The structure of chemical particles

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The possibility of predicting on a purely theoretical basis the existence of some "elementary" particles composing chemical particles (atoms, molecules) is studied. For this purpose the notion of Fock theories in separable Hilbert spaces is introduced. By using the mathematical structure of Fock theory—which is a nontrivial generalization of the Fock space—the notion of particle as sharp entity is defined. It is proved that chemical changes cannot be described by those Fock theories, which consider particles as sharply defined entities. This is a consequence of quantum-mechanical dynamical postulate concerning time evolutions of conservative systems. Finally it is shown that a category of Fock theories may describe changes in the number of chemical particles during conservative evolutions. This result is naturally obtained if the hypothesis about existence of some "elementary particles" composing chemical particles is accepted. Another simultaneously obtained conclusion is that chemical particles involved in chemical processes cannot be sharply defined.

1. Preliminaries

At the beginnings of chemistry as an exact science the so-called fundamental laws of chemistry were those, which suggested that chemical substances are composed of atoms and molecules (chemical particles). These laws were established after careful—for those times—quantitative determinations on initial and final compositions of reacting chemical systems. The success of chemical particles in explaining a lot of chemical facts led automatically to the idea that they are quite well defined entities. Account taking of this, we might assume, at least in principle, the existence of chemical experiments for determining the number of chemical particles in any mixture of substances. This is a very important observation, which will be consistently used below.

Later the progress of experimental physics constrained the scientists to accept that the matter is composed from various "elementary" particles, which imposed to consider that chemical particles have a structure. The basic elements of this structure were electrons and nuclei. Then the quantum mechanics has been developed as the appropriate theoretical apparatus for describing systems of such particularly small particles.

In this paper an interesting fact is evidenced, which may be formulated in two assertions.

(C1) The atomic-molecular structure of matter has been predicted by measurements of chemical composition for initial and final states of chemical systems, without considering the dynamic of chemical processes. In other words, for predicting the composition in "chemical particles" of matter, "static" considerations were sufficient.

(C2) The existence of some particles, which do not change during chemical processes, entering in the structure of chemical particles may be naturally predicted when one tries the description of chemical processes in the framework of traditional/Hilbert-space quantum mechanics. In other words, the necessity of considering a structure of chemical particles has a "dynamical" motivation.

This work represents an attempt to justify the assertion (C2). Concretely, we intend to study in Hilbert-space quantum mechanical theory two closely related problems. Firstly, we will try to make as clear as possible the meaning of sharply defined particles in quantum mechanical formalism. In the second paragraph we will show that this becomes possible if a special mathematical structure, which will be called Fock theory, is introduced. Secondly, it will be shown how, by using Fock theories and the conservative evolutions can be predicted the particle structure of chemical particles. This will be done in the third paragraph. Our discussion is entirely developed in the framework of general Hilbert-space formalism with a few and absolutely necessary physical interpretations of the involved mathematical objects. That is because the fundamental character of our conclusions imposes avoiding the use of some more or less "concrete" models, like L^2 spaces of wave functions or explicit forms of many-particle Hamiltonians. The reader may find the elementary mathematical notions used in the paper in the first part of the small Halmos' book about Hilbert spaces, [1].

2. Fock theories for chemical particles

In what follows we will use a Hilbert space $\mathbf{H}$ of infinite countable dimension. The inner product and the norm of the vectors x, y will be denoted by (x, y), $\|x\|$ respectively. The set of natural numbers, including 0, will be denoted by $\mathbb{N}$. The normed vectors from $\mathbf{H}$ represent the pure states of the systems, which may be described in $\mathbf{H}$. All the following discussion will refer to the pure states only. An arbitrarily fixed set of species of particles denoted by $S = \{s_1, \ldots, s_n\}$ is considered among basic objects of our work. They may be thought of as chemical particles, but this is not always necessary for our reasoning or conclusions.

As it has been already told in Preliminaries, we may affirm that there are chemical experiments—or measurements—permitting to determine the number of chemical particles in any state of an arbitrarily given system. Then it is not difficult to assume that, at least in principle, we may talk about "yes–no" experiments able

to decide if a state/system has or does not have a given composition in particles of S. Suppose $(k_1, \ldots, k_n), k_1, \ldots, k_n \in \mathbb{N}$ represents the ensemble of numbers of particles of the species $s_1, \ldots, s_n$ respectively. In other words, $(k_1, \ldots, k_n)$ denotes a possible composition in particles of an arbitrarily given state. The "yes–no" experiment corresponding to $(k_1, \ldots, k_n)$ will be indicated by the symbol $e(k_1, \ldots, k_n)$ and will be called occasionally counting test. Since $e(k_1, \ldots, k_n)$ may be measured, it represents a physical quantity. The set $E_S = \{e(k_1, \ldots, k_n); (k_1, \ldots, k_n) \in \mathbb{N}^{\times n}\}$ offers a complete description of chemical systems in terms of counting tests. This description becomes effective only if the elements of E_S may be represented in an adequate physically significant mathematical scheme. We will use the traditional Hilbert space quantum mechanics. In other words we have to find the objects corresponding to the "yes–no" experiments/observables in the Hilbert-space formalism. But we know that in the Hilbert-space quantum mechanics any observable is a selfadjoint operator. The question is what kind of selfadjoint operators may represent "yes–no" observables. In his famous book on Hilbert-space quantum mechanics von Neumann discusses the problem of orthogonal projectors as observables, [2]. We know that the selfadjoint operator P is an orthogonal projector in a Hilbert space $\mathbf{H}$ if $P^2 = P$. Any projector P has only two possible eigenvalues, 0 and 1. Since a "yes–no" experiment has only two possible results, i.e. "yes" and "no", it results without equivoque that the only selfadjoint operators, which may represent counting tests are orthogonal projectors (in what follows they will be called simply projectors). Therefore, the representation of the family E_S of counting tests in the Hilbert space $\mathbf{H}$ must be a family $H_S = \{P(k_1, \ldots, k_n); (k_1, \ldots, k_n) \in \mathbb{N}^{\times n}\}$ of projectors. Obviously, the correspondence between counting tests and projectors from H_S, $e(k_1, \ldots, k_n) \mapsto P(k_1, \ldots, k_n)$, should satisfy some specific general properties. In order to enounce them let us remember that there exists a one-to-one correspondence between projectors in $\mathbf{H}$ and the set of all closed subspaces of $\mathbf{H}$. This important result may be found in any general book of functional analysis. For our problem it is sufficient to know that the subspace corresponding to $P(k_1, \ldots, k_n)$ is $H(k_1, \ldots, k_n) \equiv P(k_1, \ldots, k_n) \mathbf{H}$, that is the range of the projector $P(k_1, \ldots, k_n)$. Obviously, the space $H(k_1, \ldots, k_n)$ contains all normed vectors describing those states whose composition in particles is surely $(k_1, \ldots, k_n)$. These vectors are eigenvectors of $P(k_1, \ldots, k_n)$ for the eigenvalue 1. The first observation is that for $(k_1, \ldots, k_n) \neq (k'_1, \ldots, k'_n)$ the equality $H(k_1, \ldots, k_n) \cap H(k'_1, \ldots, k'_n) = \{0\}$ has to be valid. Indeed, otherwise we would find a state having with probability 1 two different compositions in particles. This is clearly a physical nonsense. It is useful to keep in mind that the probability of finding the composition $(k_1, \ldots, k_n)$ in the state x is given by the scalar product $(x, P(k_1, \ldots, k_n)x)$. Then we will admit that the closed linear subspace generated by the set $\bigcup_{(k_1, \ldots, k_n)} H(k_1, \ldots, k_n)$ equals $\mathbf{H}$. If this is not so, then we may replace the space $\mathbf{H}$ with the just mentioned subspace. Finally, it is intuitively clear that the subspace $H(0, \ldots, 0)$, called the vacuum of S, has to be orthogonal to all subspaces $H(k_1, \ldots, k_n)$. The family of all subspaces $H(k_1, \ldots, k_n)$ will be denoted

by H_S^σ. We are now prepared for defining the notion of a Fock theory associated to the family H_S^σ.

It is convenient to denote by $C(H_S^\sigma)$ the set of all normed vectors belonging to one of the subspaces from the family H_S^σ. The elements of $C(H_S^\sigma)$ will be called *chemical states* (C-states) of the family H_S^σ. Given $x \in \mathbf{H}$ a C-state, we say that it is a *chemically pure state* (CP-state) of H_S^σ if there exists a unique projector $P \in H_S$ such that $(x, Px) \neq 0$. *Given* $\Sigma \supset C(H_S^\sigma)$ *a set of states, we say that the pair* (H_S^σ, Σ) *is a Fock theory. If all elements of* Σ *are CP-states, then we say that* (H_S^σ, Σ) *is a particle theory.*
Obviously, a Fock theory may be constructed from any family of subspaces of $\mathbf{H}$ having the general properties of H_S^σ and any set of states containing all chemical states of that family. We will prove now an important property of particle theories.

Proposition 1. If (H_S^σ, Σ) is a particle theory, then the subspaces of H_S^σ are mutually orthogonal and $\Sigma = C(H_S^\sigma)$.

Proof. Let us consider $P, Q \in H_S, P \neq Q$ and $x, y \in \mathbf{H}$ normed vectors such that $Px = x, Qy = y$. Since (H_S^σ, Σ) is a particle theory, $(x, y) = (Px, y) = (x, Py) = 0$. It results that the ranges of P and Q are orthogonal, so that the subspaces of the theory are mutually orthogonal. Further, if z is a normed vector, which does not represent a chemical state, then we may write $z = \sum_{p \in H_S^\sigma} c_p x_p$. Since z is not a chemical state, we may find $p \neq p'$ such that $c_p, c_{p'} \neq 0$. Finally, given P, P' the projectors corresponding to subspaces p, p' respectively, we find $(z, Pz), (z, P'z) \neq 0$, which means that z is not a CP-state. The proposition is completely proved.   □

The physical meaning of Proposition 1 is almost obvious: in a particle theory particles are sharply determined entities. In other words only those states are accepted in the theory, which have a precisely determined composition in particles.

Let us observe that, besides particle theories we can imagine other two classes of theories. One of these classes is that of *orthogonal theories*. A theory (H_S^σ, Σ) is said to be orthogonal if the elements of H_S^σ are mutually orthogonal but it has states, which are not chemically pure. Obviously, all C-states of an orthogonal theory are also CP-states. The other class is that of *non-orthogonal* theories. For such a theory the elements of H_S^σ are not mutually orthogonal. It is easy to prove that, in an orthogonal theory any normed vector z, which is not a CP-state, may be represented as a normed linear combination (or series) of CP-states. Non-orthogonal theories have a property, which is important from physical point of view.

Proposition 2. In any non-orthogonal theory there exist C-states, which are not CP-states.

Proof. Let (H_S^σ, Σ) be a non-orthogonal theory. Then we may find two C-states x, z such that $(x, z) \neq 0$ and for two non-orthogonal projectors $P, Q \in H_S$, we have $Px = x$, $Qz = z$. Then we may write $(x, Px) = 1$, $(x, Qx) \neq 0$. The equality $(x, Px) = 1$ being obvious, it remains to prove that $(x, Qx) \neq 0$. But $Q = Q_z + Q'$, where Q_z is the projector on the one-dimensional subspace generated by z and Q' is a projector orthogonal on Q_z. Then we have $(x, Qx) = \big(x, (Q_z + Q')x\big) \geqslant (x, Q_z x) = |(x, z)|^2 \neq 0$. Similarly it may be proved that $(z, Pz) \neq 0$, so that both x and z are not PC-states. The proposition is proved. $\qquad\square$

At this moment it is important to make the physical meaning of Fock theories as clear as possible. It consists essentially in the fact that a Fock theory for the set $S = \{s_1, \dots, s_n\}$ is a mathematical scheme able to describe chemical systems/states containing particles of the species from S only and their time evolutions (see the next section). Of a major interest is also the observation that Fock theories represent a quite natural framework for distinguishing those particles, which are sharply defined entities. The above considerations suggest that it is better to talk about *states of a Fock theory in which the composing particles may be considered to be sharply defined*. Naturally, such states are those, which are chemically pure. Since only chemical states can be CP-states, we may prove that *a state is chemically pure if and only if it belongs to a subspace from* H_S^σ, *which is orthogonal to any other subspace of* H_S^σ. Therefore, when we talk about sharply defined particles, we understand that the particles in question are described by a state, which is chemically pure in a given Fock theory. It results that we consider meaningless the statement "some given particles are sharply defined entities" unless a theoretical framework—in our case a Fock theory—is specified. That is because we have never sufficiently many empirical data for saying that the mentioned statement is true. Therefore, the only possible procedure is to choose a theoretical framework, which describes chemical species in accord with the existing at a given moment empirical data. The chosen theory must be able to predict, at least in principle, the behavior of chemical systems. For instance to describe the time evolution of such systems. In the next paragraph the time evolution of conservative chemical systems in Fock spaces will be discussed as well as its connection with the structure of chemical particles.

3. Conservative time evolutions of chemical states

The dynamical principle of non-relativistic quantum mechanics affirms that the time evolution of any state is completely described by a family of unitary operators in **H**, denoted by (U_t), where t runs the set $\mathbb{R}$ of real numbers. We will call

(U_t) time evolution or simply evolution. The conservative systems are described by one-parameter strongly continuous groups of unitary operators. In other words, (U_t) is a so-called conservative evolution if it has the following two properties:

(e1) $U_{t+t'} = U_t U_{t'}, \quad \forall t, t' \in \mathbb{R}$;

(e2) $\lim_{t \to t'} \|U_t x - U_{t'} x\| = 0, \quad \forall t' \in \mathbb{R}, x \in \mathbf{H}$.

It is interesting to point out that the group property (e1) is justified by the homogeneity of time with respect to conservative systems, but the strong continuity (e2) is not a physically transparent property. It is only indirectly justified by the fact that a one parameter group is generated by a selfadjoint operator/Hamiltonian if and only if it is strongly continuous, (Stone's theorem). In what follows we will use conservative evolutions without any reference to their corresponding Hamiltonian or to possible concrete forms of Hamiltonians.

The dynamical principle implies clearly that any change of a state must be considered by the general evolution of the system. Therefore, any chemical change occurring in a system must be described by its evolution. It is supposed also that the conservative systems studied bellow do not exchange matter with the environment, which means that any modification of the number of particles is caused by the chemical interactions between particles contained in those systems.

In order to describe chemical processes in a Fock theory $(H_S, \Sigma)/(H_S^\sigma, \Sigma)$ we need some specific notions. Let x be a chemical state and (U_t) an evolution with the property $U_t \Sigma \subseteq \Sigma, \forall t \in [0, \infty)$ (called admissible in the (H_S^σ, Σ) theory). *For any species s_i we define the function* $C_{i,x} : [0, \infty) \to \mathbb{R}$, $C_{i,x}(t) = \sum_\alpha k_{i\alpha}(U_t x, P(\alpha) U_t x)$, *where* $k_{i\alpha} = k_i$ *if* $\alpha = (k_1, \dots, k_n)$, *which will be called composition function for the triple* $(x, (U_t), s_i)$. Let us consider that (H_S, Σ) is orthogonal. For any $k \in \mathbb{N}$ we may define the projector $P_{ik} = \sum_{(k_1, \dots, k_n) \, k_i = k} P(k_1, \dots, k_n)$. The selfadjoint operator $N_i = \sum_k k P_{ik}$ is an observable whose eigenvalues represent the number of particles of the species s_i. In this case the corresponding composition function takes the simple form $C_{i,x}(t) = (U_t x, N_i U_t x)$. Obviously, such a construction can not be done for non-orthogonal theories.

Now we are prepared for proving the central result of this paper.

Theorem. Let us consider (H_S, Σ) a particle theory and (U_t) an admissible evolution. If (U_t) defines a non-constant composition function, then it is not strongly continuous.

Proof. Let $C_{i,x}(t) \equiv C(t)$ be the non-constant composition function. Consider the following two statements:

(i) there exists $\tau \geqslant 0$ such that $\forall t' > \tau, \exists t'' \in (\tau, t')$ with the property $C(t'') \neq C(\tau)$;

(ii) for all $\tau \geqslant 0$ there exists $t' > \tau$ such that $C(t'') = C(\tau), \forall t'' \in [\tau, t')$.

One of these two statements must be true since (ii) represents the negation of (i). It will be shown that in both cases the evolution is not strongly continuous. Suppose first that (i) is true and let us take an interval (τ, t') on which $C(t)$ is not constant. Then we can find $t'' \in (\tau, t')$ such that $(U_\tau x, U_{t''} x) = 0$. Indeed, if we admit that $(U_\tau x, U_t x) \neq 0, \forall t \in (\tau, t')$, we get that $C(t)$ is constant on (τ, t') since in particle theories two non-orthogonal states belong to the same subspace of the theory, which contradicts (i). By using this fact, we can construct a sequence (t_k) such that the following is true: $\lim t_k = \tau, (U_\tau x, U_{t_k} x) = 0, \forall k$. If it is admitted that (U_t) is continuous, then obviously $\lim_k (U_\tau x, U_{t_k} x) = 0 = (U_\tau x, U_\tau x) = 1$, absurd. The obtained result is that, if (i) is true, then (U_t) is not strongly continuous. Suppose now that (ii) is true. Then there exists $[0, t_1), [t_1, t_2), \ldots, [t_n, t_{n-1}), \ldots$ an at most denumerable family of intervals whose union is the interval $[0, \infty)$ and $C(t)$ is constant on each $[t_{n-1}, t_n)$, the constants corresponding to different intervals being different. The last assertion is supported by the fact that $C(t)$ is not constant. In the interval $[t_{n-1}, t_n)$ we find a sequence $t_k^n \to_k t_n$. Suppose (U_t) is strongly continuous. Then, just as it has been done in the case (i), we get the following equalities: $\lim_k (U_{t_k^n} x, U_{t_n} x) = 0 = (U_{t_n} x, U_{t_n} x) = 1$, absurd. The theorem is completely proved. $\qquad\square$

This theorem has important physical implications. Their discussion needs a definition of chemical systems adapted for considering chemical changes. More precisely, in the framework of Fock theories any chemical change means a modification in time of the number of particles present in the system. The most natural way of giving a formal definition for chemical systems is to identify them with pairs of the type $(x, (U_t))$, where x is a chemical state and (U_t) an admissible evolution. The simplest empirical model of a chemical system is that of a closed envelope containing different particles whose number changes according to a given evolution.

The first important consequence of Theorem is that in particle Fock theories there are not conservative evolutions describing changes in the number of particles. In other words, all subspaces from H_S^σ are invariant under operators of any conservative evolution. This means that, given (U_t) a conservative evolution, we have $U_t H(k_1, \ldots, k_n) \subseteq H(k_1, \ldots, k_n), \forall t \in \mathbb{R}, (k_1, \ldots, k_n) \in \mathbb{N}^n$. We can see that particle Fock theories are perfectly adapted for describing systems of particles, which are stable in conservative conditions. In other words, *if the number of particles in any state and at any moment is perfectly determined, then it can not change under conservative evolutions. Equivalently, the sharply defined particles can not change their number in conservative systems.* The very important chemical conclusion of all these facts is that particle Fock theories reject the possibility of

chemical reactions to occur in conservative conditions. On the other hand a natural extrapolation of experimental results concerning chemical transformations lead to the conclusion that chemical substances may react in isolated systems. Taking this conclusion as a postulate we may affirm that *only those Fock theories, which are orthogonal but some of their states are not chemically pure or are non-orthogonal may describe chemical changes of the number of chemical particles in conservative conditions.*

We are now in position to combine all these considerations for obtaining the central "chemical" conclusion of this paper. It is based on the above-obtained conclusion concerning theories able to describe chemical changes. That conclusion becomes really interesting only if we are in position to construct physically meaningful conservative evolutions predicting the changes of the number of chemical particles.

Let us notice again that, if a closed system is composed from particles, which are sharply defined entities, then it can be described in a particle Fock theory. More precisely, there exists a uniquely determined subspace $H(k_1, \ldots, k_n)$ of that theory, which describes all states of the considered system. In other words the description of such a system is purely mechanical. But for such systems the standard quantum mechanics prescribes Hamiltonians of a well-known form. This fact holds for any subspace so that for particle-theories we have physically significant conservative evolutions. *Therefore, it becomes natural to assume that chemical particles are composed from other, sharply defined particles, which do not change their numbers when chemical reactions occur.* It remains to show how this hypothesis permits the construction of conservative evolutions suitable for describing changes of the number of chemical particles. Before giving the appropriate mathematical scheme, it is useful to explain intuitively what we intend to do. Firstly we will take a family of species of particles, which are assumed to compose the chemical particles. These particles are elementary, in the sense that they do not change during chemical processes. It follows naturally that they will be described by a particle theory. Then it will be assumed that any chemical particle is composed by a well-determined number of elementary particles from each species. This assumption leads naturally to the possibility of "embedding" the Fock theory for chemical particles into that for elementary particles. The important result of this procedure is that the conservative evolutions may induce changes in the number of chemical particles. Now, for proving this we have to put the problem in the precise mathematical language of Fock theories.

Let us assume that particles of the species $s_1, \ldots, s_n$ are composed from particles of the species $\varepsilon_1, \ldots, \varepsilon_m$. These particles are described by a particle Fock theory constructed in a Hilbert space **G**. The characteristic set of subspaces of this theory is $\{G(j_1, \ldots, j_m); (j_1, \ldots, j_m) \in \mathbb{N}^m\}$. Let us denote by $(\varepsilon_1 | s_i), \ldots, (\varepsilon_m | s_i)$ the number of particles of the species $\varepsilon_1, \ldots, \varepsilon_m$ respectively composing one particle of the species s_i. Taking into account that the Fock theory for the species $s_1, \ldots, s_n$ is defined in the Hilbert space **H**, we will say

that these particles are constructed from particles of the species $\varepsilon_1, \ldots, \varepsilon_m$ if there exists an linear function $f : \mathbf{H} \to \mathbf{G}$, satisfying the following requirements:

(c1) $f : \mathbf{H} \to f(\mathbf{H})$ is an isomorphism of Hilbert spaces;

(c2) the orthogonal projectors on the subspaces $f(H(k_1, \ldots, k_n))$ and $G(j_1, \ldots, j_m)$ commute for all $(k_1, \ldots, k_n) \in \mathbb{N}^n$, $(j_1, \ldots, j_m) \in \mathbb{N}^m$;

(c3) $f(H(k_1 \ldots, k_n)) \cap G(j_1, \ldots, j_m) \neq \{0\} \Rightarrow \sum_i k_i (\varepsilon_u | s_i) \leqslant j_u, \forall u, 1 \leqslant u \leqslant m$.

The (c1)–(c3) conditions have clear physical meanings. Thus, condition (c2) means that we admit that in principle the number of chemical and of "elementary" particles entering in their composition may be measured simultaneously. In fact this assumption looks natural once we accepted that the numbers $(\varepsilon_j | s_i)$ are known for all $1 \leqslant j \leqslant m, 1 \leqslant i \leqslant n$. The (c1) and (c3) conditions have an obvious meaning, so that special explanations are not necessary. It should be understood that the existence of the function f in (c1)–(c3) is nothing more than the mathematical transcription of the assumption concerning the structure of chemical particles. In Appendix we give an example, which shows that this assumption is in accord with the standard quantum-mechanical representations of chemical particles as constituted from electrons and nuclei.

Let us consider a conservative evolution (U_t) for elementary particles defined for a particle Fock theory with the subspaces $G(j_1, \ldots, j_m) \subset \mathbf{G}, (j_1, \ldots, j_m) \in \mathbb{N}^m$. We will show that it induces a conservative evolution for chemical particles, able to predict chemical changes. In order to prove this fact we need to construct a Fock theory for chemical particles in the space $\mathbf{G}$. Naturally, such a theory must be an extension of the already considered theory with the characteristic subspaces $\{H(k_1, \ldots, k_n); (k_1, \ldots, k_n) \in \mathbb{N}^n\}$. For the sake of simplicity in what follows the subspaces $f(H(k_1, \ldots, k_n))$ will be denoted also by $H(k_1, \ldots, k_n)$. To avoid any confusion it is sufficient to remember that in the rest of the paper $H(k_1, \ldots, k_n)$ are subspaces of $\mathbf{G}$. It must be kept in mind that $f(H(0, \ldots, 0)) \oplus f(\mathbf{H})^\perp = H(0, \ldots, 0)$, the right part denoting the vacuum in the space $\mathbf{G}$, according to the above-accepted convention (here $f(\mathbf{H})^\perp$ is the orthogonal complement of $f(\mathbf{H})$ and "$\oplus$" the direct sum of subspaces). That is because in most cases $f(\mathbf{H}) \neq \mathbf{G}$. The following proposition establishes some properties of the embedded into the space $\mathbf{G}$ theory and suggests that the number of chemical particles may change during conservative evolutions.

Proposition 3. The following assertions are true:

(i) $H(\alpha) = \underset{\beta \in \mathbb{N}^m}{\oplus} [H(\alpha) \cap G(\beta)], \forall \alpha \in \mathbb{N}^n$;

(ii) for any $\beta \in \mathbb{N}^m$, $G(\beta)$ is spanned by the union $\bigcup_{\alpha \in \mathbb{N}^n} [G(\beta) \cap H(\alpha)]$.

Proof. Both assertions result from a property of commuting projectors. Let $\{P_n; n \in \mathbb{N}^n\}$ be a family of projectors and $H_n, n \in \mathbb{N}$, their ranges, respectively. If Q is a projector with the property $[Q, P_n] = 0, \forall n$, then the union $\bigcup_{n \in \mathbb{N}} (G \cap H_n)$ spans the range G of Q. Taking into account the property (c2), the assertions (i), (ii) result immediately. In (i) we use the direct sum since, as it is easy to verify, the terms are mutually orthogonal. $\square$

It remains to observe now that the evolution (U_t) leaves the subspaces $G(\beta)$ invariant but, as it results from Proposition 3(ii), the number of chemical particles is changed.

The physical point is that physically meaningful conservative evolutions for elementary particles whose number does not change may predict the change of the number of chemical particles. *That is why we affirm that the chemical reactions in conservative conditions may be predicted if it is assumed that chemical particles are constituted from elementary particles, i.e. particles whose number does not change in time during chemical processes.* At this moment it may be considered that we obtained a satisfactory argumentation for the assertion (C2).

4.   Comment

In this short section we intend to discuss an important consequence of the above-presented theoretical developments. It is strictly related to the Theorem, which has been proved in the third section. In strictly chemical terms, this result claims that sharply defined chemical particles can not react in conservative conditions. It has been obtained after we accepted that the sharply defined particles are those, which may be described only by chemically pure states. This fact generates a conflictive situation. We mean that the fundamental dynamical law of quantum mechanics does not "permit" chemical reactions between sharply defined particles. On the other hand, many quantum chemical developments accept implicitly a sort of "sharpness" of atoms and molecules, even if their electronic–nuclear structure is explicitly considered. In fact quantum chemical kinetics studies mainly elementary reactions, in which the mentioned question of "sharpness" do not appear. One of the merits of Fock theories is that they offer the possibility to distinguish between sharply and non-sharply defined chemical particles.

Returning to the above-evidenced conflictive situation, we saw that it forces us to reject particle Fock theories for describing reacting chemical particles and accept implicitly that chemical particles are not sharply defined. But this only fact is obviously insufficient for our purpose. We have to find a natural way for accounting the possibility that chemical reactions may occur in conservative systems. The concrete problem is how to find meaningful conservative evolutions able to predict chemical changes. The most natural idea, based on the generally

accepted conjecture about particle description of systems is that in any chemical system there are particles, which do not change during chemical reactions and enter in the composition of chemical particles. They must be described by particle Fock theories. As it has been seen in our work, this idea was sufficient for constructing "reactive evolutions". This is the way in which the structure of chemical particles may be predicted by quantum-mechanical dynamical arguments. It is also understandable that the physical origin of the non-sharpness of chemical particles is exactly the fact that they are composed from other particles.

Appendix

Let us consider the chemical species $s_1, \ldots, s_n$ whose particles/chemical particles are constituted from "elementary" particles of the species $\varepsilon_1, \ldots, \varepsilon_m$. We will sketch the construction of a Fock theory for chemical particles embedded into a particle Fock theory for "elementary" particles, which is a Fock space

$$\mathbf{G} = \bigoplus_{(j_1, \ldots, j_m)} G(j_1, \ldots, j_m). \tag{1}$$

According to Proposition 3, if the subspaces $H(k_1, \ldots, k_n) \cap G(j_1, \ldots, j_m)$ are constructed, then the Fock theory we look for is completely determined. In order to do this, we will use a technique of clusters, which may be found in the Reed and Simon's book, [3]. Since our example is only illustrative, the embarrassing symmetry considerations will be avoided. Let us begin with the simplest situation. Consider B a finite set of "elementary" particles and denote by β the number of its elements. Consider also a family $\{C_1, \ldots, C_k\}$, $\bigcup_{i=1}^{k} C_i = B$ of mutually disjoint subsets of B. The elements of this set will be called clusters. Let us denote h_β the standard Hamiltonian for particles from B, which acts in the Hilbert space $H(B) = L^2(\mathbb{R}^{3\beta})$. For any cluster C_i we may define an "inner" Hamiltonian, which is the standard Hamiltonian for particles from C_i only. Then, according to Reed and Simon, we may represent the space $H(B)$ as a tensor product of a family of subspaces, as follows:

$$H(B) = H(T) \otimes H(T_c) \otimes H(C_1) \otimes \cdots \otimes H(C_k). \tag{2}$$

All spaces in (2) are L^2-spaces. The space H(T) corresponds to the center of mass of all particles from B, $H(T_c)$ to the center of mass of all clusters, $H(C_i)$ to the particles of the cluster C_i after the movement of their center of mass has been removed. Since we consider that all clusters represent chemical particles, it must be admitted that all inner Hamiltonians have bound states. Let $H_b(C_i)$ be the closed subspace of $H(C_i)$ spanned by the bound states of the cluster C_i. In this case we may construct the subspace

$$H_b(B) = H(T) \otimes H(T_c) \otimes H_b(C_1) \otimes \cdots \otimes H_b(C_k). \tag{3}$$

It is obvious that $H_b(B)$ is a subspace of the type $H(k_1, \ldots, k_n)$, where $n = k$, $k_i = 1$, $1 \leqslant i \leqslant n$.

The form of the subspaces $H(k_1, \ldots, k_n) \cap G(j_1, \ldots, j_m)$ is given bellow. In the next formula, the particles of the chemical species are clusters of particles of the species ε_j and $H(s_i)$ denotes the subspace of bound states of the clusters corresponding to the species s_i:

$$\begin{aligned}
H(k_1, \ldots, k_n) &\cap G(j_1, \ldots, j_m) \\
&= H(T; j_1, \ldots, j_m) \otimes H(T_c; k_1, \ldots, k_n) \otimes H(s_1)^{\otimes k_1} \otimes \cdots \otimes H(s_n)^{\otimes k_n} \otimes \\
&\quad \otimes H_r(j_1, \ldots, j_n).
\end{aligned} \tag{4}$$

The meaning of terms in the formula (4) is quite clear from the preceding example, except the last term representing the space corresponding to those particles, which do not enter in the clusters defining chemical particles. It is clear that by following this procedure, we have no chance to obtain orthogonal theories. It is also important to observe—and this fact has a transparent physical meaning—that the vacuum of such a theory must be a subspace of infinite dimension.

References

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[2] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, 1955).
[3] M. Reed and B. Simon, *Methods of Modern mathematical Physics, III Scattering Theory* (Academic Press, 1979).