisely the rays of section 1.1. Therefore it is more natural in Schrödinger theory to represent the physical states of the electron by means of rays associated to the complex wave functions; these can also be called *Schrödinger rays*. Quantum mechanicists often call them *Hilbert rays*. As a consequence the natural space of states in Schrödinger theory is a complex projective space. Complex projective spaces have been the subject of extensive study in several branches of mathematics; see section 5.15 for details. Representing physical states by rays can be considered as a simultaneous renormalization of all states.

In most presentations of Schrödinger theory and quantism the question of equivalent wave functions is seldom mentioned; in the exceptional sources where it is mentioned little use is made of it. This is equivalence is a very important detail for if the redundancy mentioned in section 2.4 is mantained then the evolution equation (see below) is linear, while if the redundancy is removed by passage to rays and projective spaces then the the evolution equation is non-linear. Also, stationary states are motionless only in the projective theory while in the linear theory they are endowed with a periodic oscillatory motion.

In conclusion, it is possible to reformulate Schrödinger wave mechanics in such way that states are the Schrödinger rays and the space of states is the complex projective space associated to the linear space of complex valued wave functions. The interpretation of wave amplitudes as charge densities requires then a modification. In the ray formulation $|\psi|^2$ is a *relative* charge density. See the discussion in section 1.1

2.5.-Energy of Schrödinger rays. The basic observable in our discussion is the energy. Generalities about the energy of waves were discussed in section 1.5. The mathematical formulas for the energy of Schrödinger rays will be

stated now.

The *internal energy* of the ray $[\psi]$ is

$$\frac{\int |\nabla\psi|^2}{\int |\psi|^2} \tag{2}$$

and this is equal to

$$\frac{(\int \nabla^2\psi)\,\bar{\psi}}{\int \psi\bar{\psi}} \tag{3}$$

This expression has traditionally been called 'normalized mean value of the kinetic energy' of the wave, instead of the more natural 'internal energy' adopted here.

The potential energy is given by

$$\frac{\int U|\psi|^2}{\int |\psi|^2} \tag{4}$$

which can be expressed as

$$\frac{\int U\psi\,\bar{\psi}}{\int \psi\bar{\psi}} \tag{5}$$

The potential energy of the electron depends on objects interacting with it (a proton for the hydrogen atom) and this is taken into account by means of the function $U = U(x, y, z)$ that appears in the previous formula.

The total energy of the wave is then equal to

$$\frac{\int (-\nabla^2\psi + U\psi)\,\bar{\psi}}{\int \psi\bar{\psi}} \tag{6}$$

The mathematical expression

$$H = -\nabla^2 + U \tag{7}$$

is called the *Schrödinger operator* and can be used to formally reformulate the total energy as

$$\frac{\int H\psi\,\bar{\psi}}{\int \psi\bar{\psi}} \tag{8}$$

and this can be further expressed as

$$\frac{\langle H\psi, \psi\rangle}{\langle \psi, \psi\rangle} \tag{9}$$

For an explanation of this notation see section 5.1.

2.6.-Schrödinger evolution law. In Schrödinger wave mechanics the movement of wave functions is described by Schrödinger evolution equation:

$$(-\imath h)\frac{\partial \psi}{\partial t} = -\nabla^2\psi + U\psi \tag{10}$$

where h is Planck constant. Note the imaginary unit $\imath$, $\imath^2 = -1$. In terms of the Schrödinger operator the evolution equation can be written as

$$(-\imath h)\frac{\partial \psi}{\partial t} = H\psi \tag{11}$$

A wave function initially equal to ψ will move in the continuous and deterministic way specified by this equation to become, after time t, equal to a certain wave function $U_t\psi$. At the more exact level of the rays, a physical wave initially equal to $[\psi]$ becomes $[U_t\psi]$. So, as explained in section 1.12, the time evolution at the linear level induces the time evolution at the projective level.

A general basic description has been given so far of states, their interpretation, the energy observable and the dynamical law of Schrödinger theory. Note however that the projective kinematics presented here was not used in the original formulation. Instead of a projective space the 'unit sphere' of the space of wave functions was used by Schrödinger and there a phase redundancy remains.

2.7.-Conservation of energy. When waves move according to Schrödinger evolution equation they do so in the continuous and deterministic way already explained and, additionally, energy is preserved during movement. Hence, the mathematical models proposed by Schrödinger wave mechanics are models of physically isolated and energetically closed systems.

2.8.-Atoms and photons. Some properties of matter and light will be discussed now.

Matter gives and takes energy in the form of light. Ordinary matter is constituted by many microscopic atoms and light is also made up of a large number of individual microscopic entities, the photons.

In empty space photons travel in straight line and they all have the same speed. But photons are not identical. They differ, besides other things, in their energy content. Different energies correspond to different colours. The various colors that make up a light ray can be separated by means of a prism and they come in the sequence red, orange, yellow, green, blue and violet; this is the order of increasing energies. There is also infrared and ultraviolet light invisible to the naked human eye. The study of the energies (colors) of the light emmited and absorbed by objects gave rise to Spectroscopy.

During emision and absorption of light, atoms and photons interact individually with each other. On the other hand, due to the extremely small size of both atoms and photons their direct experimental study as individual objects is rather difficult. For example, instead of an individual atom large collections of atoms are considered, say, a gas in a glass enclosure. If the enclosure is provided with electrodes an electrical current can be passed through the gas and it becomes incandescent. This is the way neon lights work. The many atoms in the gas emit then many photons and the individual emissions are amplified in this way. When the light emited by the gas passes trough a prism and strikes a screen the emision of very many photons of a certain energy can be inferred from the presence of a corresponding color.

The fact to be underlined is that the light emited by the atoms of a particular element does not contain all colors. When separated by the prism instead of a complete rainbow only a few colors show up forming narrow bands known as spectral lines. Each element has a characteristic sequence of spectral lines that constitute its *spectrum.*

If colors are reinterpreted as energies it can be concluded that atoms do not emit photons with arbitrary energies but rather they form a discrete and well defined succession characteristic of the element. This is the remarkable phenomenon of *discretization of energy* at atomic level. A similar discretization appears in energy absorption processes.

2.9.-Schrödinger description of a hydrogen atom. In order to examine atomic spectra along the guidelines of Schrödinger wave mechanics it will be assumed that the atom under consideration is of the simplest element, that is, a hydrogen atom.

The hydrogen atom is normally made up of one proton and one electron. The proton has positive charge and is the nucleus or central part of the atom. The electron has a negative charge and occupies the periphery. The charges have opposite signs but the magnitude (absolute value) of the proton total charge equals the one on the electron. On the other hand the proton mass is about 1830 times the electron mass.

Protons and electrons interact by mutually attracting each other. In Schrödinger wave mechanics the proton presence is taken into account by means of the potential energy it provides to the electron; see sections 1.5 and 2.5. Thus, the proton is represented by means of an electrostatic potential $U(x, y, z)$ which in the more elementary cases does not change with time. This potential is a mathematical way to express the fact that the proton attracts the electron with an electrical force that is inversely proportional to the square of the distance and pulls towards the proton center from all directions (spherical symmetry).

The electron is represented by means of a ray $[\psi]$. Therefore, when Schrödinger viewpoint is adopted the electron is considered as a structured and extended object that occurs in space.

The energy of the atom, that is, the energy of the proton-electron system, is the total energy of the wave $[\psi]$ as given by formulas 8 or 9 in section 2.5.

2.10.-Movement of atoms according to Schrödinger. Based on the equation he postulated for wave movements Schrödinger studied his model of the hydrogen atom making a detailed analysis that revealed the following.

The waves $[\psi]$ fall into two categories: motionless waves that are usually called *stationary states* (*stationary waves, proper states, eigenstates*) and waves in permanent movement.

Mathematically a wave $[\psi]$ is motionless if $[\psi] = [U_t\psi]$ for all times t. Stationary waves are electron configurations that are locked in themselves and unable to move. Non-stationary waves are endowed with a movement that in theory obeys Schrödinger evolution equation.

There are infinitely many motionless waves and these can be enumerated

$$[\psi_0], [\psi_1], [\psi_2], \ldots, [\psi_n], \ldots \tag{12}$$

The energies of the stationary waves are called *stationary energies* (or *eigenvalues*) and can be similarly enumerated

$$-\lambda_0 < -\lambda_1 < -\lambda_2 < \ldots < \lambda_n < \ldots < 0 \tag{13}$$

These energies are negative numbers due to conventions that give negative values to the energy of an electron when it is bound to a proton.

In order to mathematically calculate the stationary waves and stationary energies it is necessary to solve the *Schrödinger eigenvalue equation*:

$$-\nabla^2\psi + U\psi = \lambda\psi \tag{14}$$

or equivalently

$$H\psi = \lambda\psi \tag{15}$$

and once this is done the above enumeration of stationary states and energies follows.

Figure 1 on page 37 shows the results of the calculations for the case of the hydrogen atom. The stationary energy values are shown arranged in a column from higher values (top) to lower ones (bottom). A horizontal line has been drawn for each stationary energy. The arrows represent transitions; these are discussed in section 2.12.

The state $[\psi_0]$ with lowest possible energy is the *fundamental state* or *base state*; all other states have higher energy and whether or not stationary they are *excited states*.

Schrödinger analysis actually shows that for each excited stationary energy there are not one but rather several stationary states. More precisely, instead

of a single stationary state $[\psi_n]$ with energy $-\lambda_n$ there is a full $(n+1)^2$ dimensional vector space E_n of eigenfunctions, the *eigenspace* of $-\lambda_n$. The eigenvalue $-\lambda_n$ has multiplicity $(n+1)^2$. This is related to representations of the group of rotations of ordinary 3-space.

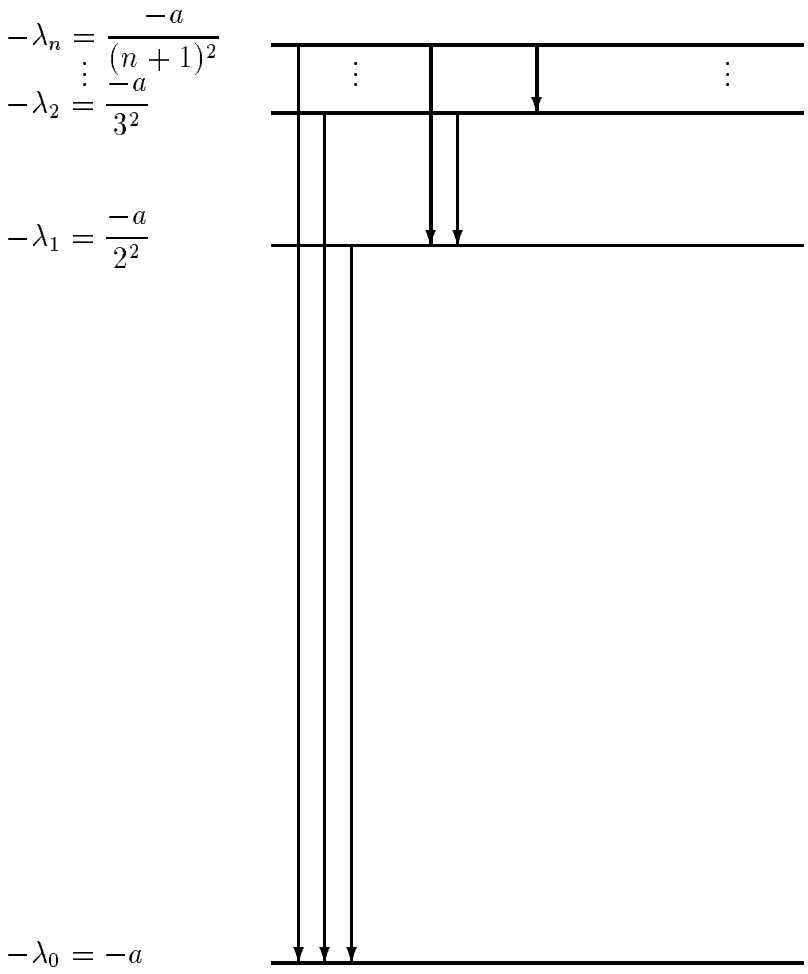

Figure 2.10-1. Stationary states and energies of the hydrogen atom

It follows that stationary states form a $((n+1)^2-1)$-dimensional complex projective subspace namely $PE_n = \{[\psi] | \psi \in E_n - \{0\}\}$. The dimension-

ality of these subspaces show up physically in phenomena like Zeeman and Stark effects. Such effects are referred to as 'symmetry breakdowns' and mathematically correspond to splittings of the multiple eigenvalues and to bifurcations of the projective flow. The interesting dynamics of the Zeeman effect is discussed, from the viewpoint of realism, in Crespin, 'Projective Spectral Theorems and Deterministic Atoms', *Acta Cientifica Venezolana*, 38, pp 570-574, 1987, referred later as [PST].

According to Schrödinger equation, electron movement in the hydrogen atom happens without change in the energy content of the wave and this is equivalent to consider the atom as an energetically closed system.

For atoms of other elements as well as for molecules similar theoretical results have been derived from Schrödinger theory; the potential and the number of electrons are changed as the case may be, arriving to other stationary waves and energy values.

2.11.-Relation of theory to experiment. The spectral lines of hydrogen, as seen in experiments, and Schrödinger theoretical calculations, are related in the followig way: The photons emited by the hydrogen atom have energies equal to differences of eigenvalues. For many other atoms and molecules similar calculations have been performed with results that agree with experimental results.

2.12.-Transitions. The relation pointed out between the the theoretical calculations and photon energies is compatible with the following hypothesis about electron behavior: The electron is a wave that, when motionless, adopts the shape of a stationary wave, as calculated from Schrödinger theory. Its movements consist in the passage from a stationary state to another one. These movements imply photon emision or photon absorption. Atoms either decrease their energy by an amount equal to the energy of the emited photon or increase it by an amount equal to the energy of the absorbed photon.

For if the electron is assumed to be in state $[\psi_m]$ its energy equals $-\lambda_m$, and if it moves to state $[\psi_k]$ the new energy will be $-\lambda_k$ so that the energy change equals the difference $\lambda_m - \lambda_k$ between the stationary energies. As pointed out before, these are the energies that, according to experiments, the emited

and the absorbed photons have.

The movement from a stationary wave to another one with a different energy is a *transition*. According to the hypothesis above, when transitions occur the atom emmits or absorbs photons.

The transition hypothesis is a fundamental descriptive contribution due to Niels Bohr. It can be reformulated as follows:

ELECTRONS IN ATOMS ARE WAVES THAT TEND TO ADOPT THE SHAPES OF STATIONARY WAVES. ELECTRON MOVEMENTS CONSIST OF TRANSITIONS.

The transition hypothesis is extremely simple and gives a reasonable description of the way atoms behave. But the description is incomplete because it does not specifies the particular way in which the waves move while transitions happen. It only says that transitions are movements between stationary states and there are, in principle, infinitely many process that carry one stationary state to another one. Now, in Schrödinger wave theory, *all* waves move at *all* times in a very specific way, that is, according to Schrödinger evolution law. In particular, as transitions occur waves have to move according to that law. As will be seen in section 2.14, this made Schrödinger wave mechanics fail.

Summing up, the electron is a stationary wave except when making transitions. As result of transitions the atom emits or absorb photons. Arrows in Figure 2.10-1 indicate transitions.

2.13.-Success of Schrödinger theory. Schrödinger wave mechanics is a general theoretical system from whose equations atomic stationary energies can be deduced. This is its paramount initial accomplishment. Furthermore, the theory defines and allows the calculation of stationary states and these provide a comprehension of various phenomena like chemical bonds, the structure of the periodic table, the disposition of electrons in molecules, etc. For the first time an accurate theoretical image of how stationary electrons look like in atoms became available.

2.14.-Failure of Schrödinger theory. As already explained (sections 1.7

to 1.12) waves generally evolve in a continuous and deterministic manner; this happens in Schrödinger theory. Such behaviour of waves is natural and expected. And furthermore, in Schrödinger theory waves move mantaining constant energy. See the end of section 2.10. However, when photons are emited the electrons lose energy; similarly, when photons are absorbed their energy increases. But if atomic electrons are waves that obey Schrödinger evolution law they should move without ever changing their energy and therefore no transitions will happen and no photons would be emmited, which contradicts experimental and quotidian facts. This contradiction made Schrödinger wave theory fail. It was originally pointed out by Bohr. See Jammer, *op cit.*pages 56, 57.

It is not enough to open the window
to see the fields and the river.
It does not suffice to be not blind
to see the trees and the flowers.
It is also necessary to have no philosophy.
With philosophy there are no trees: there are only ideas.
There is only each one of us like a cellar.
There is only a closed window and all the world outside;
and a dream of what could be seen if the window would open,
that is never what is seen when the window opens.

Fernando Pessoa

CHAPTER 3

QUANTISM

3.1.-Description of Quantism. Quantum mechanics is an attempt to rescue Schrödinger theory by direct redemption of its failure. Quantism consists of Schrödinger theory with one substitution and three (at least) additions.

Quantum mechanics and Schrödinger wave mechanics have the same space of states, observables and evolution equation; these were explained and criticized in the previous Chapter. If no other elements are taken into account they are one and the same theory. Therefore they have a common formal description of electrons in atoms and both theories have the same stationary states and stationary energies.

The substitution is a change in the interpretation of the wave amplitude. The amplitude previously thought as a charge density is now to be interpreted as a probability density; see the next section.

The additions are the Uncertainty Principle, the wave-particle duality (or complementarity principle) and the quantum jumps.

3.2.-Probalilistic interpretation. According to this interpretation the Schrödinger ray $[\psi]$ is still some sort of object in ordinary three dimensional space but now its amplitude no longer represents the electron as an electric charge distribution but rather as a *probability density.* So, the electron is not considered as a charge continuously distributed in space but rather as a pointlike charge. This infinitely small and electrically charged point moves then in an unspecified and intrinsically unpredictable way in three dimensional space, appearing in one position to vanish and reappear somewhere else. The relation between this blinking phenomenon and the amplitude is that the electron appears with higher relative frequency in regions where the

amplitude is relatively larger and more sporadically in those regions where its value is relatively smaller. Hence the statement that the amplitude is a probability wave.

According to this orthodox quantum interpretation the electron is point-like, does not obey any deterministic evolution law and additionally quantism assumes that this is a new, general and important quality of natural phenomena at microscopic level.

There is no explicit indication of how long the transient apparition of the electron at a point lasts; it is not said if it stays motionless during a finite time or if it moves following a continuous trajectory. There is even a variant (less orthodox) viewpoint that says that pointlike electrons move along a continuous curve and the amplitude measures the average time the particle stays in a region of space. It is to be presumed that the particle enters and exits the region succesively and the time inside the region is added up to calculate the average. It should be noted, however, that such trajectory has never been explicitly defined and the hypothetic continuous curve variant of the probabilistic interpretation does not seem to have the general acceptance given to other aspects of quantism.

The probabilistic interpretation is related to the original charge density interpretation of Schrödinger as follows: The apparition or insistent permanency of the electron in a given region would have the same effect than a higher charge density distributed over the region.

The interpretative probabilism introduce new elements in the general problem of description of natural processes and its proposal of fundamentally discontinuous and indeterministic processes produced a crisis that surpassed the boundaries of Physics, reflected in other branches of Science and disarranged a long scientific and philosophic tradition.

3.3.-Uncertainty principle. This principle states that it is impossible to measure with unlimited precision and simultaneously the position and momentum of a microscopic entity. The principle is supposed to be equally valid for ordinary macroscopic objects but is mathematically stated in such way that it is easy to 'prove' using elementary arithmetic that in this case

the consequences are trifling. If having a position and speed are considered inherent to the way in which objects exist, the uncertainty principle implies that the manner in which things are suffers from certain intrinsic undefinition.

The postulated uncertainty is, rather than a scientific law, the metaphysical and ideological support of the quantum project to explain transitions as truly spontaneous phenomena that do not obey any deterministic law.

3.4.-The wave-particle duality. Known also as *Principle of Complementarity,* the *Wave-Particle Duality* says that microscopic objects have both wave (extended and structured objects that occupy a volume) as well as particle (infinitely small objects that occupy a point) properties.

As pointed out in section 1.1, the idea of wave should not be restricted to vibrations or oscilations. The later are special cases where there is regularity or repetitivity over long regions. The only general requirement imposed upon waves will be that they should consist of a continuous unhomogeneity in ordinary three dimensional space.

The complementarity axiom validates a duplicity that in the last analysis is mere convenience: On one hand it allows to collect the benefits of the fine and elaborate details of a wave theory and on the other it also accepts the useful but much more elementary and simple-minded schemes and calculations of the particle-like conception.

Complementarity assumes that microscopic entities will manifest wave or pointlike properties depending on the context surrounding them. This viewpoint should be compared with the statement at the end of section 1.8.

In some popular presentations the wave particle duality pretends even to be a version of certain general dialectic principles. This duality is often invoked to pass many logically contradictory aspects of quantum theory as dialectic oppositions of nature.

3.5.-Quantum jumps. The third addition of quantism to Schrödinger theory is the *quantum jump.* This is the mechanism proposed by quantism to explain the transitions that according to Schrödinger theory do not occur

but that, as experiments show, do happen.

Quantum jumps are wave movements radically different from the ones specified by Schrödinger evolution law.

This new process of change consists of a abrupt motion that is not predictable with precision. Thanks to this movent a given stationary state suddenly becomes another one. In a more detailed way, quantism postulates that if $[\psi_m]$ is a stationary state of an electron in an isolated atom then this state will persist for an indefinite time (with a 100% probability). But due to interactions with other objects a small deviation can occur towards a nearby state $[\tilde{\psi}_m]$ endowed with a small movement ($[\tilde{\psi}_m]$=perturbation of $[\psi_m]$; $[\tilde{\psi}_m]$ is non-stationary). There is then a non-zero probability of a transformation of $[\tilde{\psi}_m]$ into a new stationary state $[\psi_k]$. This final sate is in general neither close to, nor does it resembles, the initial stationary state. This brusque change is also called *reduction of the wave packet.*

Since the electron is supposed to adjust its appearences to the dictation of the probability wave, a change in the quantum wave could perhaps be understood as a change in the electron schedule.

The most important observation here is that the quantum jump violates Schrödinger evolution law, and it is an admirable paradox of quantism the fact that both types of movement (Schrödinger evolution equation and quantum jumps) are accepted as a correct description of what takes place in the atom.

A wave that suddenly changes in a process devoid of a whole sequence of intermediate shapes constitutes a discontinuous movement of the wave. Therefore the concept of discontinuous quantum jump. From this discontinuous character and the continuous nature of the movement according to Schrödinger evolution law, it is beyond doubt that the two processes are totally different.

A form to smoother the paradox is to assume that the wave generally moves according to Schrödinger dynamics and that at some instant the movement disobeys this law; then the movement proceeds in the ilegal, unpredictable, sudden and random manner typical of quantum jumps. From this view-

point the two dynamics are not superimposed one to another but rather they complement each other, taking turns at separated times to direct electron comportment.

However, even separating the two dynamics the problem of the random nature of the jump persists. Additionally, the mechanism that suppresses one of the laws to give control to the other is not at all clear, with not much of an explanation beyond some vague invocation to the Uncertainty Principle.

Another way to deal with quantum jumps is the *quantum theory of measurements.* This theoretical apparatus concludes that the reduction of the wave packet is consequence of interactions between the atom and a measuring instrument. This gives a special role to the the observation process all the way up to the observer, introducing an undesirable subjective element in the explanation of the quantum jump.

3.6.-Occult variables. It is natural to ask whether there exists *at a deeper level inside matter* some hypothetical physical principles that could provide a basis to explain transitions within a continuous and deterministic scheme, providing a reasonable alternative to the jumps that quantism postulates and to the belief in basically random and discontinuous processes. This is the problem of the *occult variables.* They have been widely discussed from a general speculative viewpoint, but apparently have not yet been found or explicitly defined and are therefore an open problem.

3.7.-Random point vs. random wave. The the quantum interpretation of waves was discussed in section 3.2. This interpretation presumes an essentially probabilistic movement of a point-like electron that appears and vanishes randomly. The amplitude of the wave function was to be considered a portrayal of the electron preferences to show itself in various domains of space. The wave $[\psi]$ can even be motionless and nevertheless the electron keeps hurdling from one place to another in order to conform the program imposed by the wave.

In the case of quantum jumps it is not the point-like electron but rather the extended wave $[\psi_m]$ that suddenly moves and becomes the wave $[\psi_n]$. Therefore, while the probabilistic interpretation refers to the random movement of

a point-like electron, the quantum jump has to do with the random movement of an extended wave. It follows that quantism contains *two* classes of random movements.

This is confirmed by the fact that during its random trek the electron can occupy essentially an arbitrary point in space, while the quantum jump of the wave cannot land in an arbitrary wave but only in a stationary one. In other words, for the particle-like electron there are no forbidden points but for the wavelike electron only stationary waves are allowed.

The random movement of the point-like electron and the quantum jump performed by the wave happen in absence of deterministic equations; this is the very reason why they are called random. They happen even *against* the applicable evolution laws, namely, the laws of classical electromagnetism for the particle-like electron and Schrödinger equation in the case of waves; in the first case the electron would spiral down to the nucleous continuosly radiating energy until the atom would 'collapse', and in the second case the atom would never radiate.

3.8.-Success of quantism. Quantism mantains the space of states, the observables and the continuous and deterministic law of movement created by Schrödinger and for that reason it automatically collects the accomplishments of Schrödinger theory regarding stationary states and energies. See section 2.13.

Additionally quantism changes the interpretation of the wave amplitude and invents the uncertainty principle, the wave-particle duality and quantum jumps.

Postulating quantum jumps quantism pretends to 'explain' transitions raising them to the category of axioms, that is, considering them as basic facts of nature, irreductible and unexplainable in terms of simpler underlaying phenomena. In particular, these jumps are seen as unexplainable in terms of continuous and deterministic processes. This viewpoint did not exist in Schrödinger wave mechanics and has been hailed as the great triumph of quantism and of contemporary science itself. But these controversial parts of quantism contain and imply so many complexities, obscurities and contra-

dictions that perhaps they are just another scientific blunder.

3.9.-Pure probalility. In order to further clarify the content of quantism it is useful to consider the following alternative wave theory, which can be called *PP theory* , where electron movements happens in a *purely probabilistic fashion.* This theory is not proposed as physically sound but only as an artifact to emphazise the respective roles of Schrödinger evolution law and quantum jumps.

PP theory has the same space of states and observables than Schrödinger theory but *does not has an evolution equation.* Waves are to be interpreted as in Schrödinger theory. In PP wave mechanics the Schrödinger evolution law is simply dispossed off. Furthermore, to replace it, the notion of evolution law explained in section 1.12 is extended so that waves are no longer constrained to satisfy a differential equation. Any rule, even a random one, of any kind, that just specifies wave motions, will be acceptable.

PP theory then postulates that waves move executing quantum jumps of an intrinsically probabilistic nature.

These jumps happen in the following way: First, stationary states are *defined* by means of Schrödinger eigenvalue equation 2.10-1; they are states satisfying that equation. Non-stationary states will be called *virtual* states. An electron can occupy any stationary state and if perturbed will occupy nearby virtual states. When the electron stands at a virtual state there are non-zero probabilities of a quantum jump towards a stationary state.

Probabilities are calculated with the same mathematical rules of quantum theory; these depend only on the coefficients of the eigenfunction series for the virtual state and not on the evolution law.

PP theory postulates then that atoms emit photons when electrons move from a stationary state to another one with smaller energy. All this in accordance with Bohr transition hypothesis explained in section 2.12.

PP theory provides a satisfactory explanation of atomic and molecular behaviour with a random dynamics similar to the one of quantism. But, unlike

quantism, PP wave theory is self-consistent because it does not contains a continuous and deterministic dynamics that contradicts the random dynamics.

In order to dismiss PP theory as incorrect it is necesssary first to accept as physically valid the general principles of continuity and determinism explained in Chapter I. Under these assumptions PP theory is a mistaken description of the real electron movement or, at best, it should be considered only as a *provisory model* to be discarded as soon as a continuous deterministic theory that explains the same physical phenomena is available.

In conclusion, PP theory is wrong because it has no continuous and deterministic dynamics to describe wave movements. If continuity and determinism are discarded then PP theory becomes correct and has an undeniable advantage over quantism because it is self-consistent and explains the same phenomena. As for the uncertainty principle and the Wave-particle Duality, from the viewpoint of PP theory their role could be ideological but they are anyway unnecessary.

3.10.-Failure of quantism. While Schrödinger theory fails because it does not offers an explanation of transitions, quantism fails because of the nature of the explanation it provides. Indeed, quantism is logically contradictory because it postulates two movement laws that are incompatible. These laws, that quantism assumes as simultaneously correct, are Schrödinger evolution law and the quantum jumps. The laws are incompatible because if one of them holds then the other cannot be valid. To reconcile the laws stating that they alternate and apply at different times creates additional problems mentined in section 3.5.

Logical inconsistency is a serious inconvenient for any theory. Elementary Logic shows that if in a formal system contradictory statements are supposed simultaneously valid then all statements are both true and false. In the case under consideration it will be possible in principle to 'predict' any experimental fact. Still worse, if theoretical calculations disagree with experimental measurements there is a generous provision of parameters to be adjusted and match any desired numerical values. The final result is that the predictions or the *post-facto* adjusted predictions will agree with the measurements and,

by the same token, will confirm the theory.

As seen in the abundant literature on the subject, the paradoxical elements contained in quantism often stir an overwhelming temptation to state its contradictions, generally followed by attempts to resolve them. Whatever the conclusions, if inconsistent principles are accepted all arguments will eventually give rise to new contradictions.

Note also that Schrödinger wave mechanics is in fact an internally consistent theory, although it does not predict transitions. Its contradictions are not internal but rather external: They show up when the theory is compared with experiments. Nevertheless Schrödinger achievements (see section 2.13) were extremely important and have been appropiated by quantism to conceal under a cloak of validity its own more controversial aspects.

The above considerations carry the conclusion that quantum theory gives an incorrect description of microscopic phenomena. Logical consistency is an indispensable requisite to be demanded from all scientific theories and is not satisfied by quantism. This demand stems from the deeply rooted belief that Logic collects or reflects fundamental properties of the material universe at all its levels. Continuity and determinism are desirable conditions that seem obtainable from general logical considerations; continuity provides the necessary link between cause and effect while determinism afirms that there are definite causes or reasons for all phenomena.

3.11.-Failure of extensions of quantism. Theoretical amplifications of quantism like quantum electrodynamics and other quantum field theories have been created according to the idea of random quantum jump and assume as well the simultaneous validity of two incompatible dynamics. On one hand they postulate continuous and deterministic evolution laws ('unitary flows' in technical terms) predicting that particles or fields will stay forever as virtual particles and fields; on the other hand they have probabilistic and discontinuous 'creation' and 'destruction' operators responsible for the sudden appearance and vanishing of 'real 'particles from 'virtual' ones; these phenomena are supposed to occur in nature in an intrinsically random manner and are, at the level of field theory, a mockery of electronic quantum jumps. The limitations of the field evolution equations are similar to the

ones of Schrödinger evolution. They cannot, for example, deterministically predict a photon emission; if such deterministic prediction were possible the probabilistic interpretetion could be omited from quantum electrodynamics, but this is not the case.

Intelligence, give me
the exact name of the things!
... Let my word be
the thing itself,
anew created by my soul.
Let through me go all
who do not know them, to the things;
let through me go all
who now forget them, to the things;
let through me go all
the same who love them, to the things...
Intelligence, give me
the exact name, and yours
and theirs, and mine, of the things!

Juan Ramón Jiménez

CHAPTER 4

REALISM

An attempt has been made to mantain a rather discursive and informal style in this Chapter, similar to the previous ones. For a more formal and concise discussion see Chapter 5 which contains also deductions of formulas and calculations used here. The name *Realism* has been adopted because only real scalars are necessary. It is also a suggestive term with interesting philosophical implications.

The basic concepts of states, space of states, interpretation, observables, energy observable and evolution have already been discussed for wave theories in general; see Chapter 1. Schrödinger theory and elementary properties of atoms were considered in Chapter 2 and quantism was explained and criticized in Chapter 3. Everything is now ready to introduce real wave theory.

4.1.-Real states and their interpretation. Realism considers real wave functions

$$\psi : \mathbf{R}^3 \to \mathbf{R}$$

and identifies physical waves with the rays $[\psi]$. As explained in Chapter I, two non-identically zero wave functions define the same ray or *real state* if they differ in a real scalar factor. The real space of states is therefore a real projective space.

The rays are dimensionless quantities and cannot be, or do not have to be, interpreted. In other words, the rays $[\psi]$ represent states of any underlaying wave-like physical magnitude existing in three dimensional space and assuming values with one degree of freedom.

Real wave functions ψ have amplitudes $\psi^2 = |\psi|^2$ whose rays $[\psi^2]$ are also dimensionless and can be interpreted along the lines of Schrödinger theory,

that is, as dimensionless ratios of relative charge densities.

Related to this discussion is the idea that all forms of matter and radiation are space unhomogeneities and that space is a diluted or tenuous form of matter. This could mean that there exists a unique substance in the Universe. Several more or less unequivalent formulations of the idea are known (Parmenides, Sankara, Spinoza, Descartes, Faraday, Einstein and many others) and it belongs to the category of schemes that cannot be proved. See section 1.9. Nevertheless, it has considerable aesthetical appeal and even for scrupulous positivistic scientific sensibilities it can be commended as valuable orientation.

If the question of interpretation is treated along these unified or monistic guidelines, it is posible to conceive real states as space deformations, in which case the electron could be considered a space unhomogeneity, and charge density would also be a space unhomogeneity. The consistency of this rather general proposal is an open problem.

4.2.-Energy observable The *real energy observable* is a function of real states given by

$$e_H[\psi] = \frac{\int(-\nabla^2\psi + U\psi)\,\psi}{\int \psi\,\psi} = \frac{\langle H\psi, \psi\rangle}{\psi, \psi} \tag{16}$$

For a justification of this expression see Chapters I and II. This is in principle the same as formulas 8 or 9 in section 2.5, but now the wave function ψ is real valued.

4.3.-Real evolution. At the level of wave functions the real evolution equation is

$$\frac{\partial\psi}{\partial t} = (-2/h)H\psi \tag{17}$$

Note the absence of the imaginary unit, in contrast with the evolution equation 11.

This equation is known as a *diffusion equation*; these are widely studied and at the level of wave functions do not seem at all related to atomic transition phenomena.

But *at the level of rays* this equation predicts deterministic continuous transitions between stationary states with sensitive dependency on initial conditions, a situation fashionably referred to as *chaos.* Recall that consideration of the rays instead of the associated wave functions is equivalent to a global renormalization of states and results in a non-linear theory. see section 2.4. As will be seen, the consequence is a behavior of physical states deeply different from the one obtained from Schrödinger evolution equation.

4.4.-Analysis of movements. If the energy e_H is considered as a numerical function (sometimes called a *functional*) with domain the real projective space of rays then equation 17 is the same as an evolution way down the energy gradient

$$[\dot{\psi}] = (-2/h)\nabla e_H[\psi] \tag{18}$$

This formula is proved in Crespin, 'Stability of Dynamical Systems and Quantum Mechanics, I' referred later as [SDSQM]. The formula tells that states move in a way that decreases energy in the most efficient manner. This gradient form of the evolution equation suggests, when compared to Morse Theory, that the pecularities of atomic behaviour are consequence of global geometric properties of the space of states, that is, of the topology of infinite dimensional real projective space. See section 4.11.

As is done in general with all evolution equations when studied as dynamical systems, real states are sorted out into two classes. One is the class of motionless states (stationary states, critical states) and the other is the class of states endowed with movement. The stationary states of realism are rays configured in such way that they are locked in themselves, unable to move. But all other states will move and change so that energy is radiated in the most efficient manner.

A real state $[\psi]$ is stationary precisely when it is a critical point of the energy observable e_H. This is the same as being a zero of the energy gradient and is also equivalent as the real wave function ψ being a real eigenfunction of the Schrödinger eigenvalue equation; see section 2.6. Therefore $[\psi]$ is stationary if and only if $\psi = \psi_j$ is a real valued eigenfunction.

The stationary energies of the system are by definition the energies of the

stationary states, but these are just the eigenvalues of equation 15 (or 16), section 2.6. The eigenvalues are exactly the same of section 2.10 and therefore they can be enumerated

$$-\lambda_0 < -\lambda_1 < -\lambda_2 < \ldots < \lambda_n < \ldots < 0$$

resulting in a corresponding enumeration of stationary states

$$[\psi_0], [\psi_1], [\psi_2], \ldots, [\psi_n], \ldots \tag{19}$$

The real eigenfunctions are almost, but nor exactly, the same as complex ones. In fact, important differences between the real and complex rays have to be taken into account if an external magnetic field or other types of symmetry breakdowns are considered. These are treated in [PST].

The following is helpful heuristics: Visualize the space of states as a surface of infinite genus, with states corresponding to surface points, the energy as a real valued function defined on the surface and excited stationary states as saddle points. The energy gradient will be a field of vectors tangent to the surface, orthogonal to the level lines and pointing downward. The evolution can then be thought as movement of points along the flow lines defined by the vector field.

Some additional terminology will be of help at this point. A state is *quasistationary* if it is not stationary but is close to an excited stationary state. In other words, quasistationary states are perturbations of excited stationary states. They form neighborhoods of the saddle points.

If the quasistationary state $[\tilde{\psi}_m]$ is close to the stationary state $[\psi_m]$ then their total energies are practically the same and will be considered equal: $e_H[\tilde{\psi}_m] = e_H[\psi_m] = -\lambda_m$.

Also, since quasistationary states are close to stationary ones, under the real evolution they initially move very slowly and while they remain close to the stationary state a negligible amount of energy is radiated. But a faster movement eventually builds up and the radiated energy will suddenly increase. The movement and energy radiation will reach a peak and afterward will slow down as a new quasistationary state is reached.

In more detail, suppose that an initial quasistationary state $[\tilde{\psi}_m]$ with energy $-\lambda_m$ evolves in time and results in a new quasistationary state $[\tilde{\psi}_k]$ with energy $-\lambda_k$. What is in fact physically measured in this situation is the radiated energy difference $\Delta\lambda = \lambda_k - \lambda_m$. Therefore it will look as if a transition from the stationary state $[\psi_m]$ to the stationary state $[\psi_k]$ had occurred. Strictly speaking stationary states do not move and cannot undergo transitions; the nearby quasistationary states are the ones that effectively change.

However it can be said, and will be said in situations involving quasistationary states, that a transition from the stationary state $[\psi_m]$ to the stationary state $[\psi_k]$ has happened. Transitions involving only two stationary states or energies will be called *simple.* If three stationary energies are involved then the transition is *double,* and similarly there are triple transitions, etc. tro be called *multiple.* These transitions between stationary states, both simple and multiple, are exactly the kind of evolution predicted by equation 18. Starting with a quasistationary state the system will make transitions from one stationary state to another until the ground state is reached. And this process is a direct consequence of the evolution equation in the continuous and deterministic manner of classical theories.

In absence of external perturbations the transitions are determined by the initial state. But arbitrarily small changes in the initial condition can result in large, often qualitative, differences in the evolution of the state. This is the already mentioned phenomenon of sensitive dependency on initial conditions or chaos which explains, from a continuous and deterministic viewpoint, certain aspects of transitions so far considered by quantism as intrinsically random phenomena.

The following is illustrative. An excited stationary state has an infinite lifetime but if it is perturbed then the resulting quasistationary state has a finite lifetime. Also, a small change in the perturbation can result in a large change in the lifetime. In particular, quasistationary states that are relatively close to stationary ones will have a relatively long lifetime, independently of the transition energy (see sections 4.7 and 5.13 for a precise definition of lifetime.) In well controlled experimental situations is possible to increase in a large amount the lifetime of highly excited stationary states, against the quantum theoretical prediction that 'larger energies imply shorter lifetimes.'

Quasistationary states with higher excitations not only have a variable lifetime but can also make transitions towards any of a set of several quasistationary states with lesser energy; towards which one of these the evolution will occur is also a process with sensitive dependency in initial conditions. Again chaos is present.

For example, assume that three stationary energies $-\lambda_k < -\lambda_m < -\lambda_n$ are involved. Certain initial quasistationary states with energy $-\lambda_n$ will result in a transition to a quasistationary state with the lowest of the three energies $-\lambda_k$ while others will result in transitions to one with intermediate energy $-\lambda_m$. In the last case, after certain relaxation time during which the state remains quasistationary, further evolution will result in a second transition to the lowest energy $-\lambda_k$. The evolution that actually occurs varies, possibly in a considerable manner, if the initial quasistationary state undergoes a small change. The same situation arises when more than three stationary energies are involved. The relaxation time considered itself is sensitively dependent on the perturbation.

Summing up, the real evolution equation predicts transitions between quasistationary states with variable lifetimes and variable intermediate stationary states. This is done within a deterministic and continuous context. From the experimentally known physical behaviour of atomic systems these are expected predictions. Because Schrödinger evolution equation could not make these predictions, quantism was created with its *ad-hoc* assumptions or axioms. These theoretical quantum appendages and some of their undesirable consequences have been explained in Chapter 3.

4.5.-Stability of the ground state. If the electron and the nucleus attract each other, why does the electron stops at the ground state instead of attaining states with lower energy until the atom 'collapses' For realism the answer is very simple. Considering the real projective space of states as an energy well with a complicated architecture, no state has lower energy than the ground state because the ground state is the bottom of the well. It is the absolute minimum of the energy and lower energies are impossible. Therefore, the stability of atoms can be explained by realism in the most natural of the ways and without appeal to the rather suspicious uncertainty principle.

4.6.-Analysis of energy radiation. According to realism the atom radiates energy as consequence of the way in wich states evolve. The radiated energy $G_{rad}(t)$ can be calculated as a function of time if the initial quasistationary state is given. For simple transitions the radiated energy is a logistic (sigmoid, smooth step) function. The logistically radiated energy function has the following interpretation. There is an initial time interval with no energy emmision; the length of this interval is the *lifetime* of the given initial quasistationary state. There follows a time interval where the system starts to radiate, and then the amount of radiated energy increases in a sudden, albeit continuous, way. The emmision then slows down and eventually the amount energy radiated becomes zero. The total energy emmited is an eigenvalue difference $\Delta\lambda = \lambda_k - \lambda_m$.

For multiple transitions the radiated energy is in many cases a succession smooth steps. However, cases do exist in which the radiation follows a more complicated pattern and these will be discussed later.

4.7.-Energy pulses. The energy radiation can be further studied by means of the rate of change of the radiated energy

$$g\,dt = dG_{rad}$$

This quantity is the *energy pulse, energy intensity, radiance* or *luminosity* of the transition.

For simple transitions the energy intensity g is a smooth wavelet. As a function of the time variable t this wavelet has the following properties. During the time interval corresponding to the lifetime of the initial quasistationary state the pulse is nil. Afterwards there is a sharp increase of g until a peak energy intensity is reached; the pulse then diminishes and finally becomes nil again. The energy carried by g is

$$\int_{-\infty}^{\infty} g\,dt = G_{rad}(\infty) - G_{rad}(-\infty) = \Delta\lambda$$

which is the transition energy. Also, the peak or amplitude of g can be calculated and turns out to be equal to $(\Delta\lambda)^2/h$.

Most of the radiation occurs during a time interval around the peak instant. To determine this interval consider a square wavelet w in time variables t that

approximates g and which is defined as follows: w is centered at the peak instant and has the same amplitude and carries the same amount of energy as g. It then follows that w is constant equal to the peak value $(\Delta\lambda)^2/h$ over a time interval of length $\Delta\lambda/h$. It is during this interval that most of the transition energy is emitted. Let therefore the interval length $\Delta\lambda/h$ be defined as the transition time. Note that during the evolution there is, before the transition time, a variable lifetime of the initial quasistationary state.

If a decreasing sequence of stationary energies is specified there will be initial quasistationary states with energy pulse equal to a succession of simple energy pulses, each simple pulse corresponding to a simple transition. However, there are the 'anomalous' cases that have a more complicated energy pulse.

4.8.-Einstein formula. Assume that the energy radiated during simple transitions is carried away as a photon. The photon will be assumed to be a three dimensional electromagnetic wavelet and the only relevant physical fact to be used here is that it travels in space moving parallel, say, to the $x-$axis with constant speed c (there seems to be conflict with Maxwell equations but, since photons do stay localized while traveling in straight line this just means that Maxwell equations are inadequate for individual photons.) The energy distribution along the $x-$axis direction is therefore $g\,dx$ with $x = ct$. In space variables x the maximum of g is $\mu = (\Delta\lambda)^2/hc$. The photon wavelength is naturally defined as $\Lambda = \Delta\lambda/\mu$ and this is equivalent to Einstein formula

$$\Delta\lambda = \frac{hc}{\Lambda} \tag{20}$$

The energy density of the photon wavelet is concentrated near the maximum $(\Delta\lambda)^2/hc$. Note that this maximum is proportional to the square $(\Delta\lambda)^2$ of the transition energy. This proportionality explains why photons with higher energies have shorter wavelengths. Note also that for simple transitions there is a single wavelet with a single peak and not several peaks as usually supposed when dealing with the concept of wavelength. These considerations provide a partial resolution of the fine structure of photons.

For multiple transitions, if the energy pulse is a sequence of well separated traveling wavelets then there will be a series of successive photons, each satisfying 4.9.-1. The relaxation time separating the various pulses will be

variable and the distance between the peaks is not in general correlated to the wavelength. But in some 'anomalous' multiple transitions Einstein formula (20) does not hold; in such cases the photons have a maximum energy density less than $(\Delta\lambda)^2/h$. Equivalently, these photons have a wavelength longer than expected for their energy.

The previous discussion implies that realism has the conceptual simplicity of Schrödinger theory, obtains the same stationary energies and also essentially the same stationary states. Realism explains transitions as deterministic, continuous processes consistent with variable lifetimes and variable intermediate quasistationary states. Realism predicts the stability of the ground state from the kinematics and the evolution law and can deduce and interpret Einstein formula. Additionally, realism defines with precision radiated energy, radiated energy pulses, lifetimes and emission times and partially resolves the fine structure of photons. Furthermore, realism avoids the conceptual and logical complications of quantism, providing a much more natural, reasonable and understandable description of basic physical phenomena.

4.9.-Assessment. From a rather general perspective realism is an attempt to provide a simple and natural description of basic atomic phenomena. If quantum formalism and the initial history of quantism are reexamined, an initial mathematical accomplishment that turned into a major difficulty can be identified. The acomplishment is Schrödinger eigenvalue equation which, in view of its spectrum and eigenfunctions, is obviously relevant to atomic phenomena. The difficulty is Schrödinger evolution equation that does not predict transitions.

If the evolution equation is to be related to the eigenvalues and eigenfunctions then equation 17 above is a natural candidate. But as it stands it does not predicts transitions and, still worse, non-zero states diverge towards infinity. Therefore Schrödinger was forced to introduce the imaginary unit that appears in equation 10, section 2.10. This resulted in an energy conservative system of the kind appearing in Hamiltonian classical mechanics with the virtue that states no longer diverged towards infinity; rather, according to quantism states oscillate. But the conservation of energy implied by quantum evolution also meant that transitions could not be predicted. Quantum theorists then proposed the non-deterministic quantum jumps explained in

Chapter 3.

The alternative presently proposed by realism is to keep equation 17 *and renormalize all states.* The global renormalization is the passage from wave functions to their associated rays and implies a delinearization of the space of states. This predicts transitions and preserves (or reinstates) continuity and determinism.

4.10.-Role of Topology and Global Analysis. The heuristical remarks in section 4.4 can be given more content as follows. Projective spaces constructed from spaces of wave functions can be thought as infinite dimensional objects with a complicated architecture. To illustrate the sense of this statement consider that a plane, a sphere, a torus (surface of a ring), a double torus (surface of two welded rings or of a solid figure eight), a triple torus (surface of three welded rings), etc. are two dimensional objects with increasingly complex architectures; the plane is the simplest and being flat is devoid of architectural richness. The geometric qualities behind this architectonical complexity can be given mathematical content by introducing the *fundamental group* or *1-dimensional homotopy group.* Other mathematical apparata created for similar purposes are the *homology groups* in dimensions 0, 1, 2 and the cohomology groups, also in dimensions 0, 1, 2; a further arabesque is added by the fact that these homology and cohomlogy groups can be constructed using various types of coefficients. The above groups count holes and twisting in the surfaces, this subject being one of the basic topics in Algebraic Topology.

The notion of surface can be generalized to higher dimensions including infinite dimensions; the resulting objects are called *manifolds.* The projective spaces of quantism and realism are examples of infinite dimensional manifolds. Similarly there are higher dimensional homotopy and homology groups that count higher dimensional holes and twisting. Calculations can be performed then to show that the infinite dimensional projective space has homological and cohomological holes and/or twisting in an infinite range of dimensions; this gives mathematical substance to the affirmation that they have a complicated or rich architecture. By contrast, in all positive dimensions the homotopy, homology and cohomology groups of linear spaces are always zero. This means that linear spaces have neither holes nor twisting.

A branch of Differential Topology known as Morse theory establishes a connection between the cohomology groups of a manifold and the critical points of numerical valued functions with domain the manifold. Since the real projective space (and the complex projective space as well) has non-zero cohomology in an infinite range of dimensions, real valued functions are generically expected to have infinitely many critical points and values. This is the case with the energy map e_H whose critical points are of the form $[\psi_j]$, with ψ_j an eigenfunction and with critical values the eigenvalues λ_j of Schrödinger operator. Therefore, from the viewpoint of Morse theory, stationary states and stationary energies of atoms are forced by the topology of the domain. Still more, they will persist if the system is perturbed. Therefore the existence and persistence of energy eigenfunctions and eigenvalues can be considered as a consequence of the topology of the space of states, as previously indicated.

The topology of projective spaces provides a basic understanding of the kinematics of both quantism and realism. But the eventual goal is to clarify the dynamics of the systems under study and this is done with the methods and results of the theory of Dynamical Systems and the closely related Global Analysis. These provide the general setting of infinite dimensional symplectic and riemmannian manifolds as well as the concepts of vector fields, flows, critical points, stable and unstable manifolds, etc. necessary to orient and carry on a development like the present one. More formal statements can be found in section 5.15.

God is subtle, but He is not malicious.

Albert Einstein

CHAPTER 5

ELEMENTARY REAL AND QUANTUM FORMALISMS

This Chapter explains explains both quantism and realism at an elementary but more formal level than Chapters 3 and 4. It has been made largely independent of the previous material by repeating whenever necessary arguments or definitions already considered. This produces redundancies, but is convenient for readers already familiar with quantum theory that may prefer to skeep the first four chapters. The exposition underlines on one hand the existing parallelism and on the other hand the differences between quantism and realism.

5.1.-Terminology. The *inner product* of the complex valued functions $\psi = \psi(x,y,z)$ $\phi = \phi(x,y,z)$ is $\langle \psi, \phi \rangle = \int \psi \bar{\phi}\, dx\, dy\, dz$ which in case the functions are real valued reduces to $\int \psi\phi\, dx\, dy\, dz$. The *norm* of ψ is $\|\psi\| = \langle \psi, \psi \rangle^{1/2}$ and ψ is *square integrable* if $\|\psi\| < \infty$. The functions ψ, ϕ, etc. will be assumed always square integrable. The collection of all complex valued square integrable functions defined on $\mathbf{R}^3$ is a linear space. More precisely, the operations of sum of functions and product of scalars and functions give rise to a complex vector space that together with the inner product is a *complex Hilbert space* . This space is customarily designated as $L^2_{\mathbf{C}}(\mathbf{R}^3)$ but in this discussion will be denoted $E^{\mathbf{C}}$. Similarly, the set of all real valued square integrable functions defined on $\mathbf{R}^3$ together with the real inner product is a *real Hilbert space* to be denoted E. A square integrable function ψ is *normalized* if $\|\psi\| = 1$. Convergence or limits of sequences of functions and of parametrized families of functions are with respect to the norm defined by the inner product.

Recall that a number λ is an *eigenvalue* of a linear operator operator H if there exists a non-zero element ψ in the domain of H such that $H\psi = \lambda\psi$. Let $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ be the Laplace operator in $\mathbf{R}^3$, U a potential, Coulomb potential say. The Schrödinger self-adjoint hamiltonian

operator $H = -\nabla^2 + U$ with real negative eigenvalues

$$-\lambda_0 < -\lambda_1 < \ldots < -\lambda_n < \ldots < 0$$

can be considered as an operator on complex functions or as an operator on real functions. For the sake of clarity $H^{\mathbf{C}}$ will denote the Schrödinger operator acting on complex valued functions and H will be the operator acting on real ones.

In the complex case the eigenspaces are

$$F_j^{\mathbf{C}} = \{\psi : \mathbf{R}^3 \to \mathbf{C} | H^{\mathbf{C}}\psi_j = -\lambda_j\psi_j\}$$

forming a sequence $F_0^{\mathbf{C}}, F_1^{\mathbf{C}}, \ldots, F_n^{\mathbf{C}}, \ldots$ of mutually orthogonal complex vector subspaces of $E^{\mathbf{C}}$. The non-zero functions $\psi_j \in F_j^{\mathbf{C}}$ are *complex eigenfunctions* of the eigenvalue $-\lambda_j$.

In the real case the eigenspaces are

$$F_j = \{\psi : \mathbf{R}^3 \to \mathbf{R} | H\psi_j = -\lambda_j\psi_j\}$$

and these form a sequence $F_0, F_1, \ldots, F_n, \ldots$ of mutually orthogonal real vector subspaces; the *real eigenfunctions* of the eigenvalue $-\lambda_j$ are the non-zero elements of F_j. Note the contention $F_j \subseteq F_j^{\mathbf{C}}$. Also, if $\psi = \Re\psi + \imath\Im\psi$ is a complex eigenfunction of $-\lambda_j$ then, if the real and imaginary parts $\Re\psi, \Im\psi$ are non-zero, they are real eigenfunctions of $-\lambda_j$; equivalently $F_j^{\mathbf{C}} \subseteq F_j + \imath F_j$.

It will be also assumed that the eigenspaces form a *complete* family; this means that any square integrable function ψ is a series of eigenfunctions

$$\psi = \sum_{0 \leq j < \infty} \psi_j$$

with $\psi_j \in F_j^{\mathbf{C}}$ (complex case) or $\psi_j \in F_j$ (real case). For a given ψ each ψ_j in the above sum is uniquely determined; it is the *j-th component* of of ψ. Generally ψ_j is not normalized. In order to explicitly find the *j-th*component assume first that the *j-th*eigenspace has finite dimension n_j and let $\psi_j^1, \ldots, \psi_j^{n_j}$ be an orthonormal basis. Then ψ_j is the finite sum $\psi_j = \sum_{1 \leq s \leq n_j} \langle \psi, \psi_j^s \rangle \psi_j^s$. At the level of rays one has

$$[\psi] = [\sum_{0 \leq j < \infty} \psi_j]$$

If $n_j = \infty$ a similar procedure applies and ψ_j is then a series instead of a finite sum.

Quantum formalism

5.2.-Quantum states. By definition *quantum states* correspond with the *complex rays* (or *Hilbert rays*)

$$[\psi] = \{\lambda\psi | \lambda \in \mathbf{C}\}$$

Here $\psi : \mathbf{R}^3 \to \mathbf{C}$ is non identically zero, complex valued and square integrable, that is, $\psi \in E^{\mathbf{C}} - \{0\}$. The *quantum space of states* is the set of all complex rays or *complex projective space* associated to $E^{\mathbf{C}}$ and denoted $PE^{\mathbf{C}}$. Since $[\psi] = [\psi/\|\psi\|]$, states can always be represented by normalized functions. The sum of functions $\psi + \phi$ is defined as usual but *the sum of of states cannot be defined* since the expression $[\psi + \phi]$ depends on choices. More precisely, $[\psi] = [\lambda\psi]$ and $[\psi] = [\mu\psi]$ for all non-zero λ and μ, but $[\psi + \phi] \neq [\lambda\psi + \mu\phi]$ whenever $[\psi] \neq [\phi]$. Therefore states (rays) cannot be added and the space of states $PE^{\mathbf{C}}$ is a *nonlinear* space. Addition of quantum states cannot be well defined and therefore is an inconsistent mathematical operation.

Remark: The standard quantum mechanical paradoxical and paradigmatic interpretation of double slit diffraction is based in the above inconsistent mathematical manipulation.

Complex rays obey the following formal manipulation rules:

1.- Invariance under multiplication by complex scalars: $[\psi] = [\lambda\psi]$ for all $0 \neq \lambda \in \mathbf{C}$.

2.- Limits of sequences: The sequence of states $[\psi^{(n)}]$ converges to the state $[\psi]$, denoted $\lim_{n\to\infty}[\psi^{(n)}] = [\psi]$ if there is a sequence $\lambda^{(n)}$ of complex scalars such that the sequence of functions $\lambda^{(n)}\psi^{(n)}$ converges to the function ψ.

3.- Limits of functions: If $\psi(s) = \psi(s, x, y, z), \psi(s) : \mathbf{R}^3 \to \mathbf{C}$ is a function that depends on the parameter s then the equality $\lim_{s\to s_0}[\psi(s)] = [\psi]$ holds

in $PE^{\mathbf{C}}$ whenever there exists a complex scalar $\lambda(s)$ depending also on s such that, as functions, $\lim_{s\to s_0} \lambda(s)\psi(s) = \psi$ holds.

5.3.-Quantum energy observable. It is usually stated that in quantism the energy observable is the Schrödinger Hamiltonian operator $H^{\mathbf{C}}$. But observables are real valued functions of state, therefore the *quantum energy observable* is not the operator but rather the expression

$$e_H[\psi] = \frac{\langle H^{\mathbf{C}}\psi, \psi\rangle}{\langle \psi, \psi\rangle}$$

defining a function $e_H : PE^{\mathbf{C}} \to \mathbf{R}$. In quantism this formula is known as *normalized mean value of the energy* . If $\|\psi\| = 1$ and ψ is expressed as a sum of eigenfunctions $\psi = \sum_{0\le j<\infty} \psi_j$ then

$$e_H[\psi] = \sum_{0\le j<\infty} -\lambda_j \|\psi_j\|^2$$

5.4.-Quantum dynamics. Quantum states move according to *Schrödinger evolution equation*, which expressed at the level of functions is

$$\frac{\partial \psi}{\partial t} = (\imath/h) H^{\mathbf{C}}\psi$$

where h is Planck constant and $\imath$ is the imaginary unit $\imath^2 = -1$.

An initial state $[\psi] = [\psi^{(0)}] = [\sum_{0\le j<\infty} \psi_j]$ becomes, after time t, equal to

$$[\psi^{(t)}] = [\sum_{0\le j<\infty} exp(-(i/h)\lambda_j t)\psi_j]$$

In particular, $[\psi]$ is a *stationary state* (*fixed point, critical point*) if and only if $\psi = \psi_j \in F_j^{\mathbf{C}}$ for some j, that is, if and only if ψ is an eigenfunction.

As a consequence of this evolution equation the energy is constant along trajectories: $e_H[\psi^{(t)}] = e_H[\psi^{(0)}]$ for all t. Therefore the quantum evolution law implies that energy is not radiated and in particular there are no transitions between stationary states. Historically this lack of concordance between

theory and physical facts led to the probabilistic quantum jumps and other typically quantum concepts.

5.5.-Interpretation and quantum jumps. Quantum jumps are introduced as follows. Let ψ_k be an eigenfunction and $\eta = \sum_{j\neq k} \psi_j$ a small vector, $\|\eta\| = \epsilon$, so that $[\psi] = [\psi_k + \eta]$ can be considered a perturbation of $[\psi_k]$. Assume further that ψ is normalized, $\|\psi\| = 1$, and let ψ_m be the $m-th$-component of ψ. Then, the probability of a sudden, random, discontinuous quantum jump from the state $[\psi]$ (which is close to the stationary state $[\psi_k]$ and has energy close to $-\lambda_k$) to the eigenstate $[\psi_m]$ with energy $-\lambda_m$ is the number $\|\psi_m\|^2 = \langle \psi_m, \psi_m \rangle$. If the quantum jump occurs then a photon with energy $\lambda_m - \lambda_k$ is emitted.

Within the same random circle of ideas the *amplitude* $|\psi|^2$ of a normalized wave function ψ is interpreted as a probability density. If V is a volume in three-dimensional space then the probability of finding inside V the particle described by means of the wave function ψ is $\int_V |\psi|^2 \, dx \, dy \, dz$. Several versions or variants of this interpretation can be found in the abundant quantum literature.

Real formalism

5.6.-Real states. Real states are the *real rays*

$$[\psi] = \{\lambda\psi | \lambda \in \mathbf{R}\}$$

where $\psi : \mathbf{R}^3 \to \mathbf{R}$ is a non-zero real valued function that is also assumed to be square integrable. The *real space of states* is the set of all these real rays or *real projective space* associated to E and denoted PE. As is the case with the complex rays, the sum of real rays cannot be defined and the real projective space is nonlinear. The following formal rules for real rays are similar to the ones for complex rays.

1.- Invariance under multiplication by real scalars: If $0 \neq \lambda \in \mathbf{R}$ then $[\lambda\psi] = [\psi]$.

2.- Limits of sequences: Let $[\psi^{(n)}]$ be a sequence of real states; this sequence converges to $[\psi]$ if there is a sequence $\lambda^{(n)}$ of real scalars such that the sequence of functions $\lambda^{(n)}\psi^{(n)}$ converges to to the function ψ.

3.- Limits of functions: If $\psi(s) : \mathbf{R}^3 \to \mathbf{R}$ is a function that depends on the parameter s then $\lim_{s\to s_0}[\psi(s)] = [\psi]$ if there exists a real scalar $\lambda(s)$ depending also on s such that $\lim_{s\to s_0} \lambda(s)\psi(s) = \psi$

5.7.-Real interpretation. Since real rays $[\psi]$ are dimensionless ratios no interpretation is in principle required. However rays can be interpreted as relative space unhomogeneities and the wave amplitude ψ^2 can be interpreted in the way originally proposed by Schrödinger, that is, as a relative charge density. See section 5.2.

5.8.-Real energy. The real energy observable is the same expression as in the quantum case. The energy of the real state $[\psi]$ is

$$e_H[\psi] = \langle H\psi, \psi\rangle / \langle \psi, \psi\rangle$$

But note that $[\psi]$ is now a real state, not a quantum state and therefore the real energy is a function with domain the real projective space $e_H : PE \to \mathbf{R}$. Again, if ψ is normalized and expressed as a sum of (real) eigenfunctions $[\psi] = \sum_{0\le j<\infty}[\psi_j]$ then

$$e_H[\psi] = \sum_{0\le j<\infty} -\lambda_j \|\psi_j\|^2$$

and if $[\psi] = [\psi_j]$ is stationary then $e_H[\psi_j] = -\lambda_j$.

5.9.-Real dynamics. At the level of functions the real evolution equation is

$$\frac{\partial\psi}{\partial t} = (-2/h)H\psi \tag{21}$$

Note the absence of the imaginary unit $\imath$ typical of the quantum evolution and that the equation is dimensionally correct. A function initially equal to $\psi = \psi^{(0)} = \sum_{0\le j<\infty} \psi_j$ evolves to become in time t equal to $\psi^{(t)} = \sum_{0\le j<\infty} exp((2/h)\lambda_j t)\psi_j$. But since physical states are not given by functions but rather by the real rays, the physically relevant evolution occurs

at the level of rays . Therefore a real state initially equal to $[\psi^{(0)}]$ becomes, after time t, equal to

$$[\psi^{(t)}] = [\sum_{0 \leq j < \infty} exp((2/h)\lambda_j t)\psi_j]$$

Hence $[\psi]$ is a stationary (motionless) real state if and only if $[\psi] = [\psi_j]$ with $[\psi_j] \in PF_j$ for some j. For the purpose of a realistic description of microscopic phenomena the real evolution equation is always understood as an evolution equation in the space of real states, that is, in the projective space associated to the space of real wave functions.

5.10.-Energy radiation. Consider an initial state $[\psi^{(0)}]$ with real trajectory $[\psi^{(t)}] \in PE$. The real energy of $[\psi^{(t)}]$ is given by

$$e_H[\psi^{(t)}] = \frac{\langle H\psi^{(t)}, \psi^{(t)} \rangle}{\langle \psi^{(t)}, \psi^{(t)} \rangle}$$

With this formula energy radiation can be deterministically studied.

A direct calculation shows that

$$\frac{d}{dt} e_H[\psi^{(t)}] \leq 0$$

and furthermore the above expression equals 0 only if the initial state $[\psi] = [\psi^{(0)}]$ is stationary. Therefore, for real systems, non-stationary initial states radiate energy and stationary initial states have constant energy. Actually the energy of a stationary state is constant because the state itself is motionless. However, except for the ground state, these stationary states are unstable, as will be shown in the next section.

Meanwhile, let $[\psi] = [\psi^{(0)}]$ be an initial state evolving into $[\psi^{(t)}]$ after time t. Then the energy of the system at time t is

$$G_{sys}(t) = e_H[\psi^{(t)}]$$

and the energy radiated up to time t equals

$$\begin{aligned} G_{rad}(t) &= G_{sys}(0) - G_{sys}(t) \\ &= e_H[\psi^{(0)}] - e_H[\psi^{(t)}] \end{aligned}$$

so that

$$\begin{aligned} G_{sys}(t) + G_{rad}(t) &= e_H[\psi^{(0)}] \\ &= constant \end{aligned}$$

which expresses the principle of conservation of energy.

The *energy intensity* (*power, luminosity*) at time t of the energy radiated by the system is the time derivative

$$g(t) = G'_{rad}(t)$$

This magnitude will later enter in the deduction of Einstein formula. Note that, in contrast with the real theory, quantum mechanical radiation cannot be obtained from the evolution equation.

5.11.-Two-level transitions. Consider now eigenvalues $-\lambda_0 < -\lambda_1 < 0$ with normalized eigenfunctions $\psi_0 \in F_0, \psi_1 \in F_1$, and let $\Delta\lambda = \lambda_0 - \lambda_1$ be the *transition energy*. The function $\psi = \psi_0 + \psi_1$ is a superposition of two eigenfunctions and defines a non-stationary real state to be taken now as initial state $[\psi] = [\psi^{(0)}] = [\psi_0 + \psi_1]$. This gives to the system a radiated energy function

$$\begin{aligned} G_{rad}(t) &= G^{(0)}_{rad}(t) \\ &= \frac{\lambda_0 exp((4/h)\lambda_0 t) + \lambda_1 exp((4/h)\lambda_1 t)}{exp((4/h)\lambda_0 t) + exp((4/h)\lambda_1 t)} - \frac{\lambda_0 + \lambda_1}{2} \\ &= \frac{\lambda_1 + \lambda_0 exp((4/h)\Delta\lambda t)}{1 + exp((4/h)\Delta\lambda t)} - \frac{\lambda_0 + \lambda_1}{2} \end{aligned}$$

and an energy pulse

$$\begin{aligned} g(t) &= g^{(0)}(t) \\ &= \frac{4(\Delta\lambda)^2}{h} \cdot \left(\frac{1}{exp((2/h)\Delta\lambda\, t) + exp(-(2/h)\Delta\lambda\, t)} \right)^2 \end{aligned}$$

The maximum value $(\Delta\lambda)^2/h$ of the energy pulse occurs at at $t = 0$. This maximum or *energy intensity peak* is also the *amplitude* of the energy pulse.

Consider now a new initial state obtained by applying a time shift s to the initial state above, that is, let

$$\begin{aligned}[\tilde{\psi}^{(0)}] &= [(\psi_0+\psi_1)^{(s)}] \\ &= [exp((2/h)\lambda_0 s)\psi_0 + exp((2/h)\lambda_1 s)\psi_1] \\ &= [\psi_0 + exp((2/h)\delta\lambda s)\psi_1]\end{aligned}$$

The corresponding radiated energy and energy intensity are

$$\tilde{G}_{rad}(t) = G^{(s)}_{rad}(t) = G^{(0)}_{rad}(t-s)$$

and

$$\tilde{g}(t) = g^{(s)}(t) = g^{(0)}(t-s)$$

But for any pair of coefficients α , β such that $\alpha\beta > 0$ the state $[\tilde{\psi}^{(0)}] = [\alpha\psi_0 + \beta\psi_1] = [\psi_0 + |\beta/\alpha|\,\psi_1]$ is such a time shift with

$$s = \frac{h}{\Delta\lambda}(\log|\alpha| - \log|\beta|)$$

(if $\alpha\beta < 0$ recall that $-\psi_1$ is also an eigenstate and use $[\alpha\psi_0 + \beta\psi_1] = [\psi_0 + |\beta/\alpha|\,(-\psi_1)]$). Hence, for two-level transitions an appropiate choice of α and β places the energy peak at any desired time s.

Note that for large negative values of s the shifted state $[\psi^{(0)}] = [(\psi_0+\psi_1)^{(s)}]$ is close to $[\psi_1]$ and for large positive s it is close to $[\psi_0]$.

5.12.-Einstein formula. The physical assumption will now be made that the energy radiated by the system occupies a volume in space and travels as an energy wavelet that moves parallel to a straight line with constant speed c. This is the energy carried by a photon.

With notation as in the previous section assume without loss of generality that $\alpha = \beta = 1$. The pulse wavelet $g(t)$ can be approximated by a square wavelet with the same amplitude $g(0)$ and carrying the same total energy as $g(t)$. The *emission time* of a the energy pulse is then

$$\tau = \frac{1}{g(0)}\int_{-\infty}^{\infty} g(t)\,dt = \frac{G_{rad}(\infty) - G_{rad}(-\infty)}{g(0)} = \frac{\Delta\lambda}{g(0)} = \frac{h}{\Delta\lambda}$$

with *emmision time interval* $-\tau/2 \leq t \leq \tau/2$ (or $-s(-\tau/2) \leq t \leq -s + (\tau/2)$ if there is a time shift s). Therefore the *wavelenght* Λ of a photon is given by

$$\Lambda = \tau \cdot c$$

Example: if $\Lambda = 6000\mathring{A}$ then $\tau = 2 \cdot 10^{-15}$ seconds.

Since $g(0) = (\Delta\lambda)^2/h$ it follows that

$$\Delta\lambda = \frac{hc}{\Lambda}$$

which is Einstein formula relating the energy and wavelenght of a photon. A crucial fact in this deduction has been that the amplitude of the energy intensity is proportional to the square of the transition energy, a fundamental physical consequence of real wave theory. The formula was postulated by Einstein based on experimental results dealing with the photoelectric effect. It was also incorporated into quantism, but as a postulate rather than as a corollary deduced from first principles. For two-level transitions it has been easily obtained from realism. The more general case of multiple transitions will be discussed below in section 5.14.

5.13.-Further consequences. The emission time and emission intervals deterministically defined above for individual two-level transitions are fundamental physical quantities unobtainable by quantism. Also, the *lifetime* Υ of a given two-level initial state $[\tilde{\psi}^{(0)}] = [\alpha\psi_0 + \beta\psi_1]$ is now definable as $\Upsilon = s - \frac{\tau}{2}$, giving a measure of the time it remains in the initial stationary energy level. In a statistical situation the lifetimes will have a certain distribution that will depend on the distribution of the initial states. This illustrates how random physical quantities arise in a natural way from the deterministic equations of real wave theory.

Some additional calculations can be instructive. Assume, again without loss of generality, that $\alpha = \beta = 1$. The fraction of the transition energy $\Delta\lambda$ radiated during the emmision interval $-\tau/2 \leq t \leq \tau/2$ is

$$\frac{G_{rad}(-\tau/2) - G_{rad}(\tau/2)}{\Delta\lambda} = \frac{e^2 - 1}{e^2 + 1} = .76$$

independent of $\Delta\lambda$ and more generally for the time interval $-n\tau/2 \leq t \leq n\tau/2$ the fraction is

$$\frac{G_{rad}(-n\tau/2) - G_{rad}(n\tau/2)}{\Delta\lambda} = \frac{e^{2n}-1}{e^{2n}+1}$$

Also, comparing $g(0)$ with $g(n\tau/2)$ gives the energy pulse decay

$$\frac{g(n\tau/2)}{g(0)} = \frac{1}{(e^{2n}+e^{-2n})^2} \sim e^{-4n}$$

In particular $g(\tau/2)/g(0) = .018$

5.14.-Multiple transitions. Multiple transitions refer to initial states that emit several succesive photons. Consider a finite set of eigenvalues of H, say $-\lambda_0 < \lambda_1 < \ldots < \lambda_p < 0$, and let $t_1, t_2, \ldots, t_p$ be given instants in time. From the previous section it follows that there are eigenfunctions $\psi_0, \psi_1, \ldots, \psi_p$ and initial states $[\tilde{\psi}_p] = [\alpha_p\psi_p + \beta_p\psi_{p-1}], [\tilde{\psi}_{p-1}] = [\alpha_{p-1}\psi_{p-1} + \beta_{p-1}\psi_{p-2}], \ldots, [\tilde{\psi}_1] = [\alpha_1\psi_1 + \beta_1\psi_0]$ at time $t = 0$ such that the corresponding energy intensities $g_p(t), g_{p-1}(t), \ldots, g_1(t)$ attain their peak at $t_p, t_{p-1}, \ldots, t_1$ respectively.

Since the transitions are succesive it is natural to assume that $0 < t_p < t_{p-1} < \ldots < t_1$. Furthermore, the system should relax (become stationary) after each transition and before the next one. This requires a certain time lapse between transitions, for example, $t_p > \tau_p$ and $t_j - t_{j-1} > \tau_j + \tau_{j-1}, p < j < 1$ suffices; in this regard let D denote the smallest of the quantities $t_j - t_{j-1} - (\tau_j + \tau_{j-1}), j = p, p-1, \ldots, 1$. Under such conditions

$$\tilde{\psi} = \tilde{\psi}_p + \tilde{\psi}_{p-1} + \ldots + \tilde{\psi}_1$$

is a linear combination of eigenfunctions such that for the initial state $[\tilde{\psi}]$ the energy intensity satisfies $g(t) = g_p(t) + g_{p-1}(t) + \ldots + g_1(t)$ up to a term that decays exponentially with D. Therefore $g(t)$ is a superposition of non-overlaping two-level transitions, each satisfying Einstein formula.

On the other hand, if the relaxation conditions do not hold, say $D < 0$, then some pair of succesive energy pulses will overlap non-linearly. If the overlap is only partial the individual pulses that form the wavetrain $g(t)$ will *not* satisfy

Einstein formula. The corresponding photons will have a longer wavelenght and smaller energy intensity peak than expected from its energy in the two-level case. But as the overlapping increases the wavelenght becomes shorter and eventually there will be, instead of a pair of pulses that do not satisfying Einstein relation, a single one satisfying it.

5.15.-Mathematical properties of spaces of states. The following additional information about $PE^{\mathbf{C}}$ and PE is more technical and not essential for the previous exposition. Use is made of concepts from Global Analysis and Algebraic Topology.

1.- Local structure of $PE^{\mathbf{C}}$: The quantum mechanical space of states is a smooth connected Hilbert manifold modeled on hyperplanes of the complex Hilbert space $E^{\mathbf{C}}$.

2.- Symplectic structure of $PE^{\mathbf{C}}$: The complex projective space admits a natural symplectic 2-form. In fact $PE^{\mathbf{C}}$ is in a natural way a Hermitian and Kähler manifold and the corresponding symplectic form is the imaginary part of the Kḧaler form.

3.- Homotopy groups of $PE^{\mathbf{C}}$: The Hopf bundle is a principal bundle over $PE^{\mathbf{C}}$ with fibre the circle group and total space the infinite dimensional unit sphere of $E^{\mathbf{C}}$; this sphere is contractible. From the exact homotopy sequence for fibrations it follows that the homotopy groups of $PE^{\mathbf{C}}$ are $\mathbf{Z}$ in dimension 2 and trivial elsewhere. This means that $PE^{\mathbf{C}}$ is an Eilenberg-MacLane space $K(\mathbf{Z}, 2)$. From standard obstruction theory it then follows that $PE^{\mathbf{C}}$ is a classifying space for 2-dimensional cohomology groups with integral coefficients; in other words, for finite CW-complexes X the second cohomology group with integral coefficients, $H^2(X; \mathbf{Z})$, is isomorphic to the group of homotopy classes of maps $[X, PE^{\mathbf{C}}]$.

4.- Cohomology algebra of $PE^{\mathbf{C}}$: An explicit presentation of $PE^{\mathbf{C}}$ as union of even dimensional cells can be used to prove that the cohomology algebra of $PE^{\mathbf{C}}$ with integral coefficients is a polynomial algebra over $\mathbf{Z}$ with one generator c_1 of degree 2, that is, $H^*(PE^{\mathbf{C}}; \mathbf{Z}) \cong \mathbf{Z}[c_1]$. The generator $c_1 \in H^2(PE^{\mathbf{C}}; \mathbf{Z})$ turns out to be the first Chern class of the canonical complexline bundle $\gamma(E^{\mathbf{C}})$ over $PE^{\mathbf{C}}$.

5.- Complex line bundles and $PE^{\mathbf{C}}$: By direct geometric construction it follows that, again for finite CW-complexes X, there is a natural isomorphism between the group (under tensor product) of isomorphism classes of complex line bundles over X and the group of homotopy classes $[X, PE^{\mathbf{C}}]$. Each homotopy class $[f]$ corresponds with the isomorphism class of the pull-back by f of the canonical complex line bundle $\gamma(E^{\mathbf{C}})$.

6.- Global properties of the quantum flow: Schroedinger evolution equation in $PE^{\mathbf{C}}$ is the Hamiltonian vector field of the energy map e_H. A complete global analysis of this flow is carried out [SDSQM]. All trajectories lie in tori and the relative periods can be expressed in terms of the eigenvalues providing a characterization of periodic and quasiperiodic trajectories.

7.- Local structure of PE: The space of real states is a smooth connected Hilbert manifold modeled on hyperplanes of the real Hilbert space E.

8.- Riemannian metric on PE: The real projective space has a natural Riemannian metric with geodesics the real projective lines (one-dimensional projective subspaces of PE).

9.- Homotopy groups of PE: There is a natural two-to-one map from the infinite dimensional unit sphere of E to PE. Since this defines a covering space and the unit sphere is contractible it follows that the homotopy groups of PE are Z_2 in dimension 1 and trivial elsewhere. Hence, PE is an Eilenberg-MacLane space $K(\mathbf{Z_2}, 1)$. From obstruction theory it can then be concluded that PE is a classifiyng space for 1-dimensional cohomology groups with $\mathbf{Z_2}$ coefficients: $H^1(X; \mathbf{Z_2}) \cong [\mathbf{X}, \mathbf{PE}]$.

10.- Cohomology algebra of PE: An explicit presentation of PE as union of cells provides the basis to conclude that the cohomology algebra of PE with coefficients in Z_2 is a polynomial algebra over $\mathbf{Z_2}$ with one generator in dimension 1: $H^*(PE; \mathbf{Z_2}) \cong \mathbf{Z_2}[w_1]$. This generator $w_1 \in H^1(PE; \mathbf{Z_2})$ is the Stiefel-Whitney class of the canonical real line bundle $\gamma(E)$ over PE.

11.- PE and real line bundles: There is a natural isomorphism between the group of isomorphism classes of real line bundles over a compact CW-complex X and the group of homotopy classes of maps $[X, PE]$. Each homotopy class

$[f] \in [X, PE]$ corresponds with the equivalence class of the pull-back by f of the canonical real line bundle $\gamma(E)$.

12.- Structure of the energy map: Both in the real and complex cases the energy observable e_H is a smooth map with non-degenerated critical manifolds (Bott manifolds) equal to the projective subspaces defined by the eigenspaces. The normal bundle to these critical manifolds split into a stable and an unstable manifold. See [SDSQM]. If all eigenvalues are simple (have multiplicity 1) then each critical manifolds reduces to a critical point and the energy map becomes a Morse map.

13.- Global properties of the real flow: The real evolution equation equals (up to the factor $-2/h$) the gradient vector field of the energy map e_H. This flow can be completely analized as well. The asimptotic behaviour of all trajectories can be explicitly given in terms of eigenvalues and component eigenfunctions. For more details see [SDSQM].

As the above technicalities show, $PE^{\mathbf{C}}$ and PE are well known and much studied mathematical objects.

APPENDIX

A practical way to grasp the results of section 5.14 on multiple transitions is to run a program that numerically calculates $G_{rad}(t)$ and $g(t)$. A sample program for *Mathematica* is given below in the case of four energy levels, heuristically a 'four level atom'. A diagonalized 4×4 matrix plays the role of the Hamiltonian operator and the program calculates the radiated energy and energy pulse for this matrix. A hydrogen atom corresponds to an infinite matrix that, when diagonalized, has diagonal elements equal to stationary energies of the atom. The program can be easily modified to accomodate more than four energy levels.

The initial state given in the program is a perturbation $v = [\tilde{\psi}_3] = [(x_0, x_1, x_2, x_3)] = [(10^{-27}, 10^{-8}, 0.06, 1)]$ of the stationary state $[\psi_3] = [(0, 0, 0, 1)]$ which has 'highest energy'. The most instructive aspect is how the output changes in response to small changes in the perturbation. Therefore, the program should also be run with various other values of the perturbation $[\tilde{\psi}_3]$.

The program. To run the *Mathematica* program below just copy the code to a *Mathematica* editor. The output sould be a smooth staircase with three steps and a train of three wavelets of increasing amplitude and decreasing wavelenght.

```
x0=10^(-27) x1=0.00000001 x2=0.06 x3=1 v={x0,x1,x2,x3} a0=10
a1=a0/2 a2=a0/4 a3=a0/8 h={{-a0,0,0,0},{0,-a1,0,0},{ 0,0,-a2,0
},{ 0,0,0,-a3 }}
u[t]={{Exp[a0*t],0,0,0},{0,Exp[a1*t],0,0},{0,0,Exp[a2*t],0},{0,0,
 0,Exp[a3*t]}} x[t]=u[t].v medval[t]=h.x[t]
medval[t]=medval[t].x[t] quadnorm[t]=x[t].x[t]
vm[t]=-medval[t]/quadnorm[t] pulse=D[vm[t],t]
```

```
Plot[%%-a3,{t,0,10},PlotPoints->500,PlotRange->{0,10},AxesLabel->
 "Time,"Energy"}]
Plot[%%,[{t,0,10},PlotPoints->500,PlotRange->{0,14},AxesLabel->"T
 ime,"Energy intensity"}]
```