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Pattern Recognition in Molecular Quantum Mechanics

I. Background Dependence of Molecular States

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It is shown that the classical concept of an open system does not encompass quantal systems but has to be replaced by the non-Boolean notion of an *entangled system.* Molecular, chemical, or biological phenomena can be considered to be reduced to a fundamental theory like quantum mechanics only if the fundamental and the phenomenological theories are formally and interpretatively connected, and if the classifications used in the empirical sciences are shown to follow from a single set of fundamental dynamical laws. These conditions enforce a non-statistical and ontic interpretation of quantum mechanics, hence a non-Boolean calculus of propositions. In this interpretation the notion of a world state is well-defined, its Schmidt-decomposition defines a background-dependent model state for molecular systems and creates the phenomena we can observe. To any molecular system there is associated in an objective way a nonnegative number which we call the *integrity.* The integrity measures the inherent fuzziness of the system concept in a holistic theory, and is used to define recognizable molecular patterns.

Key words: Molecular quantum mechanics – Pattern recognition in molecular quantum mechanics

1. Introduction

The spectacular contributions of quantum mechanics to chemistry are well-known. Quite as well, every chemist knows that there are important provinces of chemistry in which quantum mechanics has contributed absolutely nothing. Since the search for regularities is the principal concern of all scientific inquiry, *classification* is a most fundamental objective of science. But at first sight, fundamental quantum mechanics is not only inefficient for chemical systematics but exhibits an entirely counter-intuitive picture of the molecular world. There is still a tremendous gap between what we know to be true empirically, and what we understand from our first principles of the theory of molecular matter. Nevertheless, it has become fashionable to claim that chemistry (or even biology) in principle can be reduced to physics. Such grandiloquent statements have an extremely meager content. In order to succeed in reducing biology or chemistry to fundamental physics, it must be shown that all experimental findings and all phenomenological theories are *logical consequences* of molecular quantum mechanics. Moreover, and very importantly, we have to require that the phenomenological theories of biology and chemistry are *interpretatively connected* with molecular quantum mechanics. That is, the regulative principles used in the phenomenological theories have to follow from the regulative principles adopted in molecular quantum mechanics. Regulative principles are of normative nature, they must be compatible with but are not implied by empirical facts and the mathematical formalism of the theory [1]. Nevertheless, they play a crucial role in the theoretical reasonings and explanations. If the regulative principles are changed when reducing one theory to another, the words used change their meaning, and no common vocabularly is available to compare the various theories. *Theories that are not interpretatively connected are incommensurable.* Most experimentalists vastly underestimate the immense conceptual difficulties of a reductionistic program. At the present time, quantum mechanics of complex systems with a large number of degrees of freedom is still in the initial state of its development. Avoiding bias and emotion, we have to state honestly that *we do not yet know whether chemistry is reducible to quantum mechanics or not.*

If we order the empirical sciences, we find that the sciences richer in empirical content (e.g. biology) use concepts (e.g. "purpose") not appearing in the more fundamental sciences (e.g. physics). Often it is claimed that such new concepts cannot even be formulated using only the notions of the more fundamental sciences. However, *it is typical for non-Boolean theories that a restriction of the universe of discourse can lead to the emergence of novel concepts.* In order to perceive this novelty, some method of *pattern recognition* has to be used. The inadequacy of classical logic for the representation of variables in the area of pattern recognition is well-known to the experts; it is directly related to the alleged impossibility to discuss notions like "novelty" or "purpose" in terms of a fundamental science. An analysis of the currently available, mathematically well-defined methods of pattern recognition reveals the interesting fact that the statistical methods of pattern recognition can be rephrased as individual (i.e. non-statistical) but non-Boolean classification methods.

We accept the working hypothesis that molecular quantum mechanics is the true fundamental theory of molecular matter, universally valid for molecular systems of any complexity[1]. In order to fulfill the postulate of the *interpretative connectability of fundamental and phenomenological theories,* we are forced to adopt an individual and ontic interpretation of quantum mechanics [1]. Such an interpretation is logically consistent and empirically correct if and only if we accept a non-Boolean calculus of propositions. That is, we admit that in our universe of discourse not every contingent and ontic proposition is either true or false. In other words, the set of all potential properties of a system is larger than the set of actual properties realized in a particular state of this system. In this sense, *molecular quantum mechanics is a non-Boolean theory.* In such a theory, the Hamiltonian time evolution can cause the emergence of new structures. The recognition of such new structures is a non-trivial matter, and requires disentangling of the genuine phenomenon from effects due to the surroundings. Adopting a non-Boolean point of view, we can unify the methods of quantum mechanics and pattern recognition, and thereby also clarify some questions of the reductionism-holism issue.

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[1] By "quantum mechanics" we mean the modern formulation of nonrelativistic quantum mechanics where Neumann's irreducibility postulate of traditional quantum mechanics is replaced by the weaker postulate that every physical state vector is eigenvector of all classical observables of the system. For a fuller discussion, compare [1].

The influence of the environment on molecular systems can be quite unexpected. Many of the problems discussed in traditional quantum chemistry are structurally instable, hence mathematically ill-posed in the sense of Hadamard. For such unstable systems, tiny causes can have big effects. A correct inclusion of the environment can have far-reaching consequences, and may even allow a logically consistent reconciliation of the fundamental principles of quantum mechanics with the *ad hoc* methods of semiempirical quantum chemistry and chemical systematics. The failure of non-empirical quantum chemistry to explain the richness of chemical systematics is related to the non-robustness of the usual models of quantum chemistry. In contrast to the *ab initio* methods, the semiempirical methods are occasionally more powerful because they accept the autochthony of chemistry. As argued convincingly by Hartmann [2], the popular attempts to "improve" the *invented* models of quantum chemistry are due to a basic misunderstanding. The role of the semiempirical models is *not* to simplify the calculation but to describe *classes* of molecules. If we reject semiempirical quantum chemistry as *ad hoc* or logically inconsistent, but nevertheless hope that a basic understanding of chemistry can be achieved by reducing it to fundamental physicals laws, we have to realize that chemical systematics does not deal with particular molecules but with *classes* of structurally diverse though functionally related molecules. *If we are to understand chemical taxonomy at all, then we have to develop a quantum mechanical theory of classes of molecules.* Moreover, if we aim to recover the familiar constructs of our everday world view from a fundamental physical theory, we need an understanding of our own pattern recognition ability. Recent progress both in the formalism and interpretation of nonrelativistic quantum mechanics, and in the theory of pattern recognition renders such an enterprice feasible.

These papers, written for the theoretical chemists, are self-contained in that they do not require any knowledge of the modern developments of quantum mechanics (like algebraic quantum mechanics or quantum logics) nor any advanced functional analysis (like the theory of *-algebras)[2]. However, we have to ask the readers for patience. In order to understand the significance of the main results, we have to discuss a few conceptual questions at some length. Unfortunately, most text books on quantum mechanics and quantum chemistry are – to put it mildly – conceptually rather naive, and do not reflect the substantial progress made in the contemporary investigations of the foundations of quantum mechanics.

The papers of this series are organized in the following way. This *first paper* is devoted to the discussion of the entanglement of molecular systems with the rest of the world. In Section 2 the importance of the environment is stressed, and the various types of open systems are reviewed. The meaning of state vector in an individual, ontic interpretation of quantum mechanics is explained in Section 3, where also the concepts of the world state and of the qualities are introduced. In Section 4 the Schmidt-decomposition of the world state is derived and used to isolate a system form the rest of the world. Section 5 introduces the model concept in non-Boolean theories, and relates patterns and reality to a restriction of the

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[2] The more mathematical aspects will be developed elsewhere [1, 3, 4].

universe of discourse by disentangling. These concepts are used in Section 6 to define molecular systems having a well-defined integrity. The notion of integrity is applied in Section 7 to define coequal molecular states and qualities in model system. The concluding remarks of the final Section 8 leads us to the *second paper* in which we will show how to describe the environment of a well-isolated molecular system in terms of quantum mechanics. In the second paper we will also give theoretically well-founded recipes for the construction of molecular models that are robust under the influence of the rest of the world. In a *third paper* we will discuss the relation of robust quantal systems and molecular patterns.

2. The Environment Must Never Be Left out of Consideration[3]

Ultimately, everything in the universe is interconnected and correlated with everything else. If we single out a "system", we have divided the universe into two parts. All we have not singled out, will be called the *environment* or the *background*. It is an empirical fact that we never can isolate a system from its environment. In molecular systems, this lack of closure can come about, for example, via the electromagnetic field associated with electrons and nuclei. In many cases these residual interactions seem to be small. However, several of the usual models in classical and quantum mechanics are characterized by an extreme instability of their motion so that even extremely weak external disturbances can cause tremendous effects. Such dynamically unstable mathematical models can give altogether misleading results unless the model is stabilized by an appropriate regularization procedure. As a rule, *the robust version gives results qualitatively different from that of the original nonregularized model.* If this is true, our simple models of molecules, and our beautiful *ab initio* calculations are in danger.

The structural instability of many models of *classical mechanics* is well-known. Already in 1887 Heinrich Burns discussed the instability of the three-body problem of classical astronomy. He proved that in the infinitesimal neighborhood of the initial conditions of a stable motion there are other initial conditions for which the perturbation theory diverges[4]. The extreme instability of complex classical systems has been used by Emile Borel to explain the macroscopic irreversibility as a manifestation of the instabilities in large mechanical systems[5]. In the same

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[3] This statement is taken from Eddington [5]. He continues: "It would be idle to develop formulae for the behaviour of an atom in conditions which imply that the rest of the matter of the universe has been annihilated ... We cannot more contemplate an atom without a physical universe to put in than we can contemplate a mountain without a planet to stand it on". Eddington's deep insight had hardly any influence on the modern theory of matter, mainly because his "Fundamental Theory" was premature and in most part underdeveloped and overambitious. Our aim is much more modest: we do not intend to understand the whole world but we propose only to investigate the influence of the background on molecular systems.

[4] Compare also the more recent work by Born [6] and Brillouin [7–9].

[5] Recall Borel's example [10]: Suppose we construct a purely mechanical model of an ideal gas and assume that we have a relative change of the gravitation potential of 10^{-100} not under our control. Such a change corresponds to an external perturbation due to a shift of 1 cm of a particle of the mass 1 gr, located on the sirius (distance from our earth: $8{,}3 \cdot 10^{16}$ m). Then the prediction of classical mechanics for the individual positions of the molecules in a macroscopic sample becomes completely wrong after 10^{-6} sec.

spirit, the irreversible behavior and the dissipativity of quantal systems can be rationalized by introducing in an *ad hoc* manner external stochastic forces [11–16]. Therefore it is tempting, but fallacious, to assume that quantal systems behave as classical systems under the influence of external perturbations. In quantum mechanics, the effects of the residual interactions of a system with the rest of the world can be much more dramatic than in classical mechanics.

Physical systems interacting with the outside world are often modelled as *open systems.* A system is called *isolated* if its properties remain unchanged whatever changes may occur in its surroundings. We speak of a *closed system* if all the variables that can influence the system have been taken into account in the initial specification [17, 18]. Any other system is called *open.* We do not possess "first principles" that are independent from far-reaching idealizations. Indeed – except perhaps cosmology – all fundamental theories refer to *closed* systems. Only by first making open systems closed, we can deduce theoretical propositions about open systems.

The dynamics that results from a projection of the global reversible dynamics of the system plus its surroundings to the system is in general no longer Hamiltonian. In this sense, open quantal systems have been extensively studied by master-equation methods and projection techniques for elucidating the irreversible character of many molecular processes. However, these techniques do not give all the information that can be obtained from the fundamental Hamiltonian equation of motion. For our problems, it is conceptually more transparent, and sometimes even technically simpler, not to use a reduced statistical description but to discuss the individual behavior in terms of the full world state.

Customarily, open systems are throught to be realizable as input-output systems. Such a restriction of the openess to energetic and material exchanges with the environment is based on common sense, engineering experience, and classical thinking, but it does by no means exhaust the possible types of non-isolated systems in quantum mechanics. In a holistic theory like quantum mechanics, the behavior of the whole cannot be deduced from the most complete knowledge of the behavior of its constituting subsystems. That is, *even the most general system-theoretic approach is not sufficient to encompass individual open quantal systems*[6]. In striking contrast to classical theories (i.e. theories with a Boolean propositional calculus), it may be impossible to define an individual state for an open quantal system, even if the interaction with the rest of the world is extremely weak. As shown by the experimentally well-established Einstein-Podolsky-Rosen effect, even systems with practically vanishing interactions can be strongly correlated. This much more complex situation reflects the intrinsically holistic character of quantum mechanics and necessitates considering open quantal systems as *entangled systems.*

The wholeness of the quantum mode of description, emphasized by Bohr [20, 21], is reflected by the fact that the world is an entangled system in the sense of Einstein *et al.* [22] and Schrödinger [23]. Generally, when two quantal systems have interacted in the past, the combined system is no longer in a product state (i.e. its state vector cannot be written as a direct product of state vectors of the

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[6] For a survey of the present trends in general system theory, compare e.g. [19].

subsystems). In such cases we speak of *entangled systems* – perhaps the most typical characteristic of the quantal world. The correlations existing between such insignificantly interacting systems are called *Einstein-Podolsky-Rosen correlations.* For example, the electromagnetic field generated by a molecule has to be included in the nontrival part of the surroundings of this molecule, so that a molecule and its electromagnetic field constitute a single quantal system rather than two coupled systems to which state vectors can be assigned. Consequently, there is no decomposition of the world state Φ into a direct product of a state Ψ describing a molecular system and a state Ξ describing the rest of the world, i.e.

$$\Phi \neq \Psi \otimes \Xi .$$

If we decide to divide the world into small pieces having an individuality, we have to realize that therewith we destroy holistic properties. Because we would like to understand *some aspects* of nature without understanding everything, *we have to learn how to isolate a subsystem from the rest of the world.* Before attacking the problem of assigning a state vector to a model system (Section 4), we will briefly review the meaning of a state vector in quantum mechanics. In the traditional interpretations of quantum mechanics it is meaningless to speak of the "state vector of the universe". Because we cannot neglect the background describing the rest of the world, we need a more general interpretation of quantum mechanics in which the notation of a world state is conceptually well-defined.

3. The State Concept. Qualities of Closed Quantal Systems

The notation of the *state of a system* is one of the most fundamental concepts for the description of nature. The conceptual definition of a quantal state characterizes the interpretation adopted. There is a widespread belief that the essence of a scientific theory is its mathematical formalism. However, it has to be emphasized that the mathematical formalism of a physical theory is not the whole theory, it determines the syntax of the theoretical concepts used but not their semantic meaning. Only interpreted mathematical formulae express empirical laws of nature. Unfortunately, no general agreement could be reached concerning the interpretation of the formalism of quantum mechanics. For our purpose, we can neither adopt the Copenhagen interpretation [24, 25] nor the orthodox ensemble interpretation [26, 27] since

(1) both interpretations do not fulfill the postulate of the interpretative connectability with the current phenomenological theories,

(2) both interpretations are meaningless when applied to the entire universe.

These difficulties are due to the fact that the traditional interpretations of quantum mechanics are either epistemic or operational. That is, they deal with our knowledge, or our measurements, but not with an objectively existing reality. A theory that refers to qualities having a real being is called *ontic*; traditionally all classical physical theories are formulated as ontic theories. An ontic interpretation of quantum mechanics is often rejected by operationalistic arguments, or by claiming logical inconsistencies. Operationalism is an empirically unverfiable philosophical position which bars propositions that cannot be tested by experiments. However, we reject operationalism as a view that confuses meaning and measurement. Logical inconsistencies cannot arise if we are prepared to accept a non-Boolean propositional calculs[7].

Fortunately, we are not forced to accept any of the traditional views with their grave limitations. Using the results of the modern investigations in the foundations of quantum mechanics, it can be shown that it is logically consistent and empirically irrefutable to adopt the following ontic interpretation which refers to individual systems [1, 4]:

(1) Conceptually, a state is defined as the set of all ontic contingent propositions that are true at a specified time.

(2) Any closed individual system is always in a well-defined state – whether we know this state or not is conceptually irrelevant.

This state concept refers to an individual system, and applies to quantal systems as well as to classical systems. All fundamental classical theories, and all non-statistical phenomenological theories are traditionally formulated in accordance with this ontic interpretation. But note that in quantum mechanics as well as in pattern recognition not all propositions one can make are either true or false. The contingent propositions refer to a certain time, they can be true now, and false, *or senseless* another time. That is, in the proposed interpretation the lattice of all ontic propositions is in general no longer Boolean. In this sense, we say that quantum mechanics and pattern recognition are *non-Boolean* theories. We call a theory *classical* if the contingent ontic propositions fulfill the laws of classical logic, i.e. if they form a Boolean (that is, distributive) lattice.

Many of the classical statistical theories (like Kolmogorov's probability theory, or the methods of statistical pattern recognition) can be rephrased efficiently as *non-Boolean* theories referring to *individual* systems. On the other hand, the orthodox ensemble interpretation of quantum mechanics, or the Copenhagen view *can be derived* from the non-Boolean, individual, and ontic interpretations, Nevertheless, the choice between statistical and individual interpretations is not entirely a matter of taste because some problems can be formulated in the individual interpretation only. Alone in an individual interpretation of quantum mechanics it makes sense to speak of the state of the whole universe of discourse. We call this state the *world state.*

In the Hilbert-space formulation of quantum mechanics a state is represented by a one-dimensional subspace, called a *ray*, of an appropriate complex, separable Hilbert space, called the *state space* $\mathfrak{H}$. Any vector generating a ray corresponding to a state, is called a *state vector.* Often, but not always, we normalize state vectors. We assume that quantum mechanics is a complete theory and universally valid. That is, we postulate

(1) a state vector characterizes an isolated individual system exhaustively (i.e. we exclude hidden variables),

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[7] The Copenhagen view is an individual, epistemic, and Boolean interpretation. The orthodox ensemble interpretation is statistical, epistemic, and Boolean. An individual, ontic, and Boolean interpretation of quantum mechanics is impossible. A logical analysis of the ontic and epistemic interpretations of quantum mechanics has been given by Scheibe [28, 29].

(2) the time-dependent Schrödinger equation is valid for any closed system (even for the whole world) at any time[8].

These two postulates are empirically unchallenged and compatible with the ontic individual interpretation. The various famous paradoxa of quantum mechanics arise only if one introduces in addition a point of view inapplicable to non-Boolean theories.

In the Hilbert-space model of quantum mechanics, the *qualities* are represented by the closed subspaces of the state space $\mathfrak{H}$. We do not exclude superselection rules, so that we do not assume that every subspace necessarily also represents a quality [1]. A quality f implies the quality g if the subspace $\mathfrak{G} \subset \mathfrak{H}$ associated with g is contained in the subspace $\mathfrak{F} \subset \mathfrak{H}$ associated with f,

$$f \text{ implies } g \quad \text{if} \quad \mathfrak{G} \subset \mathfrak{F} . \tag{1}$$

Two qualities that imply each other are called equal, hence

$$f = g \quad \textit{iff} \quad \mathfrak{F} = \mathfrak{G} . \tag{2}$$

A quality that is not implied by another quality is called an *atomic quality*. Atomic qualities are indecomposable, and are represented by one-dimensional subspaces. The set of all closed subspaces of a Hilbert space forms a complete, non-Boolean lattice under the set-theoretic inclusion $\subset$. This lattice admits an orthocomplementation induced by the inner product. Let $\mathfrak{F}$ be a closed subspace of $\mathfrak{H}$, then the orthocomplement $\mathfrak{F}^{\perp}$ of $\mathfrak{F}$ is defined to be the closed subspace containing all vectors orthogonal to all members of $\mathfrak{F}$,

$$\mathfrak{F}^{\perp} \overset{\text{def}}{=} \{\chi : \chi \in \mathfrak{H}, \langle \chi | \varphi \rangle = 0 \quad \text{for all} \quad \varphi \in \mathfrak{F}\} .$$

The characteristic property that distinguishes quantal from classical systems is the existence of *incompatible qualities* in quantum mechanics. Two qualities f and g with the associated subspaces $\mathfrak{F}$ and $\mathfrak{G}$ are called compatible, written $f \Leftrightarrow g$, if the lattice generated by $\mathfrak{F}$, $\mathfrak{F}^{\perp}$, $\mathfrak{G}$, $\mathfrak{G}^{\perp}$ is Boolean, i.e.

$$f \Leftrightarrow g \quad \textit{iff} \quad (\mathfrak{F} \cap \mathfrak{G}^{\perp}) \cup \mathfrak{G} = (\mathfrak{G} \cap \mathfrak{F}^{\perp}) \cup \mathfrak{F} . \tag{3}$$

This relation can be rephrased in an equivalent but simpler form if we introduce the projectors F and G corresponding to the subspaces $\mathfrak{F}$ and $\mathfrak{G}$, respectively[9],

$$\begin{aligned} F = F^* = F^2 , \quad & \mathfrak{F} = F\mathfrak{H} , \\ G = G^* = G^2 , \quad & \mathfrak{G} = G\mathfrak{H} , \end{aligned} \tag{4}$$

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[8] This postulate contradicts the Copenhagen view as expressed by Bohr [24] and Fock [25]. However, it is in accordance with the orthodox interpretation by Newmann [26] and by London and Bauer [27]. A consequent non-statistical development of the Neumann-London-Bauer interpretation is due to Everett [30] and Wheeler [31]. It is important to acknowledge the fact that the Hamiltonian is the generator of the time evolution, hence a self-adjoint operator on the state space, but *in general not an observable.*

[9] A projector is an idempotent and self-adjoint operator acting on the Hilbert space $\mathfrak{H}$. Here we have no need to introduce the concept of observables. Conceptually, observables are defined via external classification operators. The algebra of all observables equals the Neumann algebra generated by the set of all projectors corresponding to all possible qualities of the system. For further details, compare [1].

Two qualities f and g are compatible if and only if the associated projectors F and G commute,

$$f \Leftrightarrow g \quad \textit{iff} \quad FG = GF\,. \tag{5}$$

The lattice of all qualities of a classical system is Boolean. That is, the distributive law

$$\begin{aligned} \mathfrak{E} \cap (\mathfrak{F} \cup \mathfrak{G}) &= (\mathfrak{E} \cap \mathfrak{F}) \cup (\mathfrak{E} \cap \mathfrak{G}) \\ \mathfrak{E} \cup (\mathfrak{F} \cap \mathfrak{G}) &= (\mathfrak{E} \cup \mathfrak{F}) \cap (\mathfrak{E} \cup \mathfrak{G}) \end{aligned} \tag{6}$$

holds for the subspaces $\mathfrak{E}$, $\mathfrak{F}$, $\mathfrak{G}$ associated with every triple $\{e, f, g\}$ of qualities of a classical system. Equivalently, in a classical system the commutative law

$$FG = GF \tag{7}$$

holds for the projectors F, G associated with every pair $\{f, g\}$ of qualities.

Let Ψ be a state vector belonging to the subspace $\mathfrak{F} \subset \mathfrak{H}$,

$$\Psi \in \mathfrak{F}\,, \quad \text{or equivalently} \quad F\Psi = \Psi\,,$$

where F is the projector onto $\mathfrak{F}$, $\mathfrak{F} = F\mathfrak{H}$. Then the ontic interpretation implies that the system in the state Ψ *has* the quality f in a realistic and objective sense. It would be artificial not to attribute a certain degree of "f-ness" to a state vector that only "almost" belongs to the subspace $\mathfrak{F}$. The distance $d(\Psi, \mathfrak{F})$ of a vector Ψ from a subspace $\mathfrak{F}$ is defined by (compare [35], Section I.6)

$$d(\Psi, \mathfrak{F}) \overset{\text{def}}{=} \inf_{\Phi \in \mathfrak{F}} \|\Psi - \Phi\|\,.$$

The uniqueness theorem on orthogonal projections in a Hilbert space implies that this distance is given by

$$d(\Psi, \mathfrak{F}) = \|F^{\perp}\Psi\|\,,$$

where $F^{\perp} = 1 - F$ and $\mathfrak{F} = F\mathfrak{H}$. The tangent of the angle $\varphi(\Psi, \mathfrak{F})$ between a vector Ψ and a subspace is defined by

$$\tan \varphi(\Psi, \mathfrak{F}) = \frac{d(\Psi, \mathfrak{F})}{d(\Psi, \mathfrak{F}^{\perp})} = \frac{\|F^{\perp}\Psi\|}{\|F\Psi\|}\,. \tag{8a}$$

Accordingly, we have

$$\begin{aligned} \cos^2 \varphi(\Psi, \mathfrak{F}) &= \frac{\|F\Psi\|^2}{\|\Psi\|^2} = \frac{\langle\Psi|F|\Psi\rangle}{\langle\Psi|\Psi\rangle} \\ &= \sup_{\Phi \in \mathfrak{F}} \frac{|\langle\Psi|\Phi\rangle|^2}{\|\Psi\|^2 \|\Phi\|^2}\,, \end{aligned} \tag{8b}$$

and

$$\sin^2 \varphi(\Psi, \mathfrak{F}) = \frac{\|F^{\perp}\Psi\|^2}{\|\Psi\|^2} = \frac{\langle\Psi|F^{\perp}|\Psi\rangle}{\|\Psi\|^2}\,. \tag{8c}$$

The square of the cosine of the angle $\varphi(\Psi, \mathfrak{F})$ between Ψ and $\mathfrak{F}$ is an appropriate measure of the "f-ness" associated to the individual state Ψ. That is, if

$\cos^2\varphi(\Psi, \mathfrak{F}) \approx 1$, the state vector Ψ behaves similarly as the vector $\Psi_F \overset{\text{def}}{=} F\Psi \in \mathfrak{F}$ *having* the quality f.

In harmony with this concept of "f-ness", we measure the *proximity of two qualities* by the angle between the corresponding subspaces. We define the angle $\varphi(\mathfrak{G}, \mathfrak{F})$ between two closed subspaces of the same dimension by

$$\begin{aligned} \cos\varphi(\mathfrak{G}, \mathfrak{F}) &\overset{\text{def}}{=} \inf_{\Psi \in \mathfrak{G}} \cos\varphi(\Psi, \mathfrak{F}) \\ &= \inf_{\Psi \in \mathfrak{G}} \sup_{\Phi \in \mathfrak{F}} \frac{|\langle \Psi | \Phi \rangle|}{\|\Psi\|\,\|\Phi\|}, \end{aligned} \tag{9a}$$

so that

$$\sin\varphi(\mathfrak{G}, \mathfrak{F}) = \sup_{\Psi \in \mathfrak{G}} \frac{\|F^{\perp}\Psi\|}{\|\Psi\|} = \sup_{\Psi \in \mathfrak{H}} \frac{\|F^{\perp}G\Psi\|}{\|\Psi\|} = \|F^{\perp}G\|\,.$$

For two projectors F, G of the same rank, we have (compare [36], Section I-6.8)

$$\|F^{\perp}G\| = \|G^{\perp}F\| = \|G - F\| = \|F - G\|\,,$$

so that

$$\sin\varphi(\mathfrak{G}, \mathfrak{F}) = \|G - F\| \tag{9b}$$

(compare also [35], Section III-39). We say that two qualities f and g are *similar* if the corresponding subspaces $\mathfrak{F}$ and $\mathfrak{G}$ have the same dimension, and if the angle $\varphi(\mathfrak{F}, \mathfrak{G})$ between $\mathfrak{F}$ and $\mathfrak{G}$ is small. A natural measure of what has to be considered as small is given by the integrity I, introduced in Section 6.

4. The Schmidt-Decomposition of the World State

A system which is neither interacting nor entangled with another system will be called universe[10]. In the framework of the individual, ontic, non-Boolean interpretation of quantum mechanics it makes sense to speak about the state of the entire universe. Let $\mathfrak{H}_w$ be the state space of the universe of discourse, called the *world-state space;* we assume that $\mathfrak{H}_w$ is a *separable* Hilbert space and includes everything that is of importance for our discussion. In particular, we may include the electromagnetic radiation field which also interacts with the macroscopic objects of our world. Because we include everything of interest to us, our universe of discourse represents an isolated system in a well-defined state. At a fixed time, this state can be represented by a normalized vector $\Phi \in \mathfrak{H}_w$[11]. We call Φ the *world-state vector.* We never are interested in the whole world but only in a part of the world which we call the *system S.* A system is characterized by its non-contingent (i.e. time-independent) properties. In the Hilbert-space formulation

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[10] In our discussions, "world" or "universe" always means the *universe of discourse*, including all relevant observers and measuring apparatus. Genuinely relativistic problems are excluded in our discussion, hence "universe" never means the cosmological universe.

[11] If the universe of discourse contains infinitely many degrees of freedom (e.g. if the radiation field is included), some care is required. The world-state vector Φ is assumed to be an element of a superselection sector of the full state space $\mathfrak{H}_w$. That is, if the algebra of all observables is reducible, we require that all physical state vectors (including the world-state vector Φ) are eigenstates of all classical observables. Compare also [1].

of quantum mechanics, a system is specified by a particular tensor-product decomposition of the world-state space $\mathfrak{H}_{\mathrm{w}}$, say[12]

$$\mathfrak{H}_{\mathrm{w}}=\mathfrak{H}\otimes\mathfrak{H}_{\mathrm{e}}\,. \tag{10}$$

Thereby, $\mathfrak{H}$ is the state space of the system under discussion, and $\mathfrak{H}_{\mathrm{e}}$ is the state space of the environment of this system. The world-state vector Φ can be written in very many different ways in a form adapted to this tensor-product decomposition, say as

$$\Phi=\sum\nolimits_j\sum\nolimits_k c_{jk}\Psi_j\otimes\Xi_k\,,$$

with complex numbers c_{jk}, and

$$\Phi\in\mathfrak{H}_{\mathrm{w}}\,,\qquad \Psi_j\in\mathfrak{H}\,,\qquad \Xi_k\in\mathfrak{H}_{\mathrm{e}}\,.$$

Fortunately, there exists a unique canonical form of such an expansion in which the expansion coefficients c_{jk} are diagonal, and both the vectors Ψ_j and Ξ_k form an orthogonal system. According to a theorem due to Schmidt [32], any normalized vector $\Phi\in\mathfrak{H}\otimes\mathfrak{H}_{\mathrm{e}}$ can be represented in the form

$$\Phi=\sum\nolimits_{j=0}^{\infty}\varkappa_j\Psi_j\otimes\Xi_j\,,\qquad \Psi_j\in\mathfrak{H}\,,\qquad \Xi_j\in\mathfrak{H}_{\mathrm{e}}\,, \tag{11a}$$

$$\|\Phi\|^2=\sum\nolimits_{j=0}^{\infty}|\varkappa_j|^2=1\,, \tag{11b}$$

where the orthonormalized vectors Ψ_j, Ξ_j

$$\langle\Psi_j|\Psi_k\rangle_{\mathfrak{H}}=\langle\Xi_j|\Xi_k\rangle_{\mathfrak{H}_{\mathrm{e}}}=\delta_{jk} \tag{11c}$$

are eigenvectors, and the complex numbers $\varkappa_j$ are eigenvalues of the following coupled eigenvalue problem[13]:

$$\langle\Psi_j|\Phi\rangle_{\mathfrak{H}}=\varkappa_j\Xi_j\,, \tag{11d}$$

$$\langle\Xi_j|\Phi\rangle_{\mathfrak{H}_{\mathrm{e}}}=\varkappa_j\Psi_j\,. \tag{11e}$$

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[12] Any countably infinite-dimensional Hilbert space is isomorphic to arbitrary finite tensor products of countably infinite-dimensional Hilbert spaces. Hence, without additional information, it makes no sense to ask for a decomposition of a given state space into a tensor product of state spaces. The different possible ways to choose the state space $\mathfrak{H}$ mirror the plurality of ways seeing phenomena. The general problem of representing the state space as a meaningful tensor product is a highly important problem of molecular pattern recognition. For the present, we assume that the tensor product decomposition (10) is contextually given, and concretely defined, say via a representation of the Galilei group.

[13] Of course, in Schmidt's paper of 1907 Hilbert spaces are not mentioned but realized as $\mathfrak{L}_2$-spaces of equivalence classes of Lebesgue square integrable, complex-valued functions in the n-dimensional Euclidean space $\mathfrak{R}^n$. Let $\mathfrak{H}=\mathfrak{L}_2(\mathfrak{R}^p)$, $\mathfrak{H}_{\mathrm{e}}=\mathfrak{L}_2(\mathfrak{R}^q)$, $\mathfrak{H}_{\mathrm{w}}=\mathfrak{L}_2(\mathfrak{R}^p\times\mathfrak{R}^q)$, then we get the integral equations actually used by Schmidt:

$$\int_{\mathfrak{R}^p}\Psi_j^*(x)\Phi(x,y)\,\mathrm{d}x=\varkappa_j\Xi_j(y)\,,\qquad y\in\mathfrak{R}^q\,,$$

$$\int_{\mathfrak{R}^q}\Xi_j^*(y)\Phi(x,y)\,\mathrm{d}y=\varkappa_j\Psi_j(x)\,,\qquad x\in\mathfrak{R}^p\,,$$

where $\Phi\in\mathfrak{L}_2(\mathfrak{R}^p\times\mathfrak{R}^q)$ plays the role of an unsymmetrical kernel.

In the following, we always choose the notion such that

$$1 \geqq |\varkappa_0|^2 \geqq |\varkappa_1|^2 \geqq \ldots \geqq 0\,. \tag{11f}$$

We call this canonical expansion the *Schmidt-decomposition of the world state Φ relative to the system S.*

The Schmidt-decomposition has a remarkable optimality property. For fixed natural numbers m and n,

$$\inf \|\Phi - \textstyle\sum_{j=0}^{m} \sum_{k=0}^{m'} c_{jk} \tilde{\Psi}_j \otimes \tilde{\Xi}_k\| = \|\Phi - \sum_{j=0}^{n} \varkappa_j \Psi_j \otimes \Xi_j\|^2 = 1 - \sum_{j=0}^{n} |\varkappa_j|^2\,, \tag{12}$$

where $n = \min(m, m')$ and the infimum has to be taken over all complex numbers c_{jk}, and all vectors $\tilde{\Psi}_j \in \mathfrak{H}$, $\tilde{\Xi}_j \in \mathfrak{H}_e$. Accordingly, the best possible approximation (in the Hilbert space norm) of the world-state vector Φ by a product state Φ_0 (i.e. $n = 1$) is given by the first term of the Schmidt-decomposition,

$$\Phi_0 = \Psi_0 \otimes \Xi_0 \tag{13}$$

with

$$\|\Phi - \Phi_0\|^2 = 1 - |\varkappa_0|^2\,, \tag{14}$$

$$|\langle \Phi | \Phi_0 \rangle|^2 = |\varkappa_0|^2 \leqq 1\,. \tag{15}$$

The statement that no system can be isolated from its surroundings means that $|\varkappa_0|^2 = 1$ is impossible. If $|\varkappa_0|^2 \approx 1$, then we call $\Phi_0 = \Psi_0 \otimes \Xi_0$ the *dominant Schmidt state.*

When we speak of a *closed* system, we have already assumed that the system is disentangled from the rest of the world. That is, we have ignored certain aspects and tacitly replaced the world state space vector Φ by a product state $\Psi \otimes \Xi$ where Ψ is a vector of the state space that defines the system, and Ξ is a background state describing the rest of the world. The best possible choice for such a model state $\Psi \otimes \Xi$ is the dominant Schmidt state $\Phi_0 = \Psi_0 \otimes \Xi_0$ of the world state vector Φ. Accordingly, *we define a molecular model by a tensor product decomposition of the world-state space together with the dominant Schmidt state Φ_0 which serves as a model state.* An idealization of this type is *always* made in every application of quantum mechanics, the proposed definition gives the best possible separation of the molecular system from its surroundings.

Because the model state $\Phi_0 = \Psi_0 \otimes \Xi_0$ is a product state, we lose nothing when we restrict our discussion to the molecular state Ψ_0. Such a notational simplification is common practice. Nevertheless, the replacement of $\Psi_0 \otimes \Xi_0$ by Ψ_0 does not eliminate the effects of the surroundings, the state vector Ψ_0 is in an essential way *background dependent.* That is, we cannot expect that by restricting the discussion to the subsystem defined by the state space $\mathfrak{H}$ we are able to evaluate a reasonable approximation to the model-state vector Ψ_0. The model state Ψ_0 is defined via the Schmidt-decomposition of the world-state, hence it is a *relational concept* which refers to a system adapted to its environment.

In the individual, ontic interpretation the world-vector and its dominant Schmidt state are conceptually well-defined but, of course, lack direct operational meaning. We never know the world-state. Nevertheless, it is possible to get approximations for the dominant Schmidt state Φ_0 because we have reasonable ideas what the interactions of a molecular system with its surroundings are. As we will discuss in the second paper, the quasi-classical nature of our macroscopic world implies that the vector Ξ_M approximating the state vector of the surroundings of a well-isolated molecular system has a surprisingly simple structure. Hence we can work out the time evolution $\Phi_M(0) \to \Phi_M(t)$ of a model with a product vector

$$\Phi_M(0) \overset{\text{def}}{=} \Psi_M \otimes \Xi_M \to \Phi_M(t), \qquad t > 0 .$$

In general, $\Phi_M(t)$ will no longer be a product state but it may happen that the molecular part of the dominant Schmidt state of $\Phi_M(t)$ does not depend in an essential way on the interactions with the surroundings. In such cases we say the molecular state Ψ_M is *robust*, and we can consider Ψ_M as a useful approximation for the true but unknown model state Ψ_0. In these fortunate situations we can altogether neglect the influence of the surroundings, and hence recover the traditional methods of molecular quantum mechanics. In any other case the molecular model state Ψ_M is *structurally instable*, and does not represent an actual situation. Regularization methods for such unstable situations will be discussed in later papers [3, 33].

Preliminary Example

Consider the molecule H_2 in the Born-Oppenheimer approximation. Let $\Psi(R)$ be the electronic ground state as a function of the internuclear distance R, and let R_{eq} be the equilibrium distance defined by the minimum of the electronic energy. Empirically we know that $\Psi(R_{eq})$ is an acceptable approximation, so that we feel sure that $\Psi(R_{eq}) \otimes \Xi$ is a reasonable approximation for the world state Φ. The very same methods of traditional quantum chemistry that are empirically successful for the evaluation of the ground state of the hydrogen molecule give a curious result when applied for the case $R \to \infty$. We get

$$\lim_{R \to \infty} \Psi(R) = 2^{-1/2} \{ \varphi_1 \otimes \varphi_2 - \varphi_2 \otimes \varphi_1 \} ,$$

where φ_1 and φ_2 are two orthogonal molecular orbitals. However, if we have one proton on the earth and another on the moon, then we know empirically that the realized lowest energy state of this 2-nuclei-2-electron problem is one hydrogen atom on the earth and one hydrogen atom on the moon. That is, the appropriate approximate decomposition of the world state Φ is *either* of the type

$$(1) \qquad \Phi \cong \varphi_1 \otimes \varphi_2 \otimes \Xi_{12} ,$$

or of the type

$$(2) \qquad \Phi \cong \varphi_2 \otimes \varphi_1 \otimes \Xi_{21} ,$$

but *not* a superposition of the type

$$(3) \qquad \Phi \cong 2^{-1/2} \{ \varphi_1 \otimes \varphi_2 - \varphi_2 \otimes \varphi_1 \} \otimes \Xi ,$$

as suggested by the methods of traditional quantum chemistry. We will show at another place [3, 33] that for $R \rightarrow \infty$ the state (3) is structurally instable and decomposes under the influence of the environment into the robust states (1) or (2).

5. Models and Phenomena

If we replace the pragmatic approach to molecular quantum mechanics by the universally valid quantum mechanics in its ontic interpretation, we are confronted with problems and possibilities unknown in the traditional approach. Adopting the primacy of quantum mechanics, we have not only the burden but also the chance to *derive* the classical behavior of some systems and the existence of patterns and phenomena in our world.

In a holistic theory, notions like patterns and phenomena have no *a priori* meaning. Pattern recognition turns out to be the same as pattern creation, so that the distinction between discovery and invention breaks down. Pattern recognition is a map of the non-Boolean world into a Boolean description, whereby different recognition criteria may lead to incommensurable but equally legitimate descriptions. The selection of a particular criterion creates some patterns but makes it impossible to ask complementary questions. However, *a priori* we have no rules how to select a pattern recognition criterion. Nevertheless, the phenomena created by a given pattern recognition process can be reproduced in the universally valid quantum mechanics by a particular, theoretically well-founded model tailored to this pattern recognition criterion.

Ignorance, particularization, and artificial isolation are intrinsic in the scientific method. The erasing of not directly relevant information is the *conditio sine qua non* not only for pattern recognition but for any scientific inquiry. Any pattern recognition method singles out some directly relevant aspects, and suppresses unessential features; it can be characterized by the specification of the relevant variables together with a threshold level. The threshold level measures the amount of irrelevant information thrown away. The specification of the relevant observables can be used (for example via a representation of the Galilei group) to define the Hilbert space $\mathfrak{H}$ of the system, and therewith the tensor-product decomposition of the world-state space $\mathfrak{H}_w$. As we will discuss in detail in a later paper, the threshold level ε is related to the eigenvalue $\varkappa_0$ of the dominant Schmidt state Φ_0 of this tensor-product decomposition by $\varepsilon = 1 - |\varkappa_0|^2$. The operation that corresponds to the pattern recognition process is the replacement of the world state Φ by the model state Φ_0. The operation $\Phi \rightarrow \Phi_0$ is nonlinear, it destroys some holistic properties by dismissing the (always existing!) Einstein-Podolsky-Rosen type correlations between the system S and its surroundings, and creates new patterns. The world state Φ is patternless; only in the model state Φ_0 there are knowable patterns and actions. Both, in quantum mechanics and in pattern recognition, phenomena exist only because of abstractions. The purpose of a theoretical model is to *isolate* particular qualities and phenomena. To summarize: *disentangling a system from its surroundings creates new phenomena which can be discovered by a pattern recognition method that rejects the Einstein-Podolsky-Rosen correlations between the system and its surroundings as irrelevant.*

It would be somewhat naive to presume that there *are* real events but that theories describe idealized systems only. Reality is a very abstract construct, it is known to us only through some pattern recognition mechanism. What *we* call a real event is the result of a pattern recognition process in *our* brain[14]. Pattern recognition is a highly developed faculty of mankind, not necessarily of subjective nature even though depending on our historical origin and biological evolution. We decipher the outside world on the basis of recognition criteria derived from our own long biological evolution. The evolution of the faculty to do some categorization must have been a crucial component for the survival of living beings. These pattern recognition processes create the reality witnessed by animals and men by rejecting irrelevant informations. What passes as irrelevant is, however, neither determined by quantum mechanics nor by subjective beliefs, but by the historical biological evolution. Accordingly, human pattern recognition is not a purely logical process; the extra logical factor is given by our own history. A knowledge of the criteria man uses to recognize patterns is imperative for any practical application of universally valid quantum mechanics.

6. The Model Reference-State and Its Integrity

In order to isolate a phenomenon, we have to choose a Hilbert-space decomposition of the world-state space $\mathfrak{H}_w$, say

$$\mathfrak{H}_w = \mathfrak{H} \otimes \mathfrak{H}_e \,. \tag{16}$$

The *model reference-state* $\Psi_0 \in \mathfrak{H}$ is then defined by the dominant Schmidt state $\Phi_0 = \Psi_0 \otimes \Xi_0$ of the Schmidt decomposition (11) of the world state Φ. The absolute square of the eigenvalue $\varkappa_0$ of the dominant Schmidt state is a measure for the wholeness of the system considered; therefore we call $|\varkappa_0|^2$ the *integrity* I of the model

$$I \overset{\text{def}}{=} |\varkappa_0|^2 = |\langle \Phi | \Phi_0 \rangle|^2 \,, \tag{17}$$

$$0 < I \leqq 1 \,. \tag{18}$$

The only purely quantal system with integrity one is the whole world. A system with integrity smaller than one is entangled with its environment. Such an entanglement reflects the superposition principle, it is typical for quantum mechanics and does not occur in classical theories.

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[14] *Example:* Does the moon exist in reality as an individual entity? We are inclined to give an affirmative answer. However, the moon is composed of elementary particles with an inseparable associated electromagnetic radiation field.

Question: Does this electromagnetic field belong to the "real moon"? Note that there exists no non-arbitrary decomposition of the electromagnetic field into a part associated with the moon, a part associated with the earth, etc.

Way out: Ignore this sophistry which is not relevant to most practical problems, hence introduce an "ideal moon" not having an intrinsic radiation field.

Moral: Unprejudiced facts, and observations without data processing do not exist. Individual entities exist only as patterns created by idealizations.

The concept of integrity is called for in the individual interpretation of quantum mechanics. Conceptually, the integrity is a measure of the inherent fuzziness of the system concept in a holistic theory, but it does not concern missing information and bears no resemblance to the entropy concept of information theory. *To any system whatsoever there is associated in an objective way an inherent integrity.* Nevertheless, in a statistical interpretation the quantity $-\ln I$ can be used as an entropy. In a statistical ensemble interpretation of quantum mechanics, one would say that the system S is not in a pure state but has to be described by a non-idempotent density operator D, generated by the Schmidt-decomposition (11) of the world state-vector Φ (compare e.g. Feynman [34], p. 42),

$$D \overset{\text{def}}{=} \sum_{j=0}^{\infty} |\varkappa_j|^2 |\Psi_j\rangle\langle\Psi_j| \,. \tag{19}$$

This reduced density operator is obtained by averaging over all degrees of freedom of the environment, and gives a partial description of the world state Φ. The degree of mixture of the density operator D can be measured, for example, by a Rényi entropy H_α of order α, defined by the nonincreasing function H_α of α

$$H_\alpha \overset{\text{def}}{=} (1-\alpha)^{-1} \ln\{\operatorname{tr}(D^\alpha)\}\,, \qquad 0<\alpha<\infty\,, \qquad \alpha \neq 1\,, \tag{20}$$

$$H_\alpha \leqq H_\beta \quad \textit{if} \quad \alpha > \beta\,. \tag{21}$$

The Shannon entropy H_1 is given by the limit

$$H_1 = \lim_{\alpha \to 1} H_\alpha = -\operatorname{tr}\{D \ln D\}\,, \tag{22}$$

while H_∞ is defined by

$$H_\infty \overset{\text{def}}{=} \lim_{\alpha \to \infty} H_\alpha = -\ln\|D\| = -\ln I\,. \tag{23}$$

The norm of D equals the largest eigenvalue $|\varkappa_0|^2$ of the reduced density operator (19), so that $H_\alpha \geqq -\ln I$, or

$$I \geqq \exp(-H_\alpha)\,, \qquad 0<\alpha<\infty\,. \tag{24}$$

In the statistical interpretation, the entropies H_α, $0<\alpha\leqq\infty$, are measures of the chaoticness of the ensemble described by the density operator D, and reflect our ignorance about the individual members in the ensemble. This view allows a Boolean but only partial description. We prefer the individual non-Boolean interpretation because it permits an ontic description, and allows for a transparent discussion of the holistic nature of our world. Note that there is no contradiction between these two views, and that the uninterpreted mathematical formalism is the same. However, in the individual interpretation density operators are rejected as conceptual basic elements but appear only as convenient but secondary mathematical tools. In the individual interpretation, all states are exclusively described by rays or the associated state vectors.

The usefulness of a tensor-product decomposition (16) critically depends on the value of the integrity of the associated dominant Schmidt state. Though our developments do not depend on the value of the integrity, the system concept is useful only if the integrity is sufficiently close to one, i.e. if

$$I \approx 1 . \tag{25}$$

If the condition is violated, then the tensor product decomposition used is not sensible and has to be replaced by a more appropriate one. To find a suitable tensor-product decomposition is not an easy task because in a non-Boolean theory it is not true that there exists a sequence of models that approximate more and more phenomena in an increasingly better way. Any empirical phenomenon has its clearest appearance in a particular model; adopting new models, we isolate new phenomena. Both, extending and reducing an optimal state space impairs the manifestation of the phenomenon we are looking for.

Example

Consider a (2+1)-particle system like He or H_2^+ with the center-of-mass motion separated, so that we have a problem with 6 degrees of freedom. A brute-force solution of the Schrödinger equation in the state space $\mathfrak{L}_2(\mathfrak{R}^6)$ does not reveal any of the properties by which a chemist classifies He as an atom and H_2^+ as a diatomic molecule. Of course, in the ground state both systems have spherical symmetry, hence all properties are isotropic. Only if we decide for a particular tensor-product decomposition of the state space $\mathfrak{H}$, say as

$$(1) \qquad \mathfrak{H} = \mathfrak{L}_2(\mathfrak{R}^3) \otimes \mathfrak{L}_2(\mathfrak{R}^3) ,$$

where both $\mathfrak{L}_2$-spaces are defined by a projective representation of the Galilei group with respect to the two identical particles, we get the usual description of the helium atom as a system consisting of two interacting electrons in an external Coulomb potential. If we decide for the different decomposition

$$(2) \qquad \mathfrak{H} = \mathfrak{L}_2'(\mathfrak{R}^3) \otimes \mathfrak{L}_2''(\mathfrak{R}^3) ,$$

where $\mathfrak{L}_2'$ is the representing space of the distinguished particle (i.e. the electron in H_2^+, or the nucleus in He), and $\mathfrak{L}_2''$ is related to rotational and vibrational degrees of freedom, then we get the Born-Oppenheimer-type description of H_2^+ as a diatomic molecule, characterized by an internuclear distance, a moment of inertia, etc. These features of the traditional description are *created* by a particular tensor-product decomposition of the state space, they are not inherent in the (2+1)-particle problem. It is not sensible to describe the system H_2^+ according to the decomposition (1), or the system He according to the decomposition (2) because the associated integrities are too small. Needless to say, expectation values do not depend on a particular choice of the state space, we may choose $\mathfrak{L}_2(\mathfrak{R}^6)$, or the decomposition (1), or (2). Self-assured operationalists never should use (1) or (2), but stick to numbers and eliminate patterns.

Recall that in this paper we consider the world state at a fixed time only. If we relax this condition, the integrity I becomes a function of time t, $t \to I(t)$. *Stable systems* are characterized by a relation of the type

$$\text{stable systems:} \quad I(t) > I_0 \quad \text{for all} \quad t , \tag{26}$$

where I_0 is a real number close to 1. If the integrity is a nonincreasing function of t with $I(\infty)=0$, we have an *entangling system* representing a decay,

$$\text{decay:}\ \begin{cases} I(t_2)\leqq I(t_1) \quad \text{for} \quad t_2>t_1\,, \\ I(-\infty)\approx 1\,, \quad I(+\infty)\approx 0\,. \end{cases} \tag{27}$$

The most interesting case is a system with increasing integrity. If the integrity increases from a low value to a final value near one, we have a *disentangling system* describing the emergence of novelty

$$\text{emergence of novelty:}\ \begin{cases} I(t_2)\geqq I(t_1) \quad \text{for} \quad t_2>t_1\,, \\ I(-\infty)\approx 0\,, \quad I(+\infty)\approx 1\,. \end{cases} \tag{28}$$

Disentangling processes are related to the so-called "measurement process in quantum mechanics", and – more realistically and more importantly – to molecular evolution processes in the sense of bioevolution; they will be discussed in detail elsewhere.

7. Qualities of Model Systems

To speak of a physical system means to separate one aspect in spite of the inseparability of the world. Such an infringement is inevitable but requires a careful analysis in order to avoid inconsistencies. Restricting our attention to a particular dominant Schmidt-state, we determine the phenomena that can be recognized in a system S. For example, if F is a non-trivial projector with

$$F\Phi_0=\Phi_0\,,$$

then we say that the model system in the state Φ_0 *has* the property f associated with the subspace $\mathfrak{F}=F\mathfrak{H}_w$. Due to the holistic nature of quantum mechanics we cannot expect that $F\Phi_0=\Phi_0$ implies $F\Phi=\Phi$ because Φ describes the whole world but Φ_0 refers to a system isolated by ignoring the Einstein-Podolsky-Rosen correlation between the system and its environment. The fact that a larger system is not necessarily richer in recognizable patterns is typical for non-Boolean theories like quantum mechanics. Often, a restriction of the state space leads to the emergence of new patterns. Yet, the patterns of a system disentangled from the world state do not arise like bolts from the blue, they *preexist* in an approximate sense in the world prior to its decomposition into parts. Indeed, the Schmidt-decomposition of the world state Φ

$$\Phi=\varkappa_0\Phi_0+\Phi'\,, \quad \text{with} \quad \langle\Phi_0|\Phi'\rangle=0\,,$$

implies for every projector F fulfilling $F\Phi_0=\Phi_0$ the inequality

$$\langle\Phi|F|\Phi\rangle\geqq|\varkappa_0|^2\langle\Phi_0|F|\Phi_0\rangle=I\,, \tag{29}$$

hence

$$\|F\Phi-\Phi\|^2\leqq 1-I\,, \tag{30}$$

where I is the integrity of the dominant Schmidt-state Φ_0. If the subsystem has near optimal integrity, $I \approx 1$ then $F\Phi \approx \Phi$, so that we can consider the quality f as preexisting in the world state Φ.

In the terminology introduced in the context of Eq. (8), we can rephrase Eq. (29) by saying that the relation $F\Phi_0 = \Phi_0$ implies that the *f-ness of the world state is not smaller than the integrity of the dominant Schmidt-state* Φ_0. Every vector φ whose square of the cosine of the angle between φ and Φ_0 is larger than the integrity I enjoys the same property, so that it is useful to associate with the dominant Schmidt-state Φ_0 the following class $\mathfrak{C}_I^{\mathrm{w}}$ of world vectors φ

$$\mathfrak{C}_I^{\mathrm{w}} \overset{\mathrm{def}}{=} \left\{ \varphi : \varphi \in \mathfrak{H}_{\mathrm{w}}, \frac{|\langle \varphi | \Phi_0 \rangle|^2}{\|\varphi\|^2 \|\Phi_0\|^2} \geqq I \right\}. \tag{31}$$

Since $F\Phi_0 = \Phi_0$, $\|F\Phi\| \leqq 1$, and $\|\Phi_0\| = 1$ implies

$$\frac{|\langle F\Phi | \Phi_0 \rangle|^2}{\|F\Phi\|^2 \cdot \|\Phi_0\|^2} \geqq |\langle F\Phi | \Phi_0 \rangle|^2 = I\,,$$

it follows that

$$F\Phi \in \mathfrak{C}_I^{\mathrm{w}} \text{ for every projector } F \text{ with } F\Phi_0 = \Phi_0\,. \tag{32}$$

Obviously the state vector $\Phi_F \overset{\mathrm{def}}{=} F\Phi$ *has* the quality f, so that it is justifiable to say that the world state Φ has the quality f *relative* to the class $\mathfrak{C}_I^{\mathrm{w}}$ if $F\Phi \in \mathfrak{C}_I^{\mathrm{w}}$.

A product vector of the type $\varphi = \Psi \otimes \Xi_0$ is in the class $\mathfrak{C}_I^{\mathrm{w}}$ if and only if Ψ is in the class

$$\mathfrak{C}_I \overset{\mathrm{def}}{=} \left\{ \Psi : \Psi \in \mathfrak{H}, \frac{|\langle \Psi | \Psi_0 \rangle|^2}{\|\Psi\|^2 \|\Psi_0\|^2} \geqq I \right\}. \tag{33}$$

The class $\mathfrak{C}_I$ consists of all those vectors that are near to the model reference state Ψ_0, whereby the integrity I acts as a natural measure for the nearness. The inherent fuzziness of the system concept does not warrant to consider the dominant Schmidt-state Ψ_0 as the only proper model state, any vector from the class $\mathfrak{C}_I$ can serve equally well as a state vector for the disentangled system. For that reason we call $\mathfrak{C}_I$ the class of all state vectors *coequal* to the reference state vector Ψ_0. For a background-dependent system, the definition of a quality as given in Section 3 for a strictly closed system has to be replaced by a more liberal one. We define:

A system characterized by a model reference state Ψ_0 of integrity I is said to *have* the quality f if the corresponding projector F has an eigenvector coequal to Ψ_0, i.e. if (34)

$$F\Psi = \Psi \quad \text{for at least one} \quad \Psi \in \mathfrak{C}_I$$

The existence of a normalized vector $\Psi \in \mathfrak{C}_I$ with $F\Psi = \Psi$ implies that $|\langle \Psi | \Psi_0 \rangle|^2 \geqq I$, or

$$I \leqq |\langle F\Psi | \Psi_0 \rangle|^2 = |\langle \Psi | F\Psi_0 \rangle|^2 \leqq \langle \Psi | \Psi \rangle \langle F\Psi_0 | F\Psi_0 \rangle$$

$$= \langle F\Psi_0 | \Psi_0 \rangle = \frac{|\langle F\Psi_0 | \Psi_0 \rangle|^2}{\|F\Psi_0\|^2 \|\Psi_0\|^2},$$

so that $F\Psi_0 \in \mathfrak{C}_I$. On the other hand, if a projector F fulfills $F\Psi_0 \in \mathfrak{C}_I$, then the vector $\Psi_F \overset{\text{def}}{=} F\Psi_0$ has the property $F\Psi_F = \Psi_F$ and $\Psi_F \in \mathfrak{C}_I$, so that the system is in a state having the quality f. Hence, a *system with the model reference state* Ψ_0 *of integrity* I *has the property* f *if and only if* $F\Psi_0$ *is a vector coequal to* Ψ_0, or equivalently,

$$S \text{ has the quality } f \quad \textit{iff} \quad \langle \Psi_0 | \mathrm{F}\Psi_0 \rangle \geqq I. \tag{35}$$

8. Concluding Remarks

General mathematical system theory or the theory of automata and sequential machines are Boolean and do not encompass quantal systems. Quantum mechanics is a holistic theory, enforcing a radically different view on the notion of a system. Our ability to describe the world is limited by the possibilities to isolate objects. Inevitably, the state of a well-isolated quantal system is background dependent, and can – as a rule – not be evaluated by the kinematics and the dynamics of the isolated system alone. The non-Boolean system concept is displayed as nonintrinsic, but the integrity is a structural property of the chosen model. A model is always a partial "Booleanization" of the non-Boolean world, or more precisely: a model is created by ignoring the Einstein-Podolsky-Rosen correlations between system and environment. A model creates and isolates phenomena important to us. If we consider something else to be important, we need a different model. The non-Boolean structure of the world implies that there exists no all-embracing model. One man's reality is another man's "stuff as dreams are made of".

Can a practically useful theory be established within the proposed framework? It might be thought, at first sight, that our definition of the model reference state is useless because we do not know the world state. Two remarks are appropriate. First, conceptually sound but nonoperational definitions of the basic entities of a theory do not render the theory nonoperational. The universally valid quantum mechanics allows us to make qualitative as well as quantitative predictions beyond reach of the traditional pragmatic quantum mechanics. Second, we can embed a molecular system in a suitable environment, and construct a *molecular state adapted to this environment*. Such a route requires a knowledge of the structure of the environment. As we will show in the second paper, this problem can be solved.

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