# BmPa

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IX

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# Bollettino di Matematica pura e applicata

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# Mathematical Studies on Quantum Mechanics

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#### Abstract

This review paper contains some posthumous writings of Prof. Matteo Campanella on the interpretative aspects of Quantum Mechanics and on a possible derivation of Born's rule. The goal of his work was to arrive at a characterization of the state of a subsystem of a quantum system independently from any probabilistic interpretation. Starting from a natural way of defining such a state, he found that a way of characterizing it is through a partial density operator, that comes out as a consequence of the formalism and of a few reasonable assumptions, connected with the notion of a state. The density operator arises as an orbit invariant. One sees that one is forced to give it a probabilistic interpretation and that its quantitative implementation is equivalent to Born's rule. In these notes all the Hilbert spaces involved in the discussion are supposed to be finite-dimensional.

Key words: quantum mechanics; Born's rule; finite-dimensional Hilbert space. MSC: 58D30; 81P99. PACS: 03.65.-w.

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# Prologue

Prof. Matteo Campanella was born in Palermo on September 27, 1947, and he died prematurely on June 18, 2016. He was a professor at the DEIM department (Dipartimento di Energia, ingegneria dell'Informazione e modelli Matematici) of Palermo University.

This monograph contains some of his writings on the foundations on quantum mechanics and on a possible derivation of Born rule. The notes are presented as he wrote them. Prof. Matteo Campanella meant to examine some propositions in depth, but, owing to its premature death, he was not able to complete his work.

I met my husband Matteo in 1982. Right away I was fascinated by his personality. His cultural interests ranged from sciences to music, history, philosophy. His passion for the sciences was not lower than the ones for politics and for social concerns.

He loved Physics and Maths. He had always been studying the foundations of Quantum Mechanics and, in particular, its interpretation. Sometimes he spoke with me about these themes, and I always tried to persuade him to publish his work. In 2011, he told me about a new interesting result. This time, I wanted to persuade him to publish his results, but he was not fully satisfied of his writing, and intended to modify some parts of his work. Five years have passed, I often asked him what the status of his work was, and he always answered me that it wasn't entirely clear. Over these five years, he continued to study this problem. The results of his studies are in one hundred files in his computer, and in a lot of notes. I decided to publish a part of his writings on this subject, hoping that someone may continue his work.

Palermo, 20 April 2017

Maria Stella Mongiovì

## Preface

This monograph contains some posthumous mathematical writings of Prof. Matteo Campanella on some interpretative aspects of Quantum Mechanics. The general goal of this work is to arrive to the Born's rule, one of the key principles of the probabilistic interpretation of quantum mechanics, but in a way independent of any a priori probabilistic interpretation. This topic is indeed a very active line of research nowadays, because of its fundamental interest. Here we try to outline and summarize the main lines of this work.

Born's rule was proposed by Max Born in 1926, in an attempt to interpret the physical meaning of the wavefunction, by relating it to the probability of obtaining some of the allowed values of the physical quantities characterizing the system when making a measurement on the system. It thus plays an essential role in the connection between quantum theory and experiments and it has a deep conceptual interest because it was one of the ways in which indeterminism entered in fundamental physics, in parallel with Heisenberg's relations. In the standard formalism of quantum mechanics it is considered as a basic postulate. However, due to its deep implications, its operational analysis, its physical derivation and its philosophical interpretation have always deserved much interest. Recall, for instance, that the same idea of probabilistic interpretation of the wavefunction aroused much discussions between Einstein [11], for whom this probabilistic character was an indication of some missing information, and Bohr and many other researchers, for whom this probabilistic character was inherent of deep physical reality and quantum mechanics was a complete theory [4], [14].

Many attempts towards a consistent derivation of Born's rule have been made along several different lines, for instance in the many-universes interpretation [12], [7], [10], [13], or from the de Broglie-Bohm interpretation [1], [3], [5], [15]. At the turning of the century, other kinds of proposals arised: Deutsch proposed to derive Born's probabilistic rule from the non-probabilistic axioms of quantum mechanics combined with classical decision theory [2], [8], [9], [18]; Zurek proposed an environment-related derivation based on the invariance (relative to a given environment  $\mathcal{E}$ , and therefore called "envariance" in short) of entangled states under a swap of the outcomes of the system  $\mathcal{S}$  without changing the outcomes of the environment  $\mathcal{E}$ , thus implying the equiprobability of the corresponding swapped states [16], [19], [17], [20],[21].

Quantum mechanics in general, and the mentioned derivations in particular, make several important mathematical assumptions about the definition of state of the system, the invariant transformations related to it, the relation between the state and probabilities, and so on. The aim of this work is to start from the uncontroversial interpretative assumptions of quantum mechanics and from a suitable mathematical formalism, in order to derive by the combination of them the other most relevant interpretative items of quantum mechanics, especially Born's rule. The mathematical assumptions are: 0) the properties of a quantum system H can be described in terms of a Hilbert space H associated with it; 1) if the system W is a universe, a state of it may be identified as a ray of W, that is, an element of a projective space  $\mathbb{P}(W)$ ; 2) if a system L is composed of two subsystems H and K its Hilbert space is a tensor product  $H \otimes K$ ; 3) the only allowed transformations for the states of a universe W are induced by unitary transformations of its Hilbert space W. These are well accepted features in quantum mechanics. At this point, an essential part of the Campanella's program is the use of a formulation mathematically equivalent to transformations but involving a single state of an extended composite system which, seen from different partial points of view, appears as the transformation, the state "before" transformations and the state "after" transformation. In doing so, it is intended to avoid two drawbacks of a transformation involving a) the totality of states and b) the idea of an "evolution" from an old state to a new one.

In Section 2 the state of a subsystem of a quantum system is characterized independently of any probabilistic interpretation. In contrast to classical mechanics, in quantum mechanics the nature of a state of a subsystem of a given composite system is deeply different as that of the whole system, because of the presence of entanglement for the states. In the conventional setting of quantum mechanics, the state of the subsystem is described by a partial density operator, whose definition is justified by the probabilistic interpretation and the use of Born's rule. In section 2, instead, it is shown that one way of characterizing the state of a subsystem is through a partial density operator independently of any a priori probabilistic interpretation. The latter will come out as a consequence of the formalism and of a few assumptions, connected with the notion of a state. Suppose that a composite system  $\mathcal C$  consists of two parts  $\mathcal S$ (the "system") and  $\mathcal{E}$  (the "environment") with respective Hilbert spaces H and K. A key step for the introduction of a natural definition of a state of S is the formalization of the "envariance" property indicated by Zurek (namely, an "environment-assisted" invariance exhibited by entangled systems). From this assertion, and describing the states of the composite system ("the Universe") as pure states, it is concluded that the state of S associated with a pure state  $|\phi\rangle$  of the composite system may be defined as the orbit of  $|\psi\rangle$  under the action of the group  $\mathbf{I} \otimes \mathcal{U}(K)$ , being  $\mathbf{I}$  the identity operator and  $\mathcal{U}(K)$  the group of the unitary transformations in K.

According to this, the state of S is characterized as a subset of the space of the composite system. To arrive at a definition involving only points of the Hilbert space of S, any set of mathematical objects in bijection with the orbits of  $\mathbf{I} \otimes \mathcal{U}(K)$  can be as well used to define the state. Thus, the author arrives at a characterization of a state of S as a density operator arising as an orbit invariant without any a priori probabilistic interpretation.

In Section 3, the step from the above non-probabilistic definition of the state of S to a probabilistic definition is given. Two related, but distinct items about this discussion are considered. The first consists in the different ways of representing the state of S depending on whether it is considered isolated or not. Classically, the state of a composite system is described as a point in its phase space, expressed as the Cartesian product of the phase spaces of the component subsystems. If also in the classical case the state of S is defined a la Zurek, with the role of  $\mathcal{U}^Z(K)$  (the quotient group of  $\mathcal{U}(K)$  modulo its center) substituted by the role of the group of the canonical transformations of the phase space of  $\mathcal{E}$ , the orbits of the latter group can be parameterized by the points of the phase space of  $\mathcal{S}$  both in the absence and

in the presence of interaction. So in the classical case the conventional definition of states of the subsystem is compatible with Zurek's point of view. In the latter case, the projections of the initial and final points of the composite system are points of the phase space of S even if an interaction takes place. Since the final point of S depends both on the initial states of S and of  $\mathcal{E}$ , if the state of  $\mathcal{E}$  is not completely known statistical methods must be introduced, but the description of the state of S by means of a point in its phase space is not forbidden, at least in principle. The situation is quite different in the quantum case. Even if the initial state is described by a point of  $\mathbb{P}(H)$ , the final state of S (i.e. the "projection" of the final state of the composite system) is a density operator with rank > 1 and not just a one-dimensional projector if an interaction with the environment has taken place.

The second question concerns the different ways of describing the evolution of the system in the absence or in the presence of interaction. Both in classical and quantum cases the interaction precludes the possibility of establishing a functional relationship between the initial and the final states of  $\mathcal{S}$ : the only thing that can be said in general is that both are "projections" of the initial and final states of the composite system. But, in contrast to the classical case, in the quantum case a fundamental difference exists in the mathematical description of the states of  $\mathcal{S}$  depending on whether the system is considered as isolated or as a subsystem of  $\mathcal{C}$ . In the first case the states are points of  $\mathbb{P}(H)$ , while in the second one they are represented by density operators. In the most popular axiomatics of quantum mechanics the need of this difference is a consequence of the a priori introduction of a probabilistic interpretation of the theory and its quantitative expression through the Born's rule. Instead, here this difference is a direct consequence of two assumptions: that a composite system is described by a tensor product, and that the correct notion of state of a subsystem is the one implied by Zurek's considerations. Neither of these assumptions involves probability; specifically, the density operator arises merely as an orbit invariant.

Suppose we may consider the system S isolated from the environment  $\mathcal{E}$  before some instant  $t_0$ , but that the interaction is switched on, until  $t_1$ , so that, for  $t > t_1$ S and  $\mathcal{E}$  can be again modeled as mutually isolated. Before  $t_0$ , S and  $\mathcal{E}$  evolve independently; at  $t < t_0$ , S is in a well definite state  $\varsigma \in \mathbb{P}(\mathcal{H})$  and  $\mathcal{E}$  in a state  $\tau \in \mathbb{P}(\mathcal{K})$ . At  $t_0$  the interaction is switched on. Therefore the state of C after  $t_0$  becomes entangled. In particular, let  $|\psi\rangle$  denote a normalized representative of the state at  $t_1$ . At this instant the system must be considered as interacting with the environment as the "past" is concerned, and as non interacting regards to the "future". If "non interacting" were the same thing as "isolated", we could think that both descriptions of the state must hold: as an interacting system it ought to be described by  $\rho_S = tr_E |\psi\rangle \langle \psi |$ , (which means a partial specification of the state of C) and as a non interacting system by a (perhaps partial) specification of some point of  $\xi$  of  $\mathbb{P}(\mathcal{H})$ .

A careful analysis shows that, when there is in  $\rho_S$  a some kind of degeneracy, the notions of "non interacting" and "isolated" are not equivalent. This means that not for all the density operators the description in terms of states of an isolated system is possible. More precisely, it is shown that if a system  $\mathcal{H}$  can be considered isolated

there is at most a single multidimensional eigenspace of  $\rho_H$  and that, if it exists, it is the null eigenspace. The spectral expansion of  $\rho_H$  is  $\rho_H = \sum wP(w)$  where all the projectors P(w) are of rank one, and the possible states of  $\mathcal{H}$  in  $\rho_H$  as an isolated system are the states associated with these projectors.

In the next step it is seen that we are forced to give to a density operator whose non-null eigenspaces are all one-dimensional, called *generic density operator*, a probabilistic interpretation: it is shown that it is possible to fix uniquely a probability law on the set  $\Xi$  of eigenstates of  $\rho_S$ , so that the state becomes a well-defined random variable.

This result is obtained in the successive sections. Barycentric coordinates with respect to an orthogonal set of states are introduced, bringing a simplex structure together the standard topology. After a detailed mathematical analysis of the set of generic density operators, the problem of the probability of the non-null eigenstates of such operators is studied and the universality of the probability distribution is shown. Without any additional axiom, the probability of each state is shown to be equal to the corresponding eigenvalue of the density operator. Thus, Born's rule is recovered as a consequence rather than introduced as an axiom.

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#### 1 Introduction

The properties of a quantum system in different physical conditions can be described in terms of a Hilbert space H associated with it. For notational simplicity, we will denote as a rule the system and its Hilbert space with the same symbol. As long as our enquiry concerns only foundational aspects, we will avoid the technicalities needed when the dimension of H is infinite, so that it will be always supposed finitedimensional. As a rule, the physical conditions which have influence on the system depend on the state of the whole Universe. However, in many circumstances these effects can be taken into account, at least as an approximation, by considering H as a subsystem of a larger system W, which will be considered as a model of "Universe" in the specified circumstances. The system W will be called a universe, of which H is a subsystem. In contrast with the notion of Universe (which is absolute and somewhat metaphysical, and as such too dangerous to include it in a physical theory) the notion of universe is relative. Indeed, if in some circumstances the physical conditions influencing H can be described regarding it as a subsystem of the universe W. in more general circumstances W itself must be considered as a subsystem of some larger universe. In more restricted circumstances, H itself may be considered as a universe. Hence the same system may be considered or not a universe. In the latter case, it will be modeled as a subsystem of some universe.

The approach to our discussion will be roughly the following. We will state without further analysis the interpretative assumptions of Quantum Mechanics which are at present substantially uncontroversial. On the contrary we will try to derive from them and from the mathematical formalism the other most relevant interpretative items (including the Born's rule).

The first assumption we make without discussion is that, if a system W is considered as a universe, a state of it can be specified by a ray of W, that is an element of the associated projective space  $\mathbb{P}(W)$ .

An equivalent formulation is to specify the state through a projector P of rank one operating on W. We will denote  $\psi$  an element of  $\mathbb{P}(W)$  and  $|\psi\rangle$  any normalized ket representing  $\psi$  (defined up to an arbitrary phase factor). Consequently the corresponding projector is  $P = |\psi\rangle \langle \psi|$ .

The second assumption is that, if a system L is composed with the two subsystems H and K, its Hilbert space is a tensor product  $H \otimes K$  (as a Hilbert space).

We observe that a tensor product of two spaces is, strictly speaking, not a space, but a bilinear mapping whose domain is the Cartesian product  $H \times K$ . Hence we ought to say that the Hilbert space of L is the image of a tensor product. Furthermore, tensor products are defined up to isomorphisms. The choice of one or another realization of the tensor product is not essential, because we can translate in a one-to one way any statement expressed in a realization into a statement expressed in any other.

However, a natural and, for many instances, convenient realization of  $H \otimes K$  in the case of (finite dimensional) Hilbert spaces is the linear space  $Hom(H^*, K)$  of the linear mappings from the dual  $H^*$  of the space H to the space K. The scalar product  $\langle \varphi, \psi \rangle$  is defined as  $tr(\varphi^* \circ \psi)$ , where  $\varphi^*$  denotes the adjoint of  $\varphi$ .

A mapping of rank one of  $Hom(H^*, K)$  is expressed as  $|k\rangle_{KH^*} \langle h|$ . We have

$$(|k\rangle_{KH^*} \langle h|) (|x\rangle_{H^*}) = |k\rangle_{KH^*} \langle h|x\rangle_{H^*} = {}_H \langle x|h\rangle_H |k\rangle_K.$$

Simplifying the notation, an element of rank one will be expressed as  $|h\rangle |k\rangle$ , with the rule of calculation

$$(|k\rangle_{H^*} \langle h|) (|x\rangle_{H^*}) = \langle x|h\rangle |k\rangle.$$

We put  $|h\rangle \otimes |k\rangle = |h\rangle |k\rangle$ . Hence in this realization the separable elements of  $H \otimes K$  are the linear mappings of rank one. Unless differently specified, the above realization of a tensor product will be understood.

The third uncontroversial notion is that the only allowed transformations for the states of a universe W are induced by unitary transformations of its Hilbert space. This means that an allowed transformation of the elements of  $\mathbb{P}(W)$  is induced by an element of the group  $\mathfrak{U}(W)$  of the unitary transformations of W.

The notion of a transformation implies a mapping, which associates to any state "before" a corresponding state "after". This point of view has two drawbacks: it involves the totality of states and it involves the idea of an "evolution" from an old state to a new one. We would like to arrive at a mathematically equivalent formulation which involves a single state (of an extended composite system) which, seen by different partial point of views, appears as the transformation, the state "before" and the state "after". A more precise sense of what we mean will come out from the following analysis.

The key observation which allows to carry on this program is the bijection between linear mappings and elements of tensor products. To the space of linear mappings Hom(X,Y) we associate the tensor product  $X^* \otimes Y$ . Using the canonical isomorphism between  $X^* \otimes Y$  and  $L = Y \otimes X^*$ , we associate a ket of the latter space to a specific linear mapping, which can be considered as a representative of a state of a composite system L. If Z is another space,  $\psi \in Hom(X,Y)$  and  $\varphi \in Hom(Y,Z)$ , the composition  $\varphi \circ \psi$  is defined and belongs to Hom(X,Z). Introducing the tensor products  $M = Z \otimes Y^*$  and  $N = Z \otimes X^*$ , we associate to  $\psi$  and  $\varphi$  the corresponding kets  $|\psi\rangle \in L$  and  $|\varphi\rangle \in M$ . The ket  $|\varphi \circ \psi\rangle$  depends linearly on  $\varphi \circ \psi$  as well as  $|\psi\rangle$ and do on  $\psi$  and  $\varphi$ . Hence the mapping which associates to the pair  $(|\varphi\rangle, |\psi\rangle)$  the ket  $|\varphi \circ \psi\rangle$  is bilinear. Consequently there is a unique linear mapping

$$M \otimes L \xrightarrow{\kappa_Y} N$$
 such that  $|\varphi \circ \psi\rangle = \kappa_Y (|\varphi\rangle \otimes |\psi\rangle).$  (1)

There is a canonical isomorphism between the spaces  $M \otimes L$  and  $Z \otimes Y^* \otimes Y \otimes X^*$ . With an abuse of notation we will understand  $|\varphi\rangle \otimes |\psi\rangle$  as an element of the latter space, and  $\kappa_Y$  with the same space as its domain. The application of  $\kappa_Y$  will be called *contraction* in Y.

Conversely, given a ket  $|\chi\rangle \in Z \otimes Y^* \otimes Y \otimes X^*$  admitting a factorization

$$|\chi\rangle = |\varphi\rangle \otimes |\psi\rangle$$
, with  $|\varphi\rangle \in Z \otimes Y^*$  and  $|\psi\rangle \in Y \otimes X^*$ .

the factors  $|\varphi\rangle$  and  $|\psi\rangle$  are determined up to scalar factors  $\lambda$  and  $\mu$  such that  $\lambda \mu = 1$ . From the object  $|\chi\rangle$  we can thus recover the ket  $|\varphi \circ \psi\rangle$ , but not the factors of its decomposition because of the above indeterminacy. The latter is however removed if we pass to the corresponding rays.

A ray of morphisms belonging to Hom(X, Y) can be represented as a ray of  $Y \otimes X^*$ , a ray of Hom(V, Z) can be represented as a ray of  $Z \otimes V^*$ . A pair of such rays can be represented in a one-to-one way as a ray of  $Z \otimes V^* \otimes Y \otimes X^*$ . If V = Y the composition of morphisms is possible and the corresponding ray is obtained contracting on Y.

If a ray of  $Z \otimes V^* \otimes Y \otimes X^*$  is the corresponding of a pair of rays of  $Z \otimes V^*$ and  $Y \otimes X^*$ , we would like to recover the original rays through contractions. This is not possible in a direct way, but we can proceed as follows. To a ray represented by  $|x\rangle \in X$  we can associate the ray generated by the element  $|x\rangle \langle x| \in Hom(X,X)$ , which corresponds to the element  $|x\rangle \otimes \langle x| \in X \otimes X^*$ . The original ray can be uniquely recovered by the ray generated by the latter element.

We can "explain" why a state of a universe is represented by a ray and not by a ket in the following way. Consider the tensor product  $\widehat{\mathbb{C}} \otimes H$  where  $\widehat{\mathbb{C}}$  is  $\mathbb{C}$  regarded as a vector space over itself with the structure of Hilbert space defined by the scalar product  $\langle x|y \rangle = x^*y$ . All its elements are separable, and the position  $|c\rangle \otimes |x\rangle \rightarrow c |x\rangle$  defines an isomorphism between  $\widehat{\mathbb{C}} \otimes H$  and H.

We associate to a universe W an extended system that we call extended universe  $W_e$ . If W is the Hilbert space of W, we introduce for  $W_e$  the Hilbert space  $W_e = \widehat{\mathbb{C}} \otimes W$ . The states of an extended universe are kets in its Hilbert space  $W_e$ . By definition, in an extended universe different kets correspond to different states. We assume that a state  $|w_e\rangle$  of the extended universe defines uniquely the state of the corresponding universe. A state of  $W_e$  can be always represented as  $|c\rangle \otimes |x\rangle$ , but each factor is defined up to a scalar coefficient. More mathematical details can be found in the monograph [6].

# 2 The state of a quantum system as a subsystem of a composite system

An important difference between the notion of a state of a physical system in quantum and in classical mechanics is the fact that, while in the latter the nature of a state of a subsystem of a given system is the same as that of the whole system, in quantum mechanics their character is deeply different. Indeed, the presence of entanglement for the states of composite systems prevents in general the possibility of ascribing to a subsystem a definite state, in the sense of a pure state of an isolated system. In the conventional setting of the interpretative rules of quantum mechanics, the state of the subsystem is described by a partial density operator, whose definition is justified by the probabilistic interpretation and the use of Born's rule.

In this section we wish to arrive at a characterization of the state of a subsystem of a quantum system independently from any probabilistic interpretation. Starting from a natural way of defining such a state, we will find that one way of characterizing it is through a partial density operator *independently of any a priori probabilistic interpretation*. The latter will come out as a consequence of the formalism and of a few reasonable assumptions, connected with the notion of a state.

Suppose that a composite system C consists of two parts S (the "system") and  $\mathcal{E}$  (the "environment"). We denote with  $\mathcal{H}$  the Hilbert space of S and with  $\mathcal{K}$  the Hilbert space of the environment. As the goal of this work is merely an assessment of interpretative aspects of Quantum Mechanics, we will avoid the technicalities connected with infinite-dimensional Hilbert spaces, so that all the Hilbert spaces involved in our discussion will be supposed *finite-dimensional*. It is hoped that the generalization to the infinite-dimensional case does not involve significant changes of the *interpretative framework*.

A key step for the introduction of a natural definition of a state of S as a subsystem of the composite system is the formalization of a property indicated by Zurek [?]. In the words of Zurek: "Unitary transformations must act on the system to alter its state. That is, when an operator does not act on the Hilbert space of S, i.e., when it has the form  $I \otimes (\ )$ , the state of S does not change." If we agree with this assertion, and we describe the states of the composite system as pure states (according to the idea that the composite system is "the Universe"), we conclude that the state of S associated with a pure state  $|\psi\rangle$  of the composite system must depend only on the orbit of  $|\psi\rangle$  under the action of the group  $I \otimes \mathcal{U}(\mathcal{K})$ . We will suppose conversely that different orbits correspond to different states. This is not a strong assumption as it may appear at first sight. Indeed, if there were different orbits physically indistinguishable, we could always redefine the states through the passage to suitable equivalence classes.

In this way, we may tentatively define the state of S as a subsystem of the composite system associated with  $|\psi\rangle$  simply as the orbit of  $|\psi\rangle$ . According to this definition, the state of S is characterized as a subset of the space of the composite system. Instead, we would like to arrive at a definition which involves only points of the Hilbert space of S. To this purpose, we observe that any set of mathematical objects in bijection with the orbits of  $I \otimes \mathcal{U}(\mathcal{K})$  can be as well used to define the state.

If we adopt this (implicit) definition of a state of S in the presence of the environment  $\mathcal{E}$ , we can arrive in a natural way at a characterization of a state of S as a density operator. We emphasize that in this association no a priori probabilistic interpretation (and, a fortiori, no Born's rule) will be involved. Indeed, the density operator will arise as an *orbit invariant*.

We first recall that, in the finite dimensional case, there is a canonical isomorphism between  $\mathcal{H} \otimes \mathcal{K}$  and the Hilbert space  $Hom(\mathcal{H}^*, \mathcal{K})$  of all linear maps from  $\mathcal{H}^*$  to  $\mathcal{K}$ , equipped with the scalar product  $\langle \psi | \psi \rangle = tr(\psi^* \psi)$ . In this isomorphism the corresponding of the ket  $|\psi\rangle \in \mathcal{H} \otimes \mathcal{K}$  will be denoted  $\psi$ . The action of  $I \otimes V$  $(V \in \mathcal{U}(\mathcal{K}))$  on  $|\psi\rangle$  corresponds to the action  $\psi \mapsto V\psi$ . The following theorem holds:

**Theorem 2.1.** The necessary and sufficient condition for the existence of a transformation  $V \in \mathcal{U}(\mathcal{K})$  such that  $\psi' = V\psi$  is that  $\psi'^*\psi' = \psi^*\psi$ .

For a proof of this theorem, see [6].

Owing to the above theorem, the state of S corresponding to  $|\psi\rangle$  can be characterized by  $\psi^*\psi$ . The latter is a positive self-adjoint operator operating on  $\mathcal{H}^*$  on the left if  $\mathcal{H}^*$  is regarded as a space of kets, and on the right if  $\mathcal{H}^*$  is regarded as the space of bras associated with  $\mathcal{H}$ , and hence it operates on the left on  $\mathcal{H}$ . Furthermore, if  $|\psi\rangle$ is normalized,  $tr\psi^*\psi = 1$ , so that  $\psi^*\psi$  is a density operator. It easy is to prove that

$$\psi^* \psi = tr_E \left| \psi \right\rangle \left\langle \psi \right|. \tag{1}$$

Indeed, let

$$|\psi\rangle = \sum a_k |s_k\rangle |\varepsilon_k\rangle \tag{2}$$

be a Schmidt decomposition of  $|\psi\rangle$ . Denoting  $|x\rangle^*$  a bra of  $\mathcal{H}$  regarded as a ket of  $\mathcal{H}^*$ , the corresponding linear map  $\psi$  is

$$\psi = \sum a_k |\varepsilon_k\rangle(^*\langle s_k|), \tag{3}$$

so that

$$\psi^*\psi = \sum |a_k|^2 |s_k\rangle^{**} \langle s_k|.$$
(4)

If  $\langle x |$  is a bra of  $\mathcal{H}$ , it must be written  $|x\rangle^*$  when regarded as a ket of  $\mathcal{H}^*$ ; we can then write

$$\psi^*\psi |x\rangle^* = \sum |a_k|^2 |s_k\rangle^{**} \langle s_k |x\rangle^* = \sum |a_k|^2 |s_k\rangle^* \langle x|s_k\rangle.$$
(5)

Regarding the latter as a bra of  $\mathcal{H}$ , we get

$$\langle x|\psi^*\psi = \langle x|\sum |a_k|^2 |s_k\rangle \langle s_k|, \qquad (6)$$

so that

$$\psi^*\psi = \sum |a_k|^2 |s_k\rangle \langle s_k|. \tag{7}$$

On the other hand we have

$$|\psi\rangle \langle \psi| = \sum a_k a_h^* |s_k\rangle \langle s_h| \otimes |\varepsilon_k\rangle \langle \varepsilon_h|, \qquad (8)$$

and  $tr_E |\psi\rangle \langle \psi| = \sum_{k} |a_k|^2 |s_k\rangle \langle s_k| = \psi^* \psi$ .

The following theorem, which can be regarded as a kind of Schmidt decomposition theorem in an invariant form, will be useful in subsequent developments:

**Theorem 2.2.** If  $|\psi\rangle \in \mathcal{H} \otimes \mathcal{K}$ , there is a unique decomposition

$$\left|\psi\right\rangle = \sum d_{\alpha} \left|\chi_{\alpha}\right\rangle$$

such that  $d_{\alpha} > 0$  with the  $d_{\alpha}$  all different each other,  $tr_E |\chi_{\alpha}\rangle \langle \chi_{\beta}| = 0$  for  $\alpha \neq \beta$ , and the set  $\{P_{\alpha} = tr_E |\chi_{\alpha}\rangle \langle \chi_{\alpha}|\}$  is a family of orthogonal projectors of  $\mathcal{H}$ . For a proof of this theorem, see [6]. The decomposition introduced in the about theorem will be called *canonical decomposition*.

**Remark 2.1.** The kets  $|\chi_{\alpha}\rangle$  in the canonical decomposition are not normalized in general. Indeed,  $\langle \chi_{\alpha} | \chi_{\alpha} \rangle = tr | \chi_{\alpha} \rangle \langle \chi_{\alpha} | = tr_E | \chi_{\alpha} \rangle \langle \chi_{\alpha} | = n_{\alpha}$  where  $n_{\alpha}$  is the dimension of the projection space of  $P_{\alpha}$ . Sometimes it is convenient to recast the canonical decomposition in a form involving normalized kets. To this purpose we put  $|\chi'_{\alpha}\rangle = 1/\sqrt{n_{\alpha}} | \chi_{\alpha} \rangle$ , so that  $|\psi\rangle = \sum d'_{\alpha} | \chi'_{\alpha} \rangle$  with  $d'_{\alpha} = \sqrt{n_{\alpha}} d_{\alpha}$ . The ket  $|\psi\rangle$  is normalized whenever  $\sum (d'_{\alpha})^2 = 1$ . The associated density operator is  $\rho_S = \sum d^2_{\alpha} P_{\alpha}$ . Hence the normalization condition for  $\rho_S$  is  $\sum n_{\alpha} d^2_{\alpha} = 1$ .

We know that a state  $\zeta$  of an isolated system described by a Hilbert space  $\mathcal{X}$  is characterized by the ray associated with some  $|\psi\rangle$ , i.e. by the set  $\{\lambda |\psi\rangle : \lambda \in \mathbb{C}\}$  which is a point of the projective space  $\mathbb{P}(\mathcal{X})$ . The unitary group  $\mathcal{U}(\mathcal{X})$  acts naturally on the rays and hence on  $\mathbb{P}(\mathcal{X})$ . However, the action is not faithful, while the action of the quotient  $\mathcal{U}^{\mathbb{Z}}(\mathcal{X})$  of  $\mathcal{U}(\mathcal{X})$  modulo its center is. Therefore we will take  $\mathcal{U}(\mathcal{X})$  as the structure group of  $\mathbb{P}(\mathcal{X})$  (in general we will denote  $G^{\mathbb{Z}}$  the quotient group of G modulo its center).

We say that a property  $\mathfrak{P}(x)$  of the nonzero kets of  $\mathcal{X}$  is a property of the states of the system if, whenever  $\mathfrak{P}$  is true for a nonzero ket  $|x\rangle$ , it is true for all the kets of the ray generated by  $|x\rangle$ . We say that a property  $\mathfrak{D}(x)$  of the states of the system defines a state of the system if, for every property  $\mathfrak{P}(x)$  of the states of the system, the condition  $\mathfrak{P}(x) \Rightarrow \mathfrak{D}(x)$  entails  $\mathfrak{P}(x) \Leftrightarrow \mathfrak{D}(x)$ .

We say that a state is completely defined if it is constrained by a property of the type  $\mathfrak{D}(x)$ . We say that the state is partially defined if it is constrained by a weaker property of the states of the system.

The systems S and  $\mathcal{E}$  are represented by  $\mathbb{P}(\mathcal{H})$  and  $\mathbb{P}(\mathcal{K})$  respectively, while the composite system C is represented by  $\mathbb{P}(\mathcal{H} \otimes \mathcal{K})$ . Their structure groups are  $\mathcal{U}^{Z}(\mathcal{H})$ ,  $\mathcal{U}^{Z}(\mathcal{K})$  and  $\mathcal{U}^{Z}(\mathcal{H} \otimes \mathcal{K})$ . The elements of  $\mathcal{U}(\mathcal{H} \otimes \mathcal{K})$  acting on indecomposable kets as  $|h\rangle |k\rangle \mapsto |h\rangle V |k\rangle$  with  $V \in \mathcal{U}(\mathcal{K})$  will be denoted  $I \otimes V$  and form a subgroup  $Id_{\mathcal{H}} \otimes \mathcal{U}(\mathcal{K})$  of  $\mathcal{U}(\mathcal{H} \otimes \mathcal{K})$ .

We say that a property  $\mathfrak{P}(x)$  of the nonzero kets of  $\mathbb{P}(\mathcal{H} \otimes \mathcal{K})$  is a property of the states of the subsystem S of C if it is a property of the states of C and, whenever  $\mathfrak{P}$  is true for a ket  $|\psi\rangle$ , it is true for all the kets of the form  $I \otimes V |\psi\rangle$  with  $V \in \mathcal{U}(\mathcal{K})$ . Let  $\Omega$  be a nonzero orbit of  $Id_{\mathcal{H}} \otimes \mathcal{U}(\mathcal{K})$ , and  $\widehat{\Omega} = \mathbb{C}\Omega$ . Then the property  $\mathfrak{P}_{\widehat{\Omega}}(x) : \mathfrak{P}_{\widehat{\Omega}}(x)$  is true iff  $x \in \widehat{\Omega}$  " is a property of the states of the subsystem S of C. The property just defined satisfies the condition: if  $\mathfrak{P}'(x)$  is a property of the states of the subsystem S of  $\mathcal{C}$  such that  $\mathfrak{P}'(x) \Rightarrow \mathfrak{P}_{\widehat{\Omega}}(x)$ , then  $\mathfrak{P}'(x) \Leftrightarrow \mathfrak{P}_{\widehat{\Omega}}(x)$ .

We say that a property  $\mathfrak{D}(x)$  of the states of the subsystem S of C defines a state of the subsystem S of C if, whenever a property  $\mathfrak{P}(x)$  of the states of the subsystem S of C is such that  $\mathfrak{P}(x) \Rightarrow \mathfrak{D}(x)$  then  $\mathfrak{P}(x) \Leftrightarrow \mathfrak{D}(x)$ .

We say that  $\mathfrak{D}(x)$  and  $\mathfrak{D}'(x)$  define the same state of the subsystem S of C if  $\mathfrak{D}(x) \Leftrightarrow \mathfrak{D}'(x)$ . If  $\widehat{\Omega} = \mathbb{C}\Omega$ ,  $\mathfrak{P}_{\widehat{\Omega}}(x)$  defines a state of the subsystem S of C. If  $\mathfrak{D}(x)$  defines a state of the subsystem S of C there is a  $\widehat{\Omega} = \mathbb{C}\Omega$  such that  $\mathfrak{D}(x) \Leftrightarrow \mathfrak{P}_{\widehat{\Omega}}(x)$ .

Conversely, if there is a  $\widehat{\Omega} = \mathbb{C}\Omega$  such that  $\mathfrak{D}(x) \Leftrightarrow \mathfrak{P}_{\Xi}(x), \mathfrak{D}(x)$  defines a state of the subsystem  $\mathcal{S}$  of  $\mathcal{C}$ . Of course  $\mathfrak{P}_{\widehat{\Omega}}(x) \Leftrightarrow \mathfrak{P}_{\widehat{\Omega}'}(x)$  iff  $\widehat{\Omega} = \widehat{\Omega}'$ .

Let  $\mathfrak{D}(x)$  be a property of the states of the composite system  $\mathcal{C}$ . The following theorem holds:

**Theorem 2.3.**  $\mathfrak{D}(x)$  defines a state of the subsystem S of C iff there is a density operator  $\rho_S$  such that  $\mathfrak{D}(x) \Leftrightarrow \langle x | x \rangle^{-1} tr_E | x \rangle \langle x | = \rho_S$ .

 $\langle x|x\rangle^{-1}tr_E|x\rangle\langle x| = \rho_S$  and  $\langle x|x\rangle^{-1}tr_E|x\rangle\langle x| = \rho'_S$  define the same state of the subsystem S of C iff  $\rho_S = \rho'_S$ .

If  $\operatorname{Dim} \mathcal{H} \leq \operatorname{Dim} \mathcal{K}$ , for every density operator  $\rho_S$ ,  $\langle x | x \rangle^{-1} tr_E | x \rangle \langle x | = \rho_S$  defines a state of the subsystem  $\mathcal{S}$  of  $\mathcal{C}$ .

*Proof.* if  $\mathfrak{D}(x)$  defines a state of the subsystem  $\mathcal{S}$  of  $\mathcal{C}$  there is a unique  $\widehat{\Omega} = \mathbb{C}\Omega \neq 0$ (being  $\Omega$  an orbit of  $I \otimes \mathcal{U}(\mathcal{K})$ ) such that  $\mathfrak{D}(x)$  is true whenever  $x \in \widehat{\Omega}$ . Let  $|\psi\rangle$  be a nonzero ket of  $\widehat{\Omega}$ . Then  $x \in \widehat{\Omega}$  iff there are  $\lambda \in \mathbb{C}$  ( $\lambda \neq 0$ ) and  $|x'\rangle$  such that  $|x'\rangle$ belongs to the orbit of  $|\psi\rangle$  and  $|x'\rangle = \lambda |x\rangle$ . We define

$$\rho_S = \langle \psi | \psi \rangle^{-1} tr_E | \psi \rangle \langle \psi | \,.$$

Then  $|x'\rangle$  belongs to the orbit of  $|\psi\rangle$  iff  $tr_E |x'\rangle \langle x'| = \langle \psi | \psi \rangle \rho_S$ , i.e. iff  $|\lambda|^2 tr_E |x\rangle \langle x| = \langle \psi | \psi \rangle \rho_S$ . Taking the traces with respect to  $\mathcal{S}$  of both sides we get  $|\lambda|^2 = \langle x | x \rangle^{-1} \langle \psi | \psi \rangle$  and hence  $\langle x | x \rangle^{-1} tr_E | x \rangle \langle x| = \rho_S$ . Then  $\mathfrak{D}(x) \Leftrightarrow \langle x | x \rangle^{-1} tr_E | x \rangle \langle x| = \rho_S$ .

Conversely suppose that there is a density operator such that

$$\mathfrak{D}(x) \Leftrightarrow \langle x | x \rangle^{-1} tr_E | x \rangle \langle x | = \rho_S.$$

Let  $\widehat{\Omega} = \left\{ |x\rangle |\langle x|x\rangle^{-1} tr_E |x\rangle \langle x| = \rho_S \right\}$ . Let  $\mathfrak{D}(x)$  be true for  $x = |\psi\rangle$ . Therefore  $\rho_S = \langle \psi|\psi\rangle^{-1} tr_E |\psi\rangle \langle \psi|$  so that  $|\psi\rangle \in \widehat{\Omega}$ . Let  $\Omega$  be the orbit of  $|\psi\rangle$ .  $|x\rangle \in \widehat{\Omega}$  iff  $\langle x|x\rangle^{-1} tr_E |x\rangle \langle x| = \langle \psi|\psi\rangle^{-1} tr_E |\psi\rangle \langle \psi|$ . Putting  $|\psi'\rangle = \langle x|x\rangle^{-1/2} \langle \psi|\psi\rangle^{1/2} |x\rangle$  we get  $tr_E |\psi'\rangle \langle \psi'| = tr_E |\psi\rangle \langle \psi|$ , so that  $\widehat{\Omega} = \mathbb{C}\Omega$ . Therefore  $\mathfrak{D}(x) \Leftrightarrow x \in \widehat{\Omega}$  and  $\mathfrak{D}(x)$  defines a state of the subsystem S of C. As  $\widehat{\Omega} = \left\{ |x\rangle |\langle x|x\rangle^{-1} tr_E |x\rangle \langle x| = \rho_S \right\}$  and  $\widehat{\Omega}' = \left\{ |x\rangle |\langle x|x\rangle^{-1} tr_E |x\rangle \langle x| = \rho'_S \right\}$  coincide iff  $\rho_S = \rho'_S$ , the states coincide iff the latter condition holds.

Let  $\rho_S$  be a density operator. In order to show that it defines a state of the subsystem S of C, it is sufficient to prove that the equation  $\langle x|x\rangle^{-1}tr_E |x\rangle \langle x| = \rho_S$  has solutions. Starting from the spectral decomposition  $\rho_S = \sum p_\alpha P_\alpha$  we can choose an orthonormal basis adapted to the decomposition and select a bijection between this basis and an orthonormal set of vectors of  $\mathcal{K}$ . If  $|\chi_\alpha\rangle$  denotes the normalized sum of the tensor products of corresponding vectors associated with the eigenspace defined by  $P_\alpha$ , the vector of  $\mathcal{K}$  defined as  $|\psi\rangle = \sum \sqrt{p_\alpha} |\chi_\alpha\rangle$  is normalized and  $\rho_S = tr_E |\psi\rangle \langle \psi| = \langle \psi|\psi\rangle^{-1} tr_E |\psi\rangle \langle \psi|$ .

We observe that the states of the subsystem S of C have been defined indirectly, i.e. through the formulation according to which some suitable specific property of the nonzero kets of C defines a state of the subsystem S of C. Among the infinite possibilities we can, owing to Theorem 2.3, choose the property  $\mathfrak{D}_{\rho}(x) : \langle x|x \rangle^{-1} tr_E |x \rangle \langle x| =$  $\rho_S$ . We read it as " $\langle x|x \rangle^{-1} tr_E |x \rangle \langle x| = \rho_S$  defines a state of the subsystem S of C". Similarly " $\langle x|x \rangle^{-1} tr_E |x \rangle \langle x| = \rho'_S$  defines a state of the subsystem S of C"; but the two states are different if  $\rho_S \neq \rho'_S$ , so that we must label the states in order to distinguish them. We can use as labels the density operators. Therefore we write the first sentence as " $\langle x|x \rangle^{-1} tr_E |x \rangle \langle x| = \rho_S$  defines the state  $\rho_S$  of the subsystem S of C". The sentence "the state of the subsystem S of C is  $\rho_S$ " is true (by definition) iff the sentence "the state  $|x\rangle$  of C is such that  $\langle x|x \rangle^{-1} tr_E |x \rangle \langle x| = \rho_S$  is satisfied" is true.

We remember that the composite system is "the Universe", so that it is in some state defined by a ray of  $\mathbb{P}(\mathcal{H} \otimes \mathcal{K})$ , and the prescription of a state of the subsystem  $\mathcal{S}$ of  $\mathcal{C}$  is simply a constraint on the possible states of  $\mathcal{C}$ . Therefore the complete specification of the state of the subsystem  $\mathcal{S}$  of  $\mathcal{C}$  can be regarded as a partial specification of the state of  $\mathcal{C}$ .

# 3 Relation between the state of a system as isolated and as open

Naively, we can consider S sometimes as a subsystem of C and sometimes as a closed system. Our next goal is to arrive at a sharp mathematical formulation of the physical conditions under which the first or the second point of view can be adopted. A necessary condition for the second possibility is the assumption that no interactions between the system and the environment take place. This sentence implies the idea of a transformation: we say that there is no interaction when the physical conditions are such that only specific types of transformations are allowed for the composite system, i.e. those which can be represented as a tensor product of a transformation of  $\mathcal{U}(\mathcal{H})$  and a transformation of  $\mathcal{U}(\mathcal{K})$ . As already discussed, a transformation involves two states: a state "before" the transformation and a state "after" the transformation.

If we assume that S can be considered as isolated, there is no interaction and its states are modeled as elements of  $\mathbb{P}(\mathcal{H})$ . Standard quantum mechanics assumes that there is  $T \in \mathcal{U}^{\mathbb{Z}}(\mathcal{H})$  such that the possible pairs (state before, state after) are the pairs  $(\zeta, T\zeta)$  with  $\zeta \in \mathbb{P}(\mathcal{H})$ . If we assume that S is not isolated, in general it is only at the level of C (which is closed) that the states can be modeled as points of a projective space (in this case  $\mathbb{P}(\mathcal{H} \otimes \mathcal{K})$ ) but not at the level of S. In this case the state of S before is a density operator  $\rho_S$  and the state of S after is a density operator  $\rho'_S$ .

Furthermore, if an interaction takes place, it is only at the level of S that the states before and after are connected by a transformation of  $\mathcal{U}^{\mathbb{Z}}(\mathcal{H}\otimes\mathcal{K})$ ; the density operators  $\rho_S$  and  $\rho'_S$  are not connected by any simple relation: they are just "projections" (through the partial trace operation) of the initial and final states of C. To be more specific, if we represent the "evolution" of  $\mathcal{C}$  by  $T \in \mathcal{U}(\mathcal{H} \otimes \mathcal{K})$ , and the state of  $\mathcal{C}$ "before" with the normalized ket  $|\psi\rangle$ , the state of  $\mathcal{C}$  "after" is represented by  $|\psi'\rangle = T|\psi\rangle$ . The states of  $\mathcal{S}$  as a subsystem of  $\mathcal{C}$  "before" and "after" are  $\rho_S = tr |\psi\rangle\langle\psi|$ , and  $\rho'_S = tr |\psi'\rangle\langle\psi'|$ .

Even if  $|\psi\rangle = |u\rangle |v\rangle$ , i.e. "before" both S and  $\mathcal{E}$  are in well defined states as isolated systems, so that  $\rho_S = |u\rangle \langle u|$ ,  $\rho'_S$  in general is no more a one-dimensional projector. Therefore, while the state before can be represented by a point of  $\mathbb{P}(\mathcal{H})$ , the state "after" is, generally speaking, a mathematical object of a different nature.

There are two related, but distinct items raised by this discussion. The first consists in the different ways of representing the state of S depending on whether it is considered isolated or not. Classically, the state of a composite system is described as a point in its phase space, which is expressed as the Cartesian product of the phase spaces of the component subsystems.

If also in the classical case we define the state of S a la Zurek, with the role of  $\mathcal{U}^Z(\mathcal{K})$  substituted by the role of the group of the canonical transformations of the phase space of  $\mathcal{E}$ , we see that the orbits of the latter group (i.e. the states a la Zurek of S as a subsystem of  $\mathcal{C}$ ), can be parameterized by the points of the phase space of  $\mathcal{S}$ . This entails that the state of the system at each time is represented by the same object (a point in its phase space) both in the absence and in the presence of interaction. So in the classical case the conventional definition of states of the subsystem is compatible with Zurek's point of view.

In the latter case the projections of the initial and final points of the composite system are points of the phase space of S even if an interaction takes place. It is true that the final point of S depends both on the initial states of S and of  $\mathcal{E}$ , so that, if the state of the latter is not completely known (e.g. because  $\mathcal{E}$  is a complex system), statistical methods, based on the introduction of the phase density, must be introduced. But the description of the state of S by means of a point in its phase space is not forbidden, at least *in principle*. The situation is quite different in the quantum case. Even if the initial state is described by a point of  $\mathbb{P}(\mathcal{H})$ , the final state of S (i.e. the "projection" of the final state of the composite system) is a density operator with rank > 1 and not just a one-dimensional projector (which is equivalent to a point of  $\mathbb{P}(\mathcal{H})$ ) if an interaction with the environment has taken place.

The second question concerns the different ways of describing the evolution of the system in the absence or in the presence of interaction. In this respect, the classical and the quantum case are similar: in both cases the interaction precludes the possibility of establishing a functional relationship between the initial and the final states of S: the only thing that can be said in general is that both are "projections" of the initial and final states of the composite system.

Hence the main conclusion of the above discussion is that the basic difference between the classical and the quantum case in this respect is that in the latter a fundamental difference exists in the mathematical description of the states of S depending on whether the system is considered as isolated or as a subsystem of C. In the first case the states are points of  $\mathbb{P}(\mathcal{H})$ , while in the second they are represented by density operators. Of course in the most popular axiomatics of quantum mechanics the need of this difference is a consequence of the *a priori* introduction in the axioms of a probabilistic interpretation of the theory and of its quantitative expression through the Born's rule.

We emphasize that instead, in our analysis this difference is a direct consequence of two assumptions: the first is that a composite system is described by a tensor product, and the second is that the correct notion of state of a subsystem is the one implied by Zurek's considerations (we emphasize that the "philosophy" underlying the notion of the state of a subsystem is identical in the classical and in the quantum case: it is a property of the state of the composite system which is left invariant by all the transformations that involve only the environment, such that every other invariant property is a consequence of it). Neither of these assumptions involves probability; specifically, the density operator arises merely as an *orbit invariant*. We will see in the following that we are *forced* to give it a probabilistic interpretation and that its quantitative implementation is equivalent to Born's rule. To carry on this program,we carefully investigate the relation between the two possible descriptions of the states of S.

Suppose we have good reasons to consider the system isolated from the environment before some instant  $t_0$ , but that this assumption is no longer valid after, up to the instant  $t_1$ , while for  $t > t_1 S$  and  $\mathcal{E}$  can be again modeled as mutually isolated. Before  $t_0$ , S and  $\mathcal{E}$  evolve independently; at  $t < t_0$ , S is in a well definite state  $\varsigma \in \mathbb{P}(\mathcal{H})$  and S in a state  $\tau \in \mathbb{P}(\mathcal{K})$ . At  $t' < t_0$  we have  $\varsigma' = T\varsigma$  and  $\tau' = S\tau$ , with  $T \in \mathcal{U}^Z(\mathcal{H})$  and  $S \in \mathcal{U}^Z(\mathcal{K})$ . If the normalized kets  $|\sigma\rangle$  and  $|\theta\rangle$  represent  $\varsigma$  and  $\tau$  respectively, and  $|\sigma'\rangle$  and  $|\theta'\rangle$  represent  $\varsigma'$  and  $\tau'$  respectively, there are U representing T and V representing S such that  $|\sigma'\rangle = U |\sigma\rangle$  and  $|\theta'\rangle = V |\theta\rangle$ . We read the pair  $(|\sigma\rangle, |\theta\rangle)$  saying that at t S is in the state  $\varsigma$  and  $\mathcal{E}$  is in the state  $\tau$ . At the same instant  $\mathcal{C}$  is in a state  $\zeta$  represented by  $|\sigma\rangle |\theta\rangle$ . We note that  $tr_E |\sigma\rangle \langle \sigma| \otimes |\theta\rangle \langle \theta| = |\sigma\rangle \langle \sigma|$  so that the density operator is a projector on a one-dimensional space, which is a description of a pure state equivalent to a ray.

Similarly, at t' S is in the state  $\varsigma'$  and  $\mathcal{E}$  is in the state  $\tau'$ , while  $\mathcal{C}$  is in a state  $\zeta'$  represented by  $U \otimes V |\sigma\rangle |\theta\rangle$ . At  $t_0$  the interaction is switched on. Therefore the state of  $\mathcal{C}$  after  $t_0$  becomes entangled. In particular, let  $|\psi\rangle$  denote a normalized representative of the state at  $t_1$ . At this instant the system must be considered as interacting with the environment as the "past" is concerned, and as non interacting regards to the "future".

If "non interacting" were the same thing as "isolated", we may think that both descriptions of the state must hold: as an interacting system it ought to be described by  $\rho_S = tr_E |\psi\rangle \langle \psi|$ , (which means a partial specification of the state of C) and as a non interacting system by a (perhaps partial) specification of some point of  $\xi$  of  $\mathbb{P}(\mathcal{H})$ . A careful analysis will however show that not for all the density operators the description in terms of states of an isolated system is possible. We will in particular find that, when there is in  $\rho_S$  some kind of degeneracy to be specified later, an obstruction to such a description arises, so that the notions of "non interacting" and "isolated" are not equivalent.

We now assume that  $\rho_S$  is such that a description is possible, and we find the conditions which must be satisfied.

If in the same physical situation  $\rho_S$  is a state of the system as subsystem of C and  $\xi$  a state of S as an isolated system, we expect that there is a relation between  $\rho_S$  and  $\xi$ . Namely, for each allowed  $\rho_S$  there is a set  $\Xi$  of possible values for  $\xi$  such that, if it is true that the state of S as a subsystem of C is  $\rho_S$ , the state of S as an isolated system is an element of the set  $\Xi$ .

Let us consider a transformation of C represented by  $U \otimes V$  which leaves  $\rho_S$  invariant. Then there is no evolution in S as a subsystem of C. The above transformation indicates that there is no interaction, and we suppose that the description of S as an isolated system is also valid. In this description too there must be no evolution. The transformation law of the density operator is  $U\rho_S U^*$ . Let  $\rho_S = \sum p_\alpha P_\alpha$  be the spectral expansion of  $\rho_S$ . The transformation U leaves  $\rho_S$  invariant iff  $UP_\alpha U^* = P_\alpha$ ,  $\forall \alpha$ .

If  $P_0$  is the projector on the null space of  $\rho_S$ , then  $P_0 = I - \sum P_\alpha$  and  $UP_0U^* = P_0$ . On the other hand, in the isolated system description, the new state is  $T\xi$ , where  $T \in \mathcal{U}^Z(\mathcal{H})$  is represented by U. Hence, for each possible state  $\xi$  of S as an isolated system given that the state of S as a subsystem of C is  $\rho_S$ , the new state  $T\xi$  must be equal to  $\xi$ .

Let  $\mathcal{G}_{\rho}$  be the stabilizer of  $\rho$ , and  $\mathcal{G}_{\xi}$  the stabilizer of  $\xi$ . Hence  $\mathcal{G}_{\rho} \subseteq \mathcal{G}_{\xi}$  for each  $\xi \in \Xi$ , so that

$$\mathcal{G}_{\rho} \subseteq \bigcap_{\xi \in \Xi} \mathcal{G}_{\xi} \triangleq \Gamma_{\Xi}.$$
 (1)

If  $|\sigma\rangle \in \mathcal{H}$  represents  $\xi$ , and if  $U\rho_S U^* = \rho_S$ , then  $U |\sigma\rangle = \lambda |\sigma\rangle (\lambda \in \mathbb{C}, |\lambda| = 1)$ (where  $\lambda$  may depend on U); furthermore  $|\sigma\rangle$  has an expansion of the form  $|\sigma\rangle = \sum P_{\alpha} |\sigma\rangle + P_0 |\sigma\rangle$ . Hence we must have

$$\sum U P_{\alpha} |\sigma\rangle + U P_0 |\sigma\rangle = \sum \lambda P_{\alpha} |\sigma\rangle + \lambda P_0 |\sigma\rangle.$$
<sup>(2)</sup>

Multiplying both sides by  $P_{\beta}$  we get

$$UP_{\beta} \left| \sigma \right\rangle = \lambda P_{\beta} \left| \sigma \right\rangle, \tag{3}$$

and multiplying both sides by  $P_0$ ,

$$UP_0 \left| \sigma \right\rangle = \lambda P_0 \left| \sigma \right\rangle. \tag{4}$$

But the restrictions of U to the images of the projectors are arbitrary unitary transformations of these images, so that if  $P_{\beta} |\sigma\rangle$  is nonzero, Im  $P_{\beta}$  is one-dimensional. The same conclusion holds for  $P_0 |\sigma\rangle$ .

Furthermore, if  $P | \sigma \rangle \neq 0$  and  $P' | \sigma \rangle \neq 0$  with  $P \neq P'$ , we can choose U such that  $UP | \sigma \rangle = e^{i\varphi}P | \sigma \rangle$  and  $UP' | \sigma \rangle = e^{i\varphi'}P' | \sigma \rangle$  with  $e^{i\varphi} \neq e^{i\varphi'}$ . But this entails that  $e^{i\varphi} = \lambda$  and  $e^{i\varphi'} = \lambda$  and this is a contradiction. We conclude that, for each possible state  $\xi$  of S as an isolated system, given that the state of S as a subsystem of C is  $\rho_S$ ,  $\xi$  is a one-dimensional eigenspace of  $\rho_S$ . Then  $\Xi$  is a set of eigenstates of  $\rho_S$ .

The subgroup of  $\mathcal{U}^{\mathbb{Z}}(\mathcal{H})$  which leaves invariant all the elements of  $\Xi$  is nothing but  $\Gamma_{\Xi}$ . No evolution is observed in  $\mathcal{S}$  under  $\Gamma_{\Xi}$  if the only possible states of it as an isolated system are the elements of  $\Xi$ . Therefore no evolution must be observed in  $\mathcal{S}$ as a subsystem of  $\mathcal{C}$  in the state  $\rho_{\mathcal{S}}$ . Consequently  $\Gamma_{\Xi} \subseteq \mathcal{G}_{\rho}$ , so that

$$\Gamma_{\Xi} = \mathcal{G}_{\rho}.\tag{5}$$

Hence we must determine the pairs  $(\rho, \Xi)$  satisfying the above condition. If the orthogonal complement  $\mathcal{L}_{\Xi\perp}$  of the space  $\mathcal{L}_{\Xi}$  generated by  $\Xi$  is nonzero, the restriction of  $\Gamma_{\Xi}$  to it acts on it as the full unitary group. But  $\mathcal{L}_{\Xi\perp}$  is an invariant subspace of  $\rho_S$ ; as the restriction to it of  $\mathcal{G}_{\rho}$  is the full unitary group, it must consist of a single eigenspace. We conclude that, besides the elements of  $\Xi$ , there is at most a single eigenspace. If  $\mathcal{L}_{\Xi\perp} = 0$ , the set of eigenspaces of  $\rho_S$  is  $\Xi$ , so that they all are one-dimensional; if the latter is at least two-dimensional, the set of the one-dimensional eigenspaces of  $\rho_S$  is  $\Xi$ . Finally, if  $\mathcal{L}_{\Xi\perp} = 0$  is one-dimensional, the eigenspaces of  $\rho_S$  consist of  $\Xi$  and in addition the orthogonal complement of  $\mathcal{L}_{\Xi\perp}$ . All the above possibilities can be summarized in the following

**Theorem 3.1.** For each orthogonal set  $\Xi$  of rays, the density operators satisfying the equation  $\Gamma_{\Xi} = \mathcal{G}_{\rho}$  are all those whose eigenspaces are the elements of  $\Xi$  and the orthogonal complement of the subspace generated by them.

**Remark 3.1.** Remark on terminology: in order to avoid confusion, we remark that we call invariant space of an operator a subspace which is transformed into itself by the operator, while we call eigenspace of the operator a maximal invariant space. As it is usual, we call eigenvector of the operator a nonzero vector on which the operator acts as a scalar multiplier. According to our terminology, the one-dimensional subspace generated by an eigenvector is an eigenspace only if the associated eigenvalue is simple; otherwise it is only an invariant space. An eigenstate is a one-dimensional eigenspace. (Using this terminology, the null space of a density operator is the eigenspace corresponding to the zero eigenvalue).

We can write the most general expression of a density operator consistent with the conditions imposed as yet. This expression is an immediate consequence of Theorem 2.3. We have

$$\rho_S = \sum_{\xi \in \Xi} w\left(\xi\right) \left|\xi\right\rangle \left\langle\xi\right| + gP,\tag{6}$$

where  $I = \sum_{\xi \in \Xi} |\xi\rangle \langle \xi| + P$ ,  $\Xi \xrightarrow{w} \mathbb{R}_{\geq}$  is injective and  $g \notin \operatorname{Im} w$  with  $g \geq 0$ , and with the normalization condition  $\sum_{\xi \in \Xi} w(\xi) + g = 1$ .

We note that, given  $\Xi$ , the set of eigenspaces of  $\rho_S$  is completely specified. It is given by the union of  $\Xi$  and the orthogonal complement of the space generated by it. The possible  $\rho_S$  are then specified by prescribing at will the set of nonnegative different eigenvalues, satisfying the normalization condition.

The above equation shows that the orthogonal set of rays can be chosen at will and expresses the general solution for  $\rho_S$ . Conversely, suppose that  $\rho_S$  is prescribed and that we want to find all the sets  $\Xi$  satisfying the equation  $\Gamma_{\Xi} = \mathcal{G}_{\rho}$ . By Theorem 2.3, the eigendecomposition of  $\rho_S$  includes at most one eigenspace at least two-dimensional. If such a space appears in the eigendecomposition,  $\Xi$  is given by the set of the remaining eigenspaces; if all the eigenspaces are one-dimensional,  $\Xi$ is the whole set of eigenspaces with the possible exception of one of them. We can summarize the situation as follows:

**Theorem 3.2.** When the system  $\mathcal{H}$  in  $\rho_H$  can be considered isolated, there is in  $\rho_H$  at most a single eigenspace at least two-dimensional; the set  $\Xi$  of possible states of  $\mathcal{H}$  as an isolated system is the set of eigenstates of  $\rho_H$  if such an eigenspace exists; if all the eigenspaces of  $\rho_H$  are one-dimensional, the set  $\Xi$  consists of all these eigenspaces with the possible exception of one of them.

A further analysis that we will soon present will remove this indeterminacy.

We remember that  $\mathcal{H}$  is a subsystem of  $\mathcal{C}$ , and that the latter is the model of our "Universe", so that its state is represented by some  $|\psi\rangle \in \mathcal{C}$  such that  $\rho_H = tr_E |\psi\rangle \langle \psi|$ . We now investigate how the conditions just found for  $\rho_H$  are reflected in the canonical decomposition of  $|\psi\rangle$ . The latter can be put in the form

$$|\psi\rangle = \sum_{\chi \in X} d(\chi) |\chi\rangle, \tag{7}$$

with  $tr_E |\chi\rangle \langle \chi'| = 0$  for  $\chi \neq \chi'$  and  $tr_E |\chi\rangle \langle \chi| = P(\chi)$ . We get

$$\rho_H = \sum_{\chi \in X} d^2(\chi) P(\chi). \tag{8}$$

The projectors appearing in the above expression correspond to the non null eigenspaces of  $\rho_H$ ; they must be one-dimensional but at most one of them, hence the kets  $|\chi\rangle$  are indecomposable, but at most one. Each indecomposable  $|\chi'\rangle$  has the form  $|\xi'(\chi')\rangle |\eta'(\chi')\rangle$ , so that we get

$$\left|\psi\right\rangle = \sum_{\chi' \in X'} d\left(\chi'\right) \left|\xi'\left(\chi'\right)\right\rangle \left|\eta'\left(\chi'\right)\right\rangle + d\left|\delta\right\rangle,\tag{9}$$

where d = 0 if all the kets are indecomposable. We have  $P(\chi') = |\xi'(\chi')\rangle \langle \xi'(\chi')|$ , so that  $|\xi'(\chi')\rangle$  and  $|\xi'(\chi'')\rangle$  are orthogonal and hence different for  $\chi' \neq \chi''$ . The same conditions hold for the  $|\eta\rangle$ .

Imagine that  $\mathcal{E}$  is in turn a composite system, say  $\mathcal{E} = \mathcal{K} \otimes \mathcal{L}$ . We now introduce a special type of state in  $\mathcal{H} \otimes \mathcal{K} \otimes \mathcal{L}$ .

**Definition 3.1.** We say that a ket  $|\phi\rangle \in \mathcal{H} \otimes \mathcal{K} \otimes \mathcal{L}$  represents an *M*-state if there is a set *A*, a partition  $\mathcal{P}_2$  of *A*, three injections  $\mathcal{P}_2 \xrightarrow{\kappa} \mathcal{H}$ ,  $A \xrightarrow{\eta} \mathcal{K}$ ,  $A \xrightarrow{\zeta} \mathcal{L}$  satisfying

the conditions  $\langle \kappa(y) | \kappa(y') \rangle = \delta_{yy'}$ ,  $\langle \eta(a) | \eta(a') \rangle = \delta_{aa'}$ ,  $\langle \zeta(a) | \zeta(a') \rangle = \delta_{aa'}$ , and an injective mapping  $A \xrightarrow{v} \mathbb{R}_{>}$  such that

$$|\phi\rangle = \sum_{a \in A} \upsilon(a) |\kappa \circ \pi_2(a) \eta(a) \zeta(a)\rangle, \qquad (10)$$

where  $\pi_2$  is the canonical projection associated with the partition  $\mathcal{P}_2$ .

The *M*-state obtained in the way described above will be denoted  $(A, \mathcal{P}_2, \kappa, \eta, \zeta, \upsilon)$ . We prove the following

**Theorem 3.3.**  $(A, \mathcal{P}_2, \kappa, \eta, \zeta, \upsilon)$  and  $(A', \mathcal{P}'_2, \kappa', \eta', \zeta', \upsilon')$  define the same *M*-state if and only if there is a bijection  $A \xrightarrow{j} A'$  such that  $\upsilon = \upsilon' \circ j$ ,  $\mathcal{P}'_2 = j\mathcal{P}_2$ , and mappings  $\mathcal{P}_2 \xrightarrow{\lambda} \mathbb{C}_1$ ,  $A \xrightarrow{\mu} \mathbb{C}_1$ ,  $A \xrightarrow{\nu} \mathbb{C}_1$  with  $(\lambda \circ \pi_2) \mu \nu = 1$  such that  $\kappa \circ \pi_2 = (\lambda \circ \pi_2) \kappa' \circ \pi'_2 \circ j$ ,  $\eta = \mu \eta' \circ j$  and  $\zeta = \nu \zeta'$ . The mappings  $j, \lambda, \mu, \nu$  are unique.

*Proof.* the expansion that defines  $|\phi\rangle$  is its canonical expansion when  $|\phi\rangle$  is regarded as an element of  $(\mathcal{H} \otimes \mathcal{K}) \otimes \mathcal{L}$ . Hence the images of v and v' are the same. Consequently the equation  $v = v' \circ j$  has  $v'^{-1} \circ v$  as its unique solution. Furthermore the kets appearing in the expansion are in bijection with the coefficients, so that  $|(\kappa \circ \pi_2) \eta \zeta\rangle =$  $|[(\kappa' \circ \pi'_2) \eta' \zeta'] \circ j\rangle$ . The single factors in the tensor product are defined up to phase factors whose product is 1, and hence the thesis.

We have

$$\rho_{HK} = \sum_{a \in A} \upsilon(a)^2 |\kappa \circ \pi_2(a) \eta(a)\rangle \langle \kappa \circ \pi_2(a) \eta(a)|.$$

We observe that the dimension of the space generated by all the kets

 $\left|\theta\left(a\right)\right\rangle \triangleq\left|\kappa\circ\pi_{2}\left(a\right)\eta\left(a\right)\right\rangle$ 

is equal to |A|.

The dimension of  $\mathcal{K}$  is at least |A|, and at least 2, i.e.  $\dim \mathcal{K} \geq \max(2, |A|)$ , while the dimension of  $\mathcal{H}$  is at least 2. Hence the dimension of  $\mathcal{H} \otimes \mathcal{K}$  is at least  $2 \max(2, |A|)$  and the codimension of the space generated by all the  $|\theta(a)\rangle$  is at least  $2 \max(2, |A|) - |A|$ . Consequently this codimension is at least |A| if  $|A| \geq 2$  and at least 3 if |A| = 1. In any case the codimension is at least 2. Remembering Theorem 3.2, we conclude in every case that the set of possible states associated with  $\rho_{HK}$  is its set of eigenstates, which in this case are nothing but those appearing in the spectral decomposition of  $\rho_{HK}$ , i.e. non-null eigenstates.

Let us now evaluate  $\rho_H$ . We have

$$\rho_{H} = tr_{K}\rho_{HK} = \sum_{a \in A} \upsilon(a)^{2} |\kappa \circ \pi_{2}(a)\rangle \langle \kappa \circ \pi_{2}(a)| = \sum_{y \in P_{2}} |\kappa(y)\rangle \langle \kappa(y)| \sum_{a \in y} \upsilon(a)^{2}.$$
(11)

Let  $\widetilde{w}(y) \triangleq \sum_{a \in y} v(a)^2$ . If  $\mathcal{P}_1$  is the partition induced on  $\mathcal{P}_2$  by  $\widetilde{w}$ , we can uniquely

define an injective mapping  $\mathcal{P}_1 \xrightarrow{w} \mathbb{R}_>$  such that  $\widetilde{w}(y) = w(x)$  whenever  $y \in x$ . Hence we have

$$\rho_{H} = \sum_{y \in P_{2}} \widetilde{w}(y) |\kappa(y)\rangle \langle \kappa(y)| = \sum_{x \in P_{1}} \sum_{y \in x} w(x) |\kappa(y)\rangle \langle \kappa(y)|.$$
(12)

Putting  $P\left(x\right) \triangleq \sum_{y \in x} \left|\kappa\left(y\right)\right\rangle \left\langle\kappa\left(y\right)\right|$  we get

$$\rho_H = \sum_{x \in P_1} w(x) P(x), \qquad (13)$$

which, remembering the injectivity of w, is recognized to be the spectral representation of  $\rho_H$ . We will now show that

**Theorem 3.4.** If  $\rho_H$  is an arbitrary density operator of  $\mathcal{H}$ , there are Hilbert spaces  $\mathcal{K}$  and  $\mathcal{L}$  together with an M-state  $|\phi\rangle \in \mathcal{H} \otimes \mathcal{K} \otimes \mathcal{L}$  such that  $\rho_H = tr_{KL} |\psi\rangle \langle \psi|$ .

*Proof.* Indeed, suppose that  $\rho_H = \sum_{w \in W} wP(w)$  is the spectral representation of  $\rho_H$ . For each w we choose an orthonormal basis  $\widetilde{Y}_w$  for the corresponding eigenspace, so that  $P(w) = \sum_{\widetilde{y} \in \widetilde{Y}_w} |\widetilde{y}\rangle \langle \widetilde{y}|$ .

We define  $\widetilde{Y} = \bigcup_{w \in W} \widetilde{Y}_w$  and  $\widetilde{Y} \xrightarrow{\widetilde{w}} \mathbb{R}_>$  as  $\widetilde{w}(\widetilde{y}) = w$  for  $\widetilde{y} \in \widetilde{Y}_w$ . Let us further associate to each  $\widetilde{y}$  a set  $y \triangleq A(\widetilde{y})$ , with the condition that these sets are mutually disjoint, and put  $A = \bigcup_{\widetilde{y} \in \widetilde{Y}} A\left(\widetilde{Y}\right)$ . There is a bijection between the y and the  $\widetilde{y}$ , so that we can put  $\widetilde{y} = \kappa(y)$ . We denote  $\mathcal{P}_2$  the partition of A in the sets y. We introduce an injective mapping  $A \xrightarrow{\gamma} \mathbb{R}_>$  satisfying the condition  $\sum_{a \in y} \gamma(a) = \widetilde{w}(\kappa(y))$ . Such a mapping exists if and only if the cardinality of y is at least 2 for each y associated with a multiple eigenvalue of  $\rho_H$ , so we choose the sets according to this criterion.

We now choose two spaces  $\mathcal{K}$  and  $\mathcal{L}$  whose dimensionality is at least |A| and two injections  $A \xrightarrow{\eta} \mathcal{K}$  and  $A \xrightarrow{\zeta} \mathcal{L}$  such that their images are orthonormal sets. We put  $v(a) = \sqrt{\gamma(a)}$  and define

$$|\phi\rangle = \sum_{a \in A} \upsilon(a) |\kappa \circ \pi_2(a) \eta(a) \zeta(a)\rangle.$$
(14)

A straightforward computation shows that  $\rho_H = tr_{KL} |\phi\rangle \langle \phi|$ .

Suppose now that  $\mathcal{H}$  in  $\rho_H$  can be considered isolated. The state of  $\mathcal{H}$  as a subsystem of a larger system is completely described by  $\rho_H$ , so that the possibility of considering it as isolated, and the set of its possible states depend uniquely on  $\rho_H$ 

and not on the specific realization of  $\rho_H$  in terms of a larger system. Theorem 3.4 shows that  $\rho_H = tr_{KL} |\phi\rangle \langle \phi |$  for some *M*-state  $|\phi\rangle$ .

We can show that, if among the eigenspaces of  $\rho_H$  there is a (single) multidimensional eigenspace, the corresponding eigenvalue must be zero. Indeed, suppose the contrary. The corresponding projector is  $P(x) \triangleq \sum_{y \in x} |\kappa(y)\rangle \langle \kappa(y)|$  for some x.

Hence the eigenspace contains vectors  $|\kappa(y)\rangle$  appearing as factors in the expansion of  $\rho_{HK}$ . As each term of the decomposition is a possible state of  $\mathcal{H} \otimes \mathcal{K}$  as an isolated system and it is indecomposable, the vectors appearing in P(x) belong to  $\Xi$ . Thus we have found states of  $\Xi$  belonging to a multidimensional eigenspace of  $\rho_H$  and this is a contradiction. We conclude that, if all the eigenspaces of  $\rho_H$  are one-dimensional, the possible states of  $\mathcal{H}$  are exactly the non-null eigenspaces.

The results of our discussion imply the theorem:

**Theorem 3.5.** If the system  $\mathcal{H}$  can be considered isolated in  $\rho_H$ , then the only multidimensional eigenspace of  $\rho_H$ , if it exists, is the null eigenspace. The spectral expansion of  $\rho_H$  is  $\rho_H = \sum wP(w)$  where all the projectors P(w) are of rank one, and the possible states of  $\mathcal{H}$  in  $\rho_H$  as an isolated system are the states associated with these projectors.

We now introduce some terminology.

**Definition 3.2.** A density operator whose non-null eigenspaces are all one-dimensional will be called a "generic density operator".

The one-dimensional eigenspaces of  $\rho_S$  are the *eigenstates* of  $\rho_S$ . A generic density operator always possesses eigenstates. They are the eigenspaces associated with the nonzero eigenvalues and in addition the null space if it is one-dimensional. Furthermore it possesses at most one degenerate eigenvalue (the zero eigenvalue). Therefore the set  $\Xi$  is nonempty for a generic density operator: it consists of its non-null eigenstates.

The number of eigenstates of a generic density operator will be called its *type*. The dimension of its image is its *rank*.

Let m be the type of a generic density operator, r its rank and n the dimension of the Hilbert space on which it operates. If  $\rho_S = \sum p_\alpha P_\alpha$  is the spectral decomposition of  $\rho_S$ , all the projectors appearing in this expansion are eigenstates, so that the rank is the number of terms of the expansion, i.e. the number of nonzero eigenvalues, or else the number of non-null eigenstates. Hence  $m \ge r$ . Of course  $m \le r+1$  and if m = r+1, m = n because otherwise the multiplicity of the zero eigenvalue would be greater than one. Thus, if  $m = r, n \ge m$ , while, if m = r+1, n = m. Equivalently,  $n \ge r$  and if n = r+1, m = r+1, m = r+1, while if  $n \ne r+1, m = r$ . Else,  $n \ge m$  and if n = m, either r = n or r = n-1 while, if n > m, r = m.

In what follows, our goal is to obtain a *complete physical interpretation of a density operator when it is generic.* The interpretation for an arbitrary density operator will be obtained successively.

Theorem 3.5 states that  $\mathcal{H}$  can be considered isolated in  $\rho_H$  only if the latter is a generic density operator; in this case the set  $\Xi$  of its possible states as an isolated system is the set of non-null eigenstates of  $\rho_H$ , but none of them in particular is specified.

The situation is similar to the case when a number is constrained, say, by a second degree equation: a set of possibilities is selected (the set of the solutions), but not any in particular is specified.

Hence we are forced to consider the state of  $\mathcal{H}$  in  $\rho_H$  as an isolated system as a variable with values in  $\Xi$ . We have seen that the set  $\Xi$  is uniquely specified by  $\rho_H$ . When the set of its possible values is finite, we can regard a variable as an equivalence class of random variables, calling equivalent any two random variables with the same domain of their probability laws. We further note that  $\rho_H$  is specified not only by  $\Xi$ , but also by the set of eigenvalues. We will show in what follows that this set is enough to fix uniquely a probability law on  $\Xi$ , so that the state is a well defined random variable. Namely, the result of our analysis will be that of the conventional interpretation of the density operator: we will find that the probability of each state is equal to the corresponding eigenvalue of the density operator. We emphasize that this result will be derived without any additional axiom such as, for instance, a Born's rule. On the contrary, Born's rule will be recovered as a consequence.

We can synthesize the conceptual framework emerging from the above discussion as follows. The composite system C, as long as it is considered a "Universe", is in a state represented as a normalized ket  $|\psi\rangle$  which is defined up to an arbitrary phase factor. We call this state generic if the corresponding density operator  $\rho_H$  is generic. Suppose that the state of C is generic. Hence its canonical expansion has the form

$$|\psi\rangle = \sum d |\xi(d)\eta(d)\rangle.$$
(15)

Unless  $|\psi\rangle$  is indecomposable, neither the state of S nor the state of  $\mathcal{E}$  as states of isolated systems can be specified. Instead, the state of S as a subsystem of C in the sense of Zurek can be specified. This state can be characterized by the density operator

$$\rho_H = tr_K |\psi\rangle \langle\psi| = \sum d^2 |\xi(d)\rangle \langle\xi(d)|.$$
(16)

Nevertheless, as long as no interactions take place between S and C, the two subsystems can be considered as isolated, so that each of them possesses a state as an isolated system. But such a state cannot be specified, so that it must be considered as a variable. The range of this variable can be read off on the canonical decomposition. Namely, the range of the state of S is the set  $\{|\xi(d)\rangle\}$ , while the range of the state of  $\mathcal{E}$  is the set  $\{|\eta(d)\rangle\}$ . We have already anticipated that a unique law of probability is associated to these variables, so that they will become random variables.

#### 4 Universality of the probability function

Our next effort will be dedicated to the determination of the probability law. But before we afford this problem, it is useful to introduce some preliminary notions.

Let us consider an orthogonal set  $\Xi$  of states of  $\mathcal{H}$  as an isolated system. Let  $D_{\Xi}$  be the set of generic density operators having  $\Xi$  as the set of their non-null eigenstates. All the elements of  $D_{\Xi}$  have the same rank  $m = |\Xi|$ . If  $P_{\sigma}$  is the projector associated with the state  $\sigma \in \Xi$ , any  $\rho_S \in D_{\Xi}$  has the spectral expansion

$$\rho_S = \sum_{\sigma \in \Xi} p_\sigma P_\sigma,\tag{1}$$

and through this equation  $D_{\Xi}$  is in bijection with the set of the injective mappings  $\mathbf{p}$ from  $\Xi$  to the set  $\mathbb{R}_{>}$  of positive real numbers such that  $\sum_{\sigma \in \Xi} \mathbf{p}(\sigma) = 1$ . The set  $D_{\Xi}$ is a proper subset of the set  $T_{\Xi}$  of all the density operators which can be expressed in the form (1), with the coefficients  $p_{\sigma}$  belonging to  $\mathbb{R}_{\geq}$ , and relaxing the injectivity assumption on the mappings  $\mathbf{p}$ . The barycentric coordinates  $p_{\sigma}$  introduce in  $T_{\Xi}$  the structure of an (m-1)-simplex together with the standard topology. With respect to the standard topology,  $\bar{D}_{\Xi} = T_{\Xi}$ . It is useful to describe in detail the structure of a set  $D_{\Xi}$  which comes out from some theorems, whose proof is reported in [6].

**Theorem 4.1.** If the points  $\rho \in D_{\Xi}$  and  $\rho' \in D_{\Xi}$  have  $\mathbf{p}$  and  $\mathbf{p}'$  as the vectors of their barycentric coordinates,  $\hat{\mathbf{p}}$  and  $\hat{\mathbf{p}}'$  are the restrictions of  $\mathbf{p}$  and  $\mathbf{p}'$  to their images, the two points belong to the same connected component of  $D_{\Xi}$  if and only if  $\hat{\mathbf{p}}' \circ \hat{\mathbf{p}}^{-1}$  is an order isomorphism with respect to the orders induced on  $\operatorname{Im} \mathbf{p}$  and on  $\operatorname{Im} \mathbf{p}'$  by the standard order in  $\mathbb{R}$ .

**Remark 4.1.** A consequence of Theorem 4.1 is that each connected component of  $D_{\Xi}$  is convex. Indeed, two points belong to the same connected component iff the corresponding mapping  $\hat{\mathbf{p}}' \circ \hat{\mathbf{p}}^{-1}$  is an order isomorphism and, if this happens, we see from the proof of Theorem 4.1 that there is in  $D_{\Xi}$  a segment connecting them. The points of  $D_{\Xi}$  can be classified according to their belonging to its connected components; they can also be classified according to the total order relations they induce in  $\Xi$ .

Theorem 4.1 establishes an injective mapping from the set of the connected components of  $D_{\Xi}$  to the set of total order relations in  $\Xi$ . Really, this mapping is bijective. Indeed, given a total order in  $\Xi$ , we can always choose a set of values  $p_{\sigma}$  such that  $\sigma < \sigma' \Rightarrow p_{\sigma} < p_{\sigma'}$ . Hence the connected components of  $D_{\Xi}$  are in bijection with the total order relations in  $\Xi$ . If < is such a relation and  $\pi$  is a permutation of  $\Xi$ , the total order relation <' defined as  $\sigma <'\sigma'$  iff  $\pi^{-1}\sigma < \pi^{-1}\sigma'$  will be denoted  $\pi <$ . It is easily shown that the action of the permutation group of  $\Xi$  on the total order relations is simply transitive, so that, if we fix a total order relation in  $\Xi$ , the set of all total order relations can be parameterized by the elements of the permutation group of  $\Xi$ . In particular, this shows that  $D_{\Xi}$  possesses m! connected components.

Each permutation  $\pi$  defines a bijective mapping of  $T_{\Xi}$  into itself, and the image of its restriction to  $D_{\Xi}$  is  $D_{\Xi}$ , so that a bijective mapping  $\mathfrak{m}(\pi)$  of  $D_{\Xi}$  into itself is obtained. The restriction of this mapping to a connected component sends it in a connected component and defines a mapping which is an isomorphism of convex spaces. Therefore the connected components of  $D_{\Xi}$  are isomorphic convex spaces.

Let  $\Delta$  be a connected component. As it is convex, its closure  $\overline{\Delta}$  is a convex closed subspace of  $T_{\Xi}$ . We want to determine the structure of  $\overline{\Delta}$  and its relation with  $\Delta$ . As  $\Delta$  is associated with a well defined total order in  $\Xi$ , we get a well defined isomorphism of totally ordered sets between  $\Xi$  and the set  $\mathbb{N}_m$  of the first m natural numbers with the natural total order. Hence there is a bijection which associates each point of  $\Delta$ with a mapping  $\mathbb{N}_m \xrightarrow{\varpi} \mathbb{R}$  such that  $p_i > 0$ ,  $\sum p_i = 1$  and  $p_i < p_j$  for i < j. This bijection is obviously the restriction to  $\Delta$  of a bicontinuous bijection defined by the same rule between  $T_{\Xi}$  and the standard (m-1)-simplex. Calling  $\Delta_S$  the image of  $\Delta$ , the image of  $\overline{\Delta}$  is the closure  $\overline{\Delta}_S$  of  $\Delta_S$ . We have:

**Lemma 4.1.** The closure of  $\Delta_S$  is the set characterized by  $p_i \ge 0$ ,  $\sum p_i = 1$ , and  $p_i \le p_j$  for i < j.

*Proof.* For the proof see [6].

The structures of  $\bar{\Delta}_S$  and  $\Delta_S$  are completely characterized by the following theorem:

**Theorem 4.2.** The transformation:

$$x'_{1} = mx_{1}, \dots, x'_{i} = (m - i + 1)(x_{i} - x_{i-1}), \dots, x'_{m} = x_{m} - x_{m-1}$$

induces an isomorphism of convex spaces between  $\overline{\Delta}_S$  and the standard (m-1)-simplex. In this isomorphism  $\Delta_S$  and the interior of the simplex correspond each other.

*Proof.* For the proof see [6].

We can carry all the previous results back to  $D_\Xi$  and summarize them in the following theorem:

**Theorem 4.3.** If  $D_{\Xi}$  is the set of generic density operators with the same set  $\Xi$  of non-null eigenstates, each  $\rho_S \in D_{\Xi}$  can be uniquely expanded as  $\rho_S = \sum_{\sigma \in \Xi} p_{\sigma} P_{\sigma}$  where  $P_{\sigma}$  is the projector associated to the eigenstate  $\sigma$  and the expansion coefficients  $p_{\sigma}$  are arbitrary real different positive numbers such that  $\sum_{\sigma \in \Xi} p_{\sigma} = 1$ . With respect to the standard topology induced by the coordinates  $p_{\sigma}$ ,  $D_{\Xi}$  consists of m! connected components in bijection with the m! total order relations that can be defined on  $\Xi$ . The closure  $\bar{\Delta}_{<}$  of the connected component  $\Delta_{<}$  corresponding to a specific order < is a simplex whose vertices can be labeled with the states of  $\Xi$ . The vertex  $\varepsilon_{<}^{\sigma}$  of  $\bar{\Delta}_{<}$  is expressed as  $\varepsilon_{<}^{\sigma} = (\operatorname{tr} \sum_{\sigma' \geq \sigma} P_{\sigma'})^{-1} \sum_{\sigma' \geq \sigma} P_{\sigma'}$ . The component  $\Delta_{<}$  is the interior of  $\bar{\Delta}_{<}$ .

**Remark 4.2.** The positions of the vertices of  $\overline{\Delta}_<$  have a simple geometric interpretation: the vertex  $\varepsilon_<^{\sigma}$  is the barycenter of all the vertices of  $T_{\Xi}$  but those preceding  $\sigma$ . For example, if  $T_{\Xi}$  is a triangle whose set of vertices is  $\{A, B, C\}$  and the total order < is A < B < C,  $\varepsilon_<^A$  is the barycenter of the triangle,  $\varepsilon_<^B$  is the barycenter of the side BC and  $\varepsilon_<^C$  is C.

Once the structure of  $D_{\Xi}$  has been thoroughly investigated, we study the problem of the probability of the non-null eigenstates of a generic density operator.

We suppose first that the probability distribution depends uniquely on the state  $\zeta$  of the composite system. This is a reasonable assumption: its meaning is that the description of  $\mathcal{C}$  through its state is complete, so the behavior of any of its parts is completely specified by this state. We claim that, really, it depends only on  $\rho_S$ . Indeed, if we have an evolution T represented by a unitary transformation of the form  $I \otimes V$ ,  $\mathcal{H}$  can be considered as isolated and there is no evolution in it. Consequently the probability of any state  $\xi$  of  $\mathcal{H}$  as an isolated subsystem of  $\mathcal{C}$  does not change. This means that it depends only on the orbit of  $\zeta$  and hence only on  $\rho_S$ . Consequently, given the composite system and its subsystem  $\mathcal{H}$ , a mapping f arises which associates to each generic density operator  $\rho_S$  the probability distribution of its non-null eigenstates. We will now prove the following theorem:

**Theorem 4.4.** If  $\Xi$ ,  $\Xi'$  are the sets of non-null eigenstates of  $\rho_S$ ,  $\rho'_S$  and  $\mathbf{p}$ ,  $\mathbf{p}'$  the mappings which associate to each non-null eigenstate the corresponding eigenvalue then, if  $\rho_S$  and  $\rho'_S$  have the same spectrum, there is a unique bijection  $\Xi \xrightarrow{\beta} \Xi'$  such that  $\mathbf{p}' = \mathbf{p} \circ \beta^{-1}$  and, if  $\mathbf{q}$  and  $\mathbf{q}'$  are the probability distributions of  $\Xi$  and  $\Xi'$ , then  $\mathbf{q}' = \mathbf{q} \circ \beta^{-1}$ .

*Proof.* if  $\rho_S$  and  $\rho'_S$  have the same spectrum, then  $\operatorname{Im} \mathbf{p} = \operatorname{Im} \mathbf{p}'$ . Furthermore the restrictions  $\hat{\mathbf{p}}$  and  $\hat{\mathbf{p}}'$  of  $\mathbf{p}$  and  $\mathbf{p}'$  to their images are bijections. Hence  $(\hat{\mathbf{p}}')^{-1} \circ \hat{\mathbf{p}}$  is the unique required bijection  $\beta$ . This bijection can be extended (although in a non unique way) to a transformation  $T \in \mathcal{U}^Z(\mathcal{H})$ . This means that there is an evolution of the isolated system  $\mathcal{H}$  such that, whenever the state "before" is  $\xi$ , the state "after" is  $\beta(\xi)$ . This entails that  $\mathbf{q}'(\xi') = \mathbf{q} \left(\beta^{-1}(\xi')\right)$ .

We now exploit Theorem 4.4 and draw from it some useful consequences.

Let  $\Xi$  be a set of m orthogonal states and  $D_{\Xi}$  the set of generic density operators admitting  $\Xi$  as the set of its non-null eigenstates. There is a bijection  $D_{\Xi} \xrightarrow{\delta_{\Xi}} \Delta_{\Xi}$ between  $D_{\Xi}$  and the set  $\Delta_{\Xi}$  of all the injective mappings  $\mathbf{p} : \Xi \xrightarrow{\mathbf{p}} \mathbb{R}_{>}$  such that  $\sum_{\sigma \in \Xi} \mathbf{p}(\sigma) = 1$ . This bijection is defined as

$$\delta_{\Xi}(\rho_S)(\sigma) = tr\left(P_{\sigma}\rho_S\right). \tag{2}$$

We have

$$\delta_{\Xi}^{-1}(\mathbf{p}) = \sum_{\sigma \in \Xi} \mathbf{p}(\sigma) P_{\sigma}.$$
 (3)

BDP. 26 M. Campanella: Mathematical Studies on Quantum Mechanics (pp. 1 - 49) If  $f_{\Xi}$  is the restriction of f to  $D_{\Xi}$ , we define the mapping

$$\widehat{f}_{\Xi} = f_{\Xi} \circ \delta_{\Xi}^{-1}.$$
(4)

Let  $\Delta_{\mathbb{N}_m}$  be the set of injective mappings from  $\mathbb{N}_m$  to  $\mathbb{R}_>$  and  $\mathbb{N}_m \xrightarrow{\gamma} \Xi$  a bijection; we define a mapping through the position

$$g_{\Xi}^{(\gamma)}(\mathbf{m}) = \widehat{f}_{\Xi}\left(\mathbf{m} \circ \gamma^{-1}\right) \circ \gamma, \tag{5}$$

for  $\mathbf{m} \in \Delta_{\mathbb{N}_m}$ . We can prove the following

**Theorem 4.5.** The mapping  $g_{\Xi}^{(\gamma)}$  is independent of  $\gamma$ .

Proof. Let  $\beta$  be any permutation of  $\Xi$ . For each  $\mathbf{p} \in \Delta_{\Xi}$  we define  $\rho_S = \delta_{\Xi}^{-1}(\mathbf{p})$ and  $\rho'_S = \delta_{\Xi}^{-1}(\mathbf{p} \circ \beta^{-1})$ . Their spectra are Im  $\mathbf{p}$  and Im  $(\mathbf{p} \circ \beta^{-1})$  respectively, and hence they are the same. If  $\mathbf{q}$  and  $\mathbf{q}'$  are the corresponding probability distributions,  $\mathbf{q} = f_{\Xi}(\rho_S)$  and  $\mathbf{q}' = f_{\Xi}(\rho'_S)$ . Owing to theorem 4.4 we get  $f_{\Xi}(\delta_{\Xi}^{-1}(\mathbf{p} \circ \beta^{-1})) = f_{\Xi}(\delta_{\Xi}^{-1}(\mathbf{p})) \circ \beta^{-1}$  that is

$$\widehat{f}_{\Xi}\left(\mathbf{p}\circ\beta^{-1}\right)=\widehat{f}_{\Xi}\left(\mathbf{p}\right)\circ\beta^{-1}.$$

Now, if  $\mathbb{N}_m \xrightarrow{\bar{\gamma}} \Xi$  is another bijection,  $\beta \triangleq \bar{\gamma} \circ \gamma^{-1}$  is a permutation of  $\Xi$ ; further we have

$$g_{\Xi}^{(\bar{\gamma})}(\mathbf{m}) = \hat{f}_{\Xi} \left(\mathbf{m} \circ \bar{\gamma}^{-1}\right) \circ \bar{\gamma} = \hat{f}_{\Xi} \left(\mathbf{m} \circ \gamma^{-1} \circ \beta^{-1}\right) \circ \beta \circ \gamma = \\ = \hat{f}_{\Xi} \left(\mathbf{m} \circ \gamma^{-1}\right) \circ \beta^{-1} \circ \beta \circ \gamma = g_{\Xi}^{(\gamma)} \left(\mathbf{m}\right).$$

We now show that

**Theorem 4.6.** The mapping  $g_{\Xi}$  is independent of  $\Xi$ .

 $\mathit{Proof.}$  Let  $\Xi \xrightarrow{\beta} \Xi'$  be a bijection. Applying Theorem 4.4 we get

$$\widehat{f}_{\Xi'}\left(\mathbf{p}\right) = \widehat{f}_{\Xi}\left(\mathbf{p}\circ\beta\right)\circ\beta^{-1}.$$
(6)

If  $\mathbb{N}_m \xrightarrow{\gamma} \Xi'$  is a bijection, we have

$$g_{\Xi'}(\mathbf{m}) = \widehat{f}_{\Xi'}(\mathbf{m} \circ \gamma^{-1}) \circ \gamma = \widehat{f}_{\Xi}(\mathbf{m} \circ \gamma^{-1} \circ \beta) \circ \beta^{-1} \circ \gamma.$$
(7)

The mapping  $\bar{\gamma}=\beta^{-1}\circ\gamma$  is a bijection  $\mathbb{N}_m\xrightarrow{\bar{\gamma}}\Xi$  and

$$g_{\Xi'}(\mathbf{m}) = \hat{f}_{\Xi} \left( \mathbf{m} \circ \bar{\gamma}^{-1} \right) \circ \bar{\gamma} = g_{\Xi} \left( \mathbf{m} \right).$$
(8)

**Remark 4.3.** The domain of  $g_{\Xi}$  is  $\Delta_{\mathbb{N}_m}$ . For each  $\mathbf{m}$ , the value of  $g_{\Xi}$  is a mapping which associates to each element of  $\mathbb{N}_m$  the probability of the corresponding state in the set  $\Xi$  of possible states, so that this mapping is an element of the standard (m-1)-simplex  $T_m$ . Therefore  $g_{\Xi}$  is a mapping from  $\Delta_{\mathbb{N}_m}$  in  $T_m$ . We have just shown that it depends on  $\Xi$  only through its cardinality m, so that it will be denoted  $g_m$ . The domain will be more simply denoted  $\Delta_m$ , so that  $g_m$  is a mapping from  $\Delta_m$  (a subset of  $T_m$ ) in  $T_m$ . Although the argumentations developed so far do not exclude a possible dependence of  $g_m$  on the system, we will next show that this is not the case. Before we pursue this goal, it is useful to furnish an explicit expression of the restriction of f to the density operators of rank m in terms of  $g_m$ . This is given by the following theorem:

**Theorem 4.7.** If  $\rho_S$  is a generic density operator of rank m,

$$f(\rho_S) = g_m \left(\delta_{\Xi}(\rho_S) \circ \gamma\right) \circ \gamma^{-1}$$

where  $\Xi$  is the set of eigenstates appearing in the spectral decomposition of  $\rho_S$  and  $\mathbb{N}_m \xrightarrow{\gamma} \Xi$  an arbitrary bijection.

*Proof.* With the notations previously introduced, we get

$$f(\rho_S)(\sigma) = \mathbf{q}(\sigma) = \widehat{f}_{\Xi}(\mathbf{p})(\sigma).$$
(9)

If  $\mathbb{N}_m \xrightarrow{\gamma} \Xi$  is a bijection, putting  $\mathbf{p} = \mathbf{m} \circ \gamma^{-1}$  we get

$$f(\rho_S)(\sigma) = \hat{f}_{\Xi} \left( \mathbf{m} \circ \gamma^{-1} \right) \left( \gamma \circ \gamma^{-1}(\sigma) \right) = g_m(\mathbf{m}) \circ \gamma^{-1}(\sigma) \,. \tag{10}$$

But  $\mathbf{m} = \mathbf{p} \circ \gamma$ , and  $\mathbf{p} = \delta_{\Xi}(\rho_S)$ , so that  $f_m(\rho_S)(\sigma) = g_m(\delta_{\Xi}(\rho_S) \circ \gamma) \circ \gamma^{-1}(\sigma)$ .  $\Box$ 

In the sequel the following theorem will prove useful:

**Theorem 4.8.** If  $\pi$  is a permutation of  $\mathbb{N}_m$ , then  $g_m(\mathbf{m} \circ \pi) = g_m(\mathbf{m}) \circ \pi$ .

*Proof.* In theorem 4.7 the bijection  $\gamma$  is arbitrary. Hence, if  $\bar{\gamma} = \gamma \circ \pi$ ,  $g_m(\mathbf{m} \circ \pi) \circ \pi^{-1} \circ \gamma^{-1} = g_m(\mathbf{m}) \circ \gamma^{-1}$ , that is  $g_m(\mathbf{m} \circ \pi) = g_m(\mathbf{m}) \circ \pi$ .

**Remark 4.4.** The mapping  $g_m$  is defined on a subset of the standard (m-1)-simplex. The set of barycentric coordinates is not independent. Hence, when we write  $g_m(\mathbf{m})$  we must regard  $\mathbf{m}$  as a point of  $T_m$  rather than a collection of free coordinates.

In what follows, we will use for  $T_m$  a standard system of free coordinates defined as  $x_i(\mathbf{m}) = \mathbf{m}(i), i \in \mathbb{N}_{m-1}$ . This position yields a bijection between  $T_m$  and the subset  $\widehat{T}_{m-1}$  of  $\mathbb{R}^{m-1}$  defined by the inequalities  $x_i \ge 0$ ,  $\sum_{i=1}^{m-1} x_i \le 1$ .

If  $T_m \xrightarrow{\eta} \widehat{T}_{m-1}$  is this bijection, in standard coordinates we use the mapping  $\widehat{g}_m = \eta \circ g_m \eta^{-1}$ . The domain  $\Delta_m$  of  $g_m$  is given by all the sets of different positive barycentric coordinates. Hence the domain  $\widehat{\Delta}_m$  of  $\widehat{g}_m$  is given by all the sets of different standard coordinates in  $\widehat{T}_{m-1}$ , with the further conditions  $1 - \sum_{j=1}^{m-1} x_j \neq x_i, i \in \mathbb{N}_{m-1}$ , and excluding further the boundary of  $\widehat{T}_{m-1}$ .
We now pursue the goal of showing that  $g_m$  does not depend on the system (provided that the dimension of its Hilbert space is at least m).

To this purpose, let us envision a composite system SS' described by a Hilbert space  $\mathcal{H} \otimes \mathcal{K}$ . Suppose that this system interacts with an environment  $\mathcal{E}$  described by a Hilbert space  $\mathcal{L}$ , so that the total system is described by  $\mathcal{H} \otimes \mathcal{K} \otimes \mathcal{L}$ . Suppose that initially the system is in a state described by a ket  $|\phi\rangle |\kappa\rangle |\theta\rangle$ .

Assume that then an interaction between  $\mathcal{S}'$  and  $\mathcal{E}$  takes place, giving rise to a state  $|\phi\rangle \left(\sum d_{\alpha} |\kappa_{\alpha}\rangle |\theta_{\alpha}\rangle\right)$  (where the term in parentheses is the canonical decomposition of the final state of  $\mathcal{S}'\mathcal{E}$ ) with the coefficients  $d_{\alpha}$  all different each other and in number of l.

The number l and the quantities  $d_{\alpha}$  can be chosen at will provided that  $l \leq \dim \mathcal{K}$ , that the dimension of  $\mathcal{L}$  is chosen not smaller than that of  $\mathcal{K}$  and that  $\sum d_{\alpha}^2 = 1$ .

Finally, suppose to have an interaction between S' and S that brings from each  $|\phi\rangle |\kappa_{\alpha}\rangle$  to  $|\phi_{\alpha}\rangle |\kappa\rangle$ , where the  $|\phi_{\alpha}\rangle$  form an orthonormal set of  $\mathcal{H}$ . This is certainly possible if  $l \leq \dim \mathcal{H}$  because the  $|\phi\rangle |\kappa_{\alpha}\rangle$ , as well as the  $|\phi_{\alpha}\rangle |\kappa\rangle$ , are orthonormal sets in  $\mathcal{H} \otimes \mathcal{K}$ . It brings the total system from the state  $\sum d_{\alpha} |\phi\rangle |\kappa_{\alpha}\rangle |\theta_{\alpha}\rangle$  to the state  $\sum d_{\alpha} |\phi_{\alpha}\rangle |\kappa\rangle |\theta_{\alpha}\rangle$ .

Consider  $\mathcal{SS}'$  as a subsystem of  $\mathcal{SS}'\mathcal{E}$ . The initial density operator is

$$\rho_{\mathcal{SS}'} = \sum d_{\alpha}^2 \left| \phi \right\rangle \left\langle \phi \right| \otimes \left| \kappa_{\alpha} \right\rangle \left\langle \kappa_{\alpha} \right|. \tag{11}$$

The set of non-null eigenstates of  $\rho_{SS'}$  is  $X = \{ |\phi\rangle |\kappa_{\alpha}\rangle \}$ . Whenever SS' is in the state  $|\phi\rangle |\kappa_{\alpha}\rangle$ , S is in  $|\phi\rangle$  and S' is in  $|\kappa_{\alpha}\rangle$  and hence S' is in  $|\kappa_{\alpha}\rangle$ .

*Vice-versa*, whenever S' is in  $|\kappa_{\alpha}\rangle$ , SS' is in  $|\phi\rangle |\kappa_{\alpha}\rangle$  so that  $\Pr_{SS'} |\phi\rangle |\kappa_{\alpha}\rangle = \Pr_{S'} |\kappa_{\alpha}\rangle$ . Let us use the elements of  $\mathbb{N}_l$  to label the states of X, so that we define

$$\mathbb{N}_{l} \xrightarrow{\gamma} X : \gamma(\alpha) = |\phi\rangle |\kappa_{\alpha}\rangle.$$
(12)

We get  $\gamma^{-1}(|\phi\rangle |\kappa_{\alpha}\rangle) = \alpha$ . Furthermore,  $\delta_X(\rho_{\mathcal{SS}'}) \circ \gamma(\alpha) = d_{\alpha}^2$ . Hence, if  $\mathbf{m}(\alpha) \triangleq d_{\alpha}^2$ , we get

$$\Pr_{\mathcal{SS}'} \left| \phi \right\rangle \left| \kappa_{\alpha} \right\rangle = g_l^{\mathcal{SS}'} \left( \mathbf{m} \right) \left( \alpha \right)$$

In order to express  $\Pr_{\mathcal{S}'} |\kappa_{\alpha}\rangle$ , we must evaluate  $\rho_{\mathcal{S}'}$ . We have

$$\rho_{\mathcal{SS}'} = \sum d_{\alpha}^2 |\kappa_{\alpha}\rangle \langle \kappa_{\alpha}|.$$

With the same procedure we find

$$\Pr_{\mathcal{S}'} |\kappa_{\alpha}\rangle = g_l^{\mathcal{S}'} (\mathbf{m}) (\alpha) .$$

Hence in this case

$$g_l^{\mathcal{S}'}(\mathbf{m})(\alpha) = g_l^{\mathcal{SS}'}(\mathbf{m})(\alpha).$$

Similarly, the final density operator is

$$\rho_{\mathcal{SS}'}' = \sum d^2{}_{\alpha} \left| \phi_{\alpha} \right\rangle \left\langle \phi_{\alpha} \right| \otimes \left| \kappa \right\rangle \left\langle \kappa \right|.$$
(13)

Using once again the same method, we conclude that  $g_l^{\mathcal{S}}(\mathbf{m})(\alpha) = g_l^{\mathcal{SS}'}(\mathbf{m})(\alpha)$ . Hence  $g_l^{\mathcal{S}}(\mathbf{m}) = g_l^{\mathcal{S}'}(\mathbf{m})$ . Owing to the previous considerations, **m** is an arbitrary point of  $\Delta_l$ , so that  $g_{l\mathcal{S}} = g_{l\mathcal{S}'}$ .

We can express the results just obtained in the following

**Theorem 4.9.** For each m a universal mapping  $g_m$  exists such that in every system supporting density operators of rank m the probability law on the set  $\Xi$  of their possible states is expressed as

$$f(\rho_S) = g_m \left(\delta_{\Xi}(\rho_S) \circ \gamma\right) \circ \gamma^{-1}.$$

#### 5 A functional equation for $g_2$

Our next task is the determination of g. We will first determine  $g_2$ , and then we will find it for a general rank m. As for the moment our analysis is focused on m = 2, we will write it simply g. In this section we will find a functional equation which must be obeyed by g. The next section will be dedicated to its solution.

Let us consider a system  $\mathcal{W}$  composed with three systems  $\mathcal{R}$ ,  $\mathcal{S}$  and  $\mathcal{T}$ . We call  $\mathcal{H}$ ,  $\mathcal{K}$  and  $\mathcal{L}$  the Hilbert spaces of  $\mathcal{R}$ ,  $\mathcal{S}$  and  $\mathcal{T}$  respectively and  $\mathcal{M} = \mathcal{H} \otimes \mathcal{K} \otimes \mathcal{L}$  the Hilbert space of  $\mathcal{W}$ . We suppose that  $\mathcal{H}$ ,  $\mathcal{K}$  and  $\mathcal{L}$  are two-dimensional. It is useful for what follows to introduce some special states of  $\mathcal{W}$  that will be called *distinguished states*. In order to simplify the terminology, we will say "state  $|\chi\rangle$ " instead of "state specified by the ket  $|\chi\rangle$ ". Furthermore all the kets will be normalized.

**Definition 5.1.** We say that a ket  $|\chi\rangle \in \mathcal{M}$  is a distinguished state if the following conditions are satisfied:

- a) The partial density operator  $\rho_L$  is generic and with nonzero eigenvalues;
- b) In the canonical representation  $|\chi\rangle = d_1 |\psi_1\rangle |l_1\rangle + d_2 |\psi_2\rangle |l_2\rangle$  with  $d_1 \neq d_2$ ,  $d_1 > 0$ ,  $d_2 > 0$ ,  $|l_1\rangle$ ,  $|l_2\rangle$  orthonormal vectors of  $\mathcal{L}$  and  $|\psi_1\rangle$ ,  $|\psi_2\rangle$  orthonormal vectors of  $\mathcal{H}\otimes\mathcal{K}$ ,  $tr_K |\psi_1\rangle \langle\psi_1|$  and  $tr_K |\psi_2\rangle \langle\psi_2|$  are generic and have the same eigenstates.

We can show that

**Theorem 5.1.** If  $|\chi\rangle = d_1 |\psi_1\rangle |l_1\rangle + d_2 |\psi_2\rangle |l_2\rangle$  with  $d_1 \neq d_2$ ,  $d_1 > 0$ ,  $d_2 > 0$ ,  $|l_1\rangle$ ,  $|l_2\rangle$  orthonormal vectors of  $\mathcal{L}$  and

$$\left|\psi_{1}\right\rangle = \sqrt{m_{1}}\left|h_{1}\right\rangle\left|k_{1}\right\rangle + \sqrt{m_{2}}\left|h_{2}\right\rangle\left|k_{2}\right\rangle,\tag{1}$$

$$\left|\psi_{2}\right\rangle = \sqrt{m'_{1}}\left|h_{1}\right\rangle\left|k_{2}\right\rangle + \sqrt{m'_{2}}\left|h_{2}\right\rangle\left|k_{1}\right\rangle,\tag{2}$$

with  $m_i, m'_i \ge 0$ ,  $m_1 + m_2 = 1$ ,  $m'_1 + m'_2 = 1$ ,  $m_1 \ne m_2$ ,  $m'_1 \ne m'_2$ ,  $|h_1\rangle$ ,  $|h_2\rangle$  orthonormal in  $\mathcal{H}$ ,  $|k_1\rangle$ ,  $|k_2\rangle$  orthonormal in  $\mathcal{K}$ , then  $|\chi\rangle$  is a distinguished state.

*Proof.*  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are orthonormal;  $\rho_L$  is generic and with nonzero eigenvalues as a consequence of the assumptions on  $d_1$  and  $d_2$ . Furthermore

$$tr_{K} |\psi_{1}\rangle \langle \psi_{1}| = m_{1} |h_{1}\rangle \langle h_{1}| + m_{2} |h_{2}\rangle \langle h_{2}|, \qquad (3)$$

and

$$tr_{K} \left| \psi_{2} \right\rangle \left\langle \psi_{2} \right| = m'_{1} \left| h_{1} \right\rangle \left\langle h_{1} \right| + m'_{2} \left| h_{2} \right\rangle \left\langle h_{2} \right|, \tag{4}$$

so that they are generic and with the same eigenstates.

We have  $\rho_{HK} = d_1^2 |\psi_1\rangle \langle \psi_1| + d_2^2 |\psi_2\rangle \langle \psi_2|$ . Putting  $\lambda = d_1^2$ ,  $\lambda' = d_2^2$ ,  $\rho_1 = tr_K |\psi_1\rangle \langle \psi_1|$  and  $\rho_2 = tr_K |\psi_2\rangle \langle \psi_2|$ , we get

$$\rho_{HK} = \lambda |\psi_1\rangle \langle \psi_1| + \lambda' |\psi_2\rangle \langle \psi_2| \quad \text{and} \quad \rho_H = \lambda \rho_1 + \lambda' \rho_2.$$

The possible states of the system  $\mathcal{RS}$  are  $|\psi_1\rangle$  and  $|\psi_2\rangle$ . We get

$$\rho_H = \left(\lambda m_1 + \lambda' m'_1\right) \left|h_1\right\rangle \left\langle h_1\right| + \left(\lambda m_2 + \lambda' m'_2\right) \left|h_2\right\rangle \left\langle h_2\right|,$$

so that, if  $\lambda m_1 + \lambda' m'_1 \neq \frac{1}{2}$ , the system  $\mathcal{R}$  can be considered isolated in  $\rho_H$ . Hence, as long as neither  $m_1 + m'_1$  nor  $m_2 + m'_2$  are zero, when the total system is in  $|\chi\rangle$ ,  $\mathcal{R}$  is either in  $|h_1\rangle$  or in  $|h_2\rangle$ .

Suppose first that all the *m* and *m'* are nonzero. In this case each possibility for the states of  $\mathcal{RS}$  as an isolated system, i.e.  $|\psi_1\rangle$  and  $|\psi_2\rangle$ , gives rise to both possibilities for the states of  $\mathcal{R}$ , that is  $|h_1\rangle$  and  $|h_2\rangle$ . Hence we have two disjoint possibilities of obtaining  $|h_1\rangle$ : either with  $\mathcal{RS}$  in  $|\psi_1\rangle$  or with  $\mathcal{RS}$  in  $|\psi_2\rangle$ . Consequently the probability  $\bar{q}_1$  of finding  $\mathcal{R}$  in  $|h_1\rangle$  is the sum of two terms corresponding to these possibilities. Applying the Bayes rule, the first term is the product of the probability  $q_1$  of finding  $\mathcal{RS}$  in  $|\psi_1\rangle$  times the probability  $q_1^{(1)}$  of finding  $\mathcal{R}$  in  $|h_1\rangle$  given that  $\mathcal{RS}$  is in  $|\psi_1\rangle$ . Similarly, the second term is the product of the probability  $q_2$  of finding  $\mathcal{RS}$  in  $|\psi_2\rangle$  times the probability  $q_1^{(2)}$  of finding  $\mathcal{R}$  in  $|h_1\rangle$  given that  $\mathcal{RS}$  is in  $|\psi_2\rangle$ . Hence we can write

$$\bar{q}_1 = q_1^{(1)} q_1 + q_1^{(2)} q_2.$$
(5)

In the same way we get

$$\bar{q}_2 = q_2^{(1)} q_1 + q_2^{(2)} q_2, \tag{6}$$

where  $q_2^{(1)}$  is the probability of finding  $\mathcal{R}$  in  $|h_2\rangle$  given that  $\mathcal{RS}$  is in  $|\psi_1\rangle$ , and  $q_2^{(2)}$  is the probability of finding  $\mathcal{R}$  in  $|h_2\rangle$  given that  $\mathcal{RS}$  is in  $|\psi_2\rangle$ .

Denoting with  $g_{(1)}$  and  $g_{(2)}$  the two components of g, we have

$$\begin{array}{ll} q_1 = g_{(1)} \left( \lambda, \lambda' \right), & q_2 = g_{(2)} \left( \lambda, \lambda' \right), \\ q_1^{(1)} = g_{(1)} \left( m_1, m_2 \right), & q_2^{(1)} = g_{(2)} \left( m_1, m_2 \right), \\ q_1^{(2)} = g_{(1)} \left( m'_1, m'_2 \right), & q_2^{(2)} = g_{(2)} \left( m'_1, m'_2 \right). \end{array}$$

Furthermore

$$\bar{q}_1 = g_{(1)} \left( \lambda m_1 + \lambda' m'_1, \lambda m_2 + \lambda' m'_2 \right), \tag{7}$$

$$\bar{q}_2 = g_{(2)} \left( \lambda m_1 + \lambda' m'_1, \lambda m_2 + \lambda' m'_2 \right).$$
(8)

By substitution we get

$$\begin{split} g_{(1)} \left(\lambda m_1 + \lambda' m'_1, \lambda m_2 + \lambda' m'_2\right) &= g_{(1)} \left(m_1, m_2\right) g_{(1)} \left(\lambda, \lambda'\right) + g_{(1)} \left(m'_1, m'_2\right) g_{(2)} \left(\lambda, \lambda'\right), \\ g_{(2)} \left(\lambda m_1 + \lambda' m'_1, \lambda m_2 + \lambda' m'_2\right) &= g_{(2)} \left(m_1, m_2\right) g_{(1)} \left(\lambda, \lambda'\right) + g_{(2)} \left(m'_1, m'_2\right) g_{(2)} \left(\lambda, \lambda'\right). \end{split}$$

These equations hold for every  $((\lambda, \lambda'), \mathbf{m}, \mathbf{m}') \in \Delta_2^3$  (where  $\mathbf{m} = (m_1, m_2), \mathbf{m}' = (m'_1, m'_2)$ ) such that  $\lambda \mathbf{m} + \lambda' \mathbf{m}' \in \Delta_2$ . We now take  $m_1 = 1$ , maintaining the condition that neither  $m_1 + m'_1$  nor  $m_2 + m'_2$  are zero. In this case the possible state  $|\psi_1\rangle$  gives rise to the single possibility  $|h_1\rangle$ . Further  $m'_2$  must be nonzero. If in addition  $m'_2 \neq 1$ ,  $|\psi_2\rangle$  gives rise to the both possibilities  $|h_1\rangle$  and  $|h_2\rangle$ . Hence in this case we must write a single summand for  $\bar{q}_2$  and identify with  $q_1$  the summand corresponding to the possibility  $|\psi_1\rangle$  in  $\bar{q}_1$ ; this is equivalent to take  $q_1^{(1)} = 1$  and  $q_2^{(1)} = 0$ . So we find

$$\bar{q}_1 = q_1 + q_1^{(2)} q_2, \tag{9}$$

$$\bar{q}_2 = q_2^{(2)} q_2,$$
 (10)

giving rise to the equations

$$g_{(1)}(\lambda + \lambda' m'_1, \lambda' m'_2) = g_{(1)}(\lambda, \lambda') + g_{(1)}(m'_1, m'_2) g_{(2)}(\lambda, \lambda'), \quad (11)$$

$$g_{(2)}(\lambda + \lambda' m'_1, \lambda' m'_2) = g_{(2)}(m'_1, m'_2) g_{(2)}(\lambda, \lambda').$$
(12)

If  $m_1 = 1, m'_2 = 1$ ,  $|\psi_2\rangle$  gives rise to the single possibility  $|h_2\rangle$ . In this case an identity is obtained. We now take  $m_2 = 1$  and  $m'_1, m'_2$  both nonzero. This time we get  $q_1^{(1)} = 0$  and  $q_2^{(1)} = 1$  and hence

$$\bar{q}_1 = q_1^{(2)} q_2, \tag{13}$$

$$\bar{q}_2 = q_1 + q_2^{(2)} q_2, \tag{14}$$

so that

$$g_{(1)}(\lambda'm'_{1},\lambda+\lambda'm'_{2}) = g_{(1)}(m'_{1},m'_{2})g_{(2)}(\lambda,\lambda'), \qquad (15)$$

$$g_{(2)}\left(\lambda'm'_{1},\lambda+\lambda'm'_{2}\right) = g_{(1)}\left(\lambda,\lambda'\right) + g_{(2)}\left(m'_{1},m'_{2}\right)g_{(2)}\left(\lambda,\lambda'\right).$$
(16)

Similarly we take  $m'_1 = 1$  and then  $m'_2 = 1$ . In the first case we get  $q_1^{(2)} = 1$  and  $q_2^{(2)} = 0$ , in the second  $q_1^{(2)} = 0$  and  $q_2^{(2)} = 1$ . We obtain respectively

$$g_{(1)}(\lambda m_1 + \lambda', \lambda m_2) = g_{(1)}(m_1, m_2) g_{(1)}(\lambda, \lambda') + g_{(2)}(\lambda, \lambda'), \qquad (17)$$

$$g_{(2)}(\lambda m_1 + \lambda', \lambda m_2) = g_{(2)}(m_1, m_2) g_{(1)}(\lambda, \lambda'), \qquad (18)$$

and

$$g_{(1)}(\lambda m_1, \lambda m_2 + \lambda') = g_{(1)}(m_1, m_2) g_{(1)}(\lambda, \lambda'), \qquad (19)$$

$$g_{(2)}(\lambda m_1, \lambda m_2 + \lambda') = g_{(2)}(m_1, m_2) g_{(1)}(\lambda, \lambda') + g_{(2)}(\lambda, \lambda').$$
(20)

We now *define* an extension  $\tilde{g}$  of g as follows:

$$\tilde{g}(m_1, m_2) = g(m_1, m_2) \quad \text{for} \quad (m_1, m_2) \in \Delta_2; 
\tilde{g}_{(1)}(1, 0) = 1, \quad \tilde{g}_{(2)}(1, 0) = 0, \quad \tilde{g}_{(1)}(0, 1) = 0, \quad \tilde{g}_{(2)}(0, 1) = 1.$$

Defining

$$\tilde{\Delta}_2 = \Delta_2 \cup \{(1,0), (0,1)\},\$$

we can show that  $\tilde{g}$  satisfies the equations

$$\begin{split} \tilde{g}_{(1)} \left(\lambda m_1 + \lambda' m'_1, \lambda m_2 + \lambda' m'_2\right) &= \tilde{g}_{(1)} \left(m_1, m_2\right) \tilde{g}_{(1)} \left(\lambda, \lambda'\right) + \tilde{g}_{(1)} \left(m'_1, m'_2\right) \tilde{g}_{(2)} \left(\lambda, \lambda'\right) \\ \tilde{g}_{(2)} \left(\lambda m_1 + \lambda' m'_1, \lambda m_2 + \lambda' m'_2\right) &= \tilde{g}_{(2)} \left(m_1, m_2\right) \tilde{g}_{(1)} \left(\lambda, \lambda'\right) + \tilde{g}_{(2)} \left(m'_1, m'_2\right) \tilde{g}_{(2)} \left(\lambda, \lambda'\right) \end{split}$$

for every  $((\lambda, \lambda'), \mathbf{m}, \mathbf{m}') \in \tilde{\Delta}_2^3$  such that  $\lambda \mathbf{m} + \lambda' \mathbf{m}' \in \tilde{\Delta}_2$ .

Indeed, it is sufficient to verify the above equations when at least one point is (1,0) or (0,1). If  $(\lambda, \lambda') = (1,0)$  or (0,1), we obtain an identity. The other cases are a consequence of equations already established for the remaining four possibilities.

Let us express this relation in free coordinates. We put  $\mathbf{m} = \eta^{-1}(z)$  and  $\mathbf{m}' = \eta^{-1}(z')$  so that

$$\lambda \mathbf{m} + \lambda' \mathbf{m}' = \eta^{-1} \left( \lambda z + (1 - \lambda) z' \right).$$
<sup>(21)</sup>

Therefore

$$\eta \circ \tilde{g} \left( \lambda \mathbf{m} + \lambda' \mathbf{m}' \right) = \tilde{g}_{(1)} \left( \lambda z + (1 - \lambda) z' \right) \triangleq \hat{g} \left( \lambda z + (1 - \lambda) z' \right).$$

We further have

$$\eta \circ \tilde{g}(\mathbf{m}) = \hat{g}(z)$$
 and  $\eta \circ \tilde{g}(\mathbf{m}') = \hat{g}(z')$ 

finally

$$\tilde{g}_{(1)}(\lambda,\lambda') = \hat{g}(\lambda)$$
 and  $\tilde{g}_{(2)}(\lambda,\lambda') = 1 - \hat{g}(\lambda)$ .

Hence we get

$$\hat{g}\left(\lambda z + (1-\lambda)z'\right) = \hat{g}\left(\lambda\right)\hat{g}\left(z\right) + (1-\hat{g}\left(\lambda\right))\hat{g}\left(z'\right),\tag{22}$$

which holds for all the  $(\lambda, z, z')$  such that the arguments in all the occurrences of  $\hat{g}$  belong to its domain  $[0, 1/2) \bigcup (1/2, 1]$ .

The definition of  $\tilde{g}$  entails that the boundary conditions  $\hat{g}(0) = 0$  and  $\hat{g}(1) = 1$  must be satisfied.

The next section will be dedicated to the solution of this functional equation.

#### 6 Solution of the functional equation

In the previous section we have found the functional equation

$$\hat{g}\left(\lambda z + (1-\lambda)z'\right) = \hat{g}\left(\lambda\right)\hat{g}\left(z\right) + (1-\hat{g}\left(\lambda\right))\hat{g}\left(z'\right).$$
(1)

The function  $\hat{g}$  is defined in  $\Delta_2 = [0, \frac{1}{2}) \bigcup (\frac{1}{2}, 1]$ . Furthermore the boundary conditions  $\hat{g}(0) = 0$ ,  $\hat{g}(1) = 1$  must be fulfilled and its values must range between 0 and 1. This equation holds in  $\Delta_2^3$  for  $\lambda z + (1 - \lambda) z' \neq \frac{1}{2}$ .

This section is dedicated to its solution. First we make the following positions

$$x = z - \frac{1}{2}, \quad x' = z' - \frac{1}{2}, \quad \mu = \lambda - \frac{1}{2}, \quad f(x) = \hat{g}(z) - \frac{1}{2}.$$
 (2)

We have  $\lambda z + (1 - \lambda) z' = \lambda x + (1 - \lambda) x' + \frac{1}{2}$ , so that

$$f(\lambda x + (1 - \lambda) x') + \frac{1}{2} = \left(f(\mu) + \frac{1}{2}\right) \left(f(x) + \frac{1}{2}\right) + \left(\frac{1}{2} - f(\mu)\right) \left(f(x') + \frac{1}{2}\right),$$
(3)

whence

$$f\left[\left(\mu + \frac{1}{2}\right)x + \left(\frac{1}{2} - \mu\right)x'\right] = f(\mu)\left(f(x) - f(x')\right) + \frac{1}{2}(f(x) + f(x')).$$
(4)

Putting  $D = \left[-\frac{1}{2}, 0\right] \bigcup \left(0, \frac{1}{2}\right]$ , this equation holds in  $D^3$  for  $\left(\mu + \frac{1}{2}\right) x + \left(\frac{1}{2} - \mu\right) x' \neq 0$ . In particular, for x' = -x we get:

$$f(2\mu x) = f(\mu) (f(x) - f(-x)) + \frac{1}{2} (f(x) + f(-x)).$$
(5)

This equation holds in  $D^2$ .

The left side is symmetric under the exchange of  $\mu$  and x, so that we have

$$-f(\mu)f(-x) + \frac{1}{2}(f(x) + f(-x)) = -f(x)f(-\mu) + \frac{1}{2}(f(\mu) + f(-\mu)).$$
(6)

We have  $f\left(-\frac{1}{2}\right) = -\frac{1}{2}$  and  $f\left(\frac{1}{2}\right) = \frac{1}{2}$ , so that, putting  $\mu = -\frac{1}{2}$  we get

$$f(x) + f(-x) = 0,$$
 (7)

and hence

$$f(2\mu x) = 2f(\mu) f(x).$$
 (8)

We put  $F(\zeta) = 2f(\frac{1}{2}\zeta)$ , so that  $f(\zeta) = \frac{1}{2}F(2\zeta)$ . Hence we get  $F(4\mu x) = F(2\mu)F(2x)$ , that is

$$F(xy) = F(x) F(y).$$
(9)

As the domain of f is D, the domain of F is  $\Lambda = [-1,0) \bigcup (0,1]$ . The equation (9) holds for any  $(x,y) \in \Lambda \times \Lambda$ . The functional equation for f can be translated into a functional equation for F. We have

$$\frac{1}{2}F\left(\left(2\mu+1\right)x+\left(1-2\mu\right)x'\right) = \frac{1}{4}F\left(2\mu\right)\left(F\left(2x\right)-F\left(2x'\right)\right) + \frac{1}{4}\left(F\left(2x\right)+F\left(2x'\right)\right).$$
(10)

Putting  $2\mu = \xi$ , 2x = u, 2x' = v, we obtain

$$F\left[\frac{1}{2}(1+\xi)u + \frac{1}{2}(1-\xi)v\right] = \frac{1}{2}F(\xi)\left[F(u) - F(v)\right] + \frac{1}{2}\left[F(u) + F(v)\right], \quad (11)$$

which holds for any  $(\xi, u, v) \in \Lambda^3$  such that  $u + v + \xi u - \xi v \neq 0$ . We can write

$$F\left(\frac{1}{2}u + \frac{1}{2}\xi u + \frac{1}{2}v - \frac{1}{2}\xi v\right) = \frac{1}{2}F(u) + \frac{1}{2}F(\xi u) + \frac{1}{2}F(v) - \frac{1}{2}F(\xi v).$$
(12)

We restrict the above equation to the subset  $\Sigma$  of  $\Lambda^3$  satisfying the condition  $u = \xi v$ and such that  $v + \xi u \neq 0$ . In this subset we have

$$F\left(\frac{1}{2}\xi u + \frac{1}{2}v\right) = \frac{1}{2}F\left(\xi u\right) + \frac{1}{2}F\left(v\right).$$
(13)

We now put  $\alpha = \xi u = \xi^2 v$ ,  $\beta = v$ . The inverse transformation is  $\xi = \pm \sqrt{\alpha/\beta}$ ,  $u = \pm \sqrt{\alpha\beta}$ ,  $v = \beta$ . Hence we have  $0 < |\beta| \le 1$ ,  $0 < \alpha/\beta \le 1$ ,  $0 < \alpha\beta \le 1$ . This subset can be characterized by the inequalities  $0 < |\alpha| \le |\beta| \le 1$  and  $\alpha\beta > 0$ . Therefore the equation

$$F\left(\frac{1}{2}\alpha + \frac{1}{2}\beta\right) = \frac{1}{2}F\left(\alpha\right) + \frac{1}{2}F\left(\beta\right)$$
(14)

holds for  $0 < |\alpha| \le 1$ ,  $0 < |\beta| \le 1$ ,  $|\alpha| \le |\beta|$  such that  $\alpha\beta > 0$ . If  $|\alpha| > |\beta|$  we put  $\alpha' = \beta$ ,  $\beta' = \alpha$ , so that  $|\alpha'| < |\beta'|$ . We have

$$F\left(\frac{1}{2}\alpha + \frac{1}{2}\beta\right) = F\left(\frac{1}{2}\alpha' + \frac{1}{2}\beta'\right) = \frac{1}{2}F\left(\alpha'\right) + \frac{1}{2}F\left(\beta'\right) = \frac{1}{2}F\left(\alpha\right) + \frac{1}{2}F\left(\beta\right).$$

Hence eq. (14) holds for all  $(\alpha, \beta)$  such that  $0 < |\alpha| \le 1, 0 < |\beta| \le 1, \alpha\beta > 0$ .

As F(x) + F(-x) = 0, we can restrict our analysis to the interval (0, 1]. Hence we have the equations

$$F(xy) = F(x) F(y), \qquad (15)$$

$$F\left(\frac{x+y}{2}\right) = \frac{1}{2}F(x) + \frac{1}{2}F(y), \qquad (16)$$

with  $(x, y) \in (0, 1]^2$ .

Let  $X_N = \left\{ \frac{n}{2^N} | n \in \mathbb{N}, n < 2^N \right\}$ . We have the following:

**Theorem 6.1.** If F satisfies eq.(16), for any  $N \in \mathbb{N}$  and for any  $x \in X_N$ , F(x) is given by

$$F(x) = F\left(\frac{1}{2}\right) + \left[1 - F\left(\frac{1}{2}\right)\right](2x - 1).$$
(17)

*Proof.* The theorem is true for N = 1. Then we prove it by recursion on N.

If the theorem is true for a given N, all the points (x, F(x)) such that  $x \in X_N$  lie on the straight line r containing the points  $(\frac{1}{2}, F(\frac{1}{2}))$  and (1, 1).

The set  $X_{N+1}$  is obtained from  $X_N$  by adjoining to it all the middle points of the intervals  $\left(\frac{n}{2^N}, \frac{n+1}{2^N}\right)$  for  $1 \le n < 2^N - 1$  and further the two points  $\frac{1}{2^N} - \frac{1}{2^{N+1}}$  and  $\frac{2^N - 1}{2^N} + \frac{1}{2^{N+1}}$ .

If N = 1,  $X_1 = \left\{\frac{1}{2}\right\}$  and  $X_2$  is obtained by adjunction of the points  $\frac{1}{4}$  and  $\frac{3}{4}$ . Eq.(16) shows that  $F\left(\frac{3}{4}\right)$  is obtained by linear interpolation of the values  $F\left(\frac{1}{2}\right)$  and F(1) = 1, so that  $\left(\frac{3}{4}, F\left(\frac{3}{4}\right)\right)$  belongs to r. The same equation shows that the linear interpolation between the values  $F\left(\frac{1}{4}\right)$  and  $F\left(\frac{3}{4}\right)$  must yield  $F\left(\frac{1}{2}\right)$ , so that  $\left(\frac{1}{4}, F\left(\frac{1}{4}\right)\right)$  belongs to r.

For N > 1, the value of F in the middle point of each interval  $\left(\frac{n}{2^N}, \frac{n+1}{2^N}\right)$  is obtained by linear interpolation of the values in its extreme points, so that (x, F(x)) lies on r. For the point adjoined on the left,  $F\left(\frac{1}{2^N} - \frac{1}{2^{N+1}}\right)$  must be such that the linear interpolation of it with  $F\left(\frac{1}{2^N} + \frac{1}{2^{N+1}}\right)$  yields  $F\left(\frac{1}{2^N}\right)$ . Hence  $\left(\frac{1}{2^N} - \frac{1}{2^{N+1}}, F\left(\frac{1}{2^N} - \frac{1}{2^{N+1}}\right)\right)$ belongs to r. Similarly,  $F\left(\frac{2^{N-1}}{2^N} + \frac{1}{2^{N+1}}\right)$  must be such that the linear interpolation of it with  $F\left(\frac{2^N-1}{2^N} - \frac{1}{2^{N+1}}\right)$  yields  $F\left(\frac{2^N-1}{2^N}\right)$ . Therefore  $\left(\frac{2^N-1}{2^N} + \frac{1}{2^{N+1}}, F\left(\frac{2^N-1}{2^N} + \frac{1}{2^{N+1}}\right)\right)$  belongs to r.  $\Box$ 

We now use eq. (15) for  $x = y = \frac{1}{2}$ . We get  $F\left(\frac{1}{4}\right) = F\left(\frac{1}{2}\right)^2$ . But  $\frac{1}{4} \in X_2$ , so that we can use Theorem 6.1 getting  $F\left(\frac{1}{4}\right) = \frac{3}{2}F\left(\frac{1}{2}\right) - \frac{1}{2}$ . Hence  $F\left(\frac{1}{2}\right)$  satisfies the equation  $F\left(\frac{1}{2}\right)^2 - \frac{3}{2}F\left(\frac{1}{2}\right) + \frac{1}{2} = 0$  whose solutions are  $F\left(\frac{1}{2}\right) = 1$  and  $F\left(\frac{1}{2}\right) = \frac{1}{2}$ . In the first case we get F(x) = 1 and in the second F(x) = x. The first case can be excluded. Indeed, as F is odd, F(x) = sign(x). If we take, for instance,  $\xi > 0$  u > 0 and such that  $\frac{(1+\xi)u}{1-\xi} < 1$  and  $v < -\frac{(1+\xi)u}{1-\xi}$ , with the further condition that all the variables belong to  $-X_N \bigcup X_N$  for some N, the argument of F on the left side is negative, so that the latter is -1. On the other hand, the right side is F(u), and hence its value is 1. We conclude that the only possibility is F(x) = x. In this way we have proved the theorem:

**Theorem 6.2.** For every  $N \in \mathbb{N}$  the restriction of F to the set  $-X_N \bigcup X_N$  is the identity.

We are now ready to prove the next theorem.

**Theorem 6.3.** The only function F satisfying eqs. (9) and (14) and not greater than 1 in magnitude is the identity.

*Proof.* As F is an odd function, we can limit our analysis to the interval (0, 1] of the independent variable.

First we observe that in this range F is non-negative. Indeed, if  $z \in (0, 1]$ , and  $x = \sqrt{z}, x \in (0, 1]$  and, by virtue of (9), we have

$$F(z) = F(x^2) = F(x)^2 \ge 0.$$

Further, F is a non-decreasing function. Indeed, if x < y,

$$F(x) = F\left(\left(\frac{x}{y}\right)y\right) = F\left(\frac{x}{y}\right)F(y) \le F(y).$$

Let  $z \in (0, 1]$ . If  $z \in X_N$  for some N, F(z) = z by Theorem 6.2. If  $z \notin X_N$  for every N, for each N we define  $x_N$  as the greatest  $x \in X_N$  smaller than z and  $x'_N$  as the smallest  $x \in X_N$  greater than z. It is obvious that  $\{x_N\}$  is a non-decreasing sequence and  $\{x'_N\}$  is a non-increasing sequence. Let  $\bar{x} = \lim_{N \to \infty} x_N$ . We have  $\bar{x} \leq z$ . If  $\bar{x} < z$ , for each N we define  $\bar{x}_N$  as the smallest  $x \in X_N$  greater than  $\bar{x}$ . The neighbor on the left of  $\bar{x}_N$  is  $\bar{x}_N - \frac{1}{2^N}$  which, by definition of  $\bar{x}_N$ , is not greater than  $\bar{x}$ . Hence for sufficiently high values of N we have  $\bar{x}_N < z$ . But we have  $x_N \leq \bar{x} < \bar{x}_N < z$ . This is a contradiction because  $x_N$  is the greatest  $x \in X_N$  smaller than z. Therefore we have

$$\lim_{N \to \infty} x_N = z.$$

In a similar way we can show that

As

$$\lim_{N \to \infty} x'_N = z.$$
$$x_N = F(x_N) \le F(z) \le F(x'_N) = x'_N, F(z) = z.$$

Remembering the changes of variables we have made to go from  $\tilde{g}$  to F, we conclude that the unique solution of the functional equation with the conditions imposed is the identity mapping.

**Remark 6.1.** We emphasize that no continuity assumption has been made in the above argument. The only assumption on g besides the fact that it must satisfy the functional equation is that, as a probability, its values must range between 0 and 1.

#### 7 The function g for arbitrary rank

In this section we generalize the results obtained before, and find the form of the function g in the general case. To this purpose, we introduce the general notion of a *distinguished state*.

Let us consider a system  $\mathcal{W}$  composed with three systems  $\mathcal{R}$ ,  $\mathcal{S}$  and  $\mathcal{T}$ . We call  $\mathcal{H}$ ,  $\mathcal{K}$  and  $\mathcal{L}$  the Hilbert spaces of  $\mathcal{R}$ ,  $\mathcal{S}$  and  $\mathcal{T}$  respectively and  $\mathcal{M} = \mathcal{H} \otimes \mathcal{K} \otimes \mathcal{L}$  the Hilbert space of  $\mathcal{W}$ . We suppose that  $\mathcal{H}$  and  $\mathcal{K}$  are *m*-dimensional, while  $\mathcal{L}$  is supposed two-dimensional. The notion of a distinguished state in this more general case is similar to that given for two-dimensional spaces:

**Definition 7.1.** We say that a ket  $|\chi\rangle \in \mathcal{M}$  is a distinguished state if the following conditions are satisfied:

a) The partial density operator  $\rho_L$  is generic and with nonzero eigenvalues,

b) In the canonical representation  $|\chi\rangle = d_1 |\psi_1\rangle |l_1\rangle + d_2 |\psi_2\rangle |l_2\rangle$  with  $d_1 \neq d_2, d_1 > 0, d_2 > 0, d_1^2 + d_2^2 = 1, |l_1\rangle, |l_2\rangle$  orthonormal vectors of  $\mathcal{L}$  and  $|\psi_1\rangle, |\psi_2\rangle$  orthonormal vectors of  $\mathcal{H} \otimes \mathcal{K}, tr_K |\psi_1\rangle \langle\psi_1|$  and  $tr_K |\psi_2\rangle \langle\psi_2|$  are generic and have the same eigenstates.

Let  $\{|h_i\rangle\}_{i\in\mathbb{N}_m}$  and  $\{|k_i\rangle\}_{i\in\mathbb{N}_m}$  arbitrary ordered orthonormal bases of  $\mathcal{H}$  and  $\mathcal{K}$  respectively. Let  $\pi$  be a permutation of  $\mathbb{N}_m$  which displaces all its points.

Let  $\mathbb{N}_m \xrightarrow{\mathbf{m}} \mathbb{R}_{\geq}$  and  $\mathbb{N}_m \xrightarrow{\mathbf{m}'} \mathbb{R}_{\geq}$  be injective mappings with  $\sum m_i = 1$  and  $\sum m'_i = 1$ . Finally, let  $|l_1\rangle$ ,  $|l_2\rangle$  be orthonormal vectors of  $\mathcal{L}$  and  $d_1 \neq d_2$ ,  $d_1 > 0$ ,  $d_2 > 0$ . Put

$$|\psi_1\rangle = \sum \sqrt{m_i} |h_i\rangle |k_i\rangle, \qquad |\psi_2\rangle = \sum \sqrt{m'_i} |h_i\rangle |k_{\pi(i)}\rangle, \tag{1}$$

and

$$|\chi\rangle = d_1 |\psi_1\rangle |l_1\rangle + d_2 |\psi_2\rangle |l_2\rangle.$$
<sup>(2)</sup>

We can easily prove that

**Theorem 7.1.**  $|\chi\rangle$  is a distinguished state.

*Proof.* As  $\pi(i) \neq i$ ,  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are orthonormal. Hence (2) is the canonical representation of  $|\chi\rangle$ . The corresponding density operator  $\rho_L$  is given by

$$ho_L = d_1^2 \left| l_1 
ight
angle \left\langle l_1 \right| + d_2^2 \left| l_2 
ight
angle \left\langle l_2 \right|$$

Therefore  $\rho_L$  is generic and with nonzero eigenvalues. Furthermore

$$\begin{split} tr_{K} \left| \psi_{1} \right\rangle \left\langle \psi_{1} \right| &= \sum m_{i} \left| h_{i} \right\rangle \left\langle h_{i} \right|, \\ tr_{K} \left| \psi_{2} \right\rangle \left\langle \psi_{2} \right| &= \sum m'_{i} \left| h_{i} \right\rangle \left\langle h_{i} \right|, \end{split}$$

so that they are generic and with the same eigenstates.

Let us evaluate the density operator  $\rho_H$  of  $|\chi\rangle$  in  $\mathcal{R}$ . We have

$$\left|\chi\right\rangle = d_1 \sum \sqrt{m_i} \left|h_i\right\rangle \left|k_i\right\rangle \left|l_1\right\rangle + d_2 \sum \sqrt{m'_i} \left|h_i\right\rangle \left|k_{\pi(i)}\right\rangle \left|l_2\right\rangle,\tag{3}$$

which we recast in the form  $|\chi\rangle = \sum |h_i\rangle |\theta_i\rangle$  with

$$\left|\theta_{i}\right\rangle = d_{1}\sqrt{m_{i}}\left|k_{i}\right\rangle\left|l_{1}\right\rangle + d_{2}\sqrt{m'_{i}}\left|k_{\pi(i)}\right\rangle\left|l_{2}\right\rangle \tag{4}$$

The kets  $|\theta_i\rangle$  are pairwise orthogonal, so that

$$\rho_{H} = \sum \left\langle \theta_{i} | \theta_{i} \right\rangle \left| h_{i} \right\rangle \left\langle h_{i} \right| = d_{1}^{2} \rho_{1} + d_{2}^{2} \rho_{2}$$

where  $\rho_1$  and  $\rho_2$  are the density operators in  $\mathcal{R}$  corresponding to  $|\psi_1\rangle$  and  $|\psi_2\rangle$ .

We now discuss the probabilities.

Putting  $d_1^2 = \lambda$ ,  $d_2^2 = \lambda'$ , the spectral decomposition of the density operator  $\rho_{HK}$ is  $\rho_{HK} = \lambda |\psi_1\rangle \langle \psi_1| + \lambda' |\psi_2\rangle \langle \psi_2|$ . Hence the system  $\mathcal{RS}$  is in the state  $|\psi_1\rangle$  with probability  $q_1$  and in the state  $|\psi_2\rangle$  with probability  $q_2$ . Applying the results of previous section we have  $q_1 = \lambda$  and  $q_2 = \lambda'$ .

Furthermore, the spectral expansion of the density operator of  $|\psi_1\rangle$  in  $\mathcal{R}$  is  $\rho_1 = \sum m_i |h_i\rangle \langle h_i|$ , so that if  $\mathcal{RS}$  is in  $|\psi_1\rangle$ ,  $\mathcal{R}$  is in  $|h_i\rangle$  with probability  $q_i^{(1)}$ . If all the components of **m** are nonzero, the rank of  $\rho_1$  is m, so that we have  $\mathbf{q}^{(1)} = g_m(\mathbf{m})$ .

Similarly, the spectral expansion of the density operator of  $|\psi_2\rangle$  in  $\mathcal{R}$  is  $\rho_2 = \sum m'_i |h_i\rangle \langle h_i|$ , so that if  $\mathcal{RS}$  is in  $|\psi_2\rangle$ ,  $\mathcal{R}$  is in  $|h_i\rangle$  with probability  $q_i^{(2)}$ . If all the components of  $\mathbf{m}'$  are nonzero, the rank of  $\rho_2$  is m, so that we have  $\mathbf{q}^{(2)} = g_m(\mathbf{m}')$ .

But then the probability that  $\mathcal{R}$  is in  $|h_i\rangle$  is  $\bar{q}_i = q_i^{(1)}q_1 + q_i^{(2)}q_2$ , provided that  $\rho_H$  is generic. But  $\rho_H = \lambda \rho_1 + \lambda' \rho_2$  so that  $\rho_H = \sum (\lambda m_i + \lambda' m'_i) |h_i\rangle \langle h_i|$ . Hence for the validity of our argument we require that  $\lambda \mathbf{m} + \lambda' \mathbf{m}'$  belongs to the domain of  $g_m$ . We have  $\bar{\mathbf{q}} = g_m (\lambda \mathbf{m} + \lambda' \mathbf{m}')$ .

Hence by substitution we get

$$g_m \left(\lambda \mathbf{m} + \lambda' \mathbf{m}'\right) = \lambda g_m \left(\mathbf{m}\right) + \lambda' g_m \left(\mathbf{m}'\right).$$
(5)

We must be careful about the range of validity of the above equation. In our derivation we have supposed  $\lambda > 0$ ,  $\lambda' > 0$  and  $\lambda \neq \lambda'$ . Furthermore **m** and **m'** must belong to the domain of  $g_m$ , as well as  $\lambda \mathbf{m} + \lambda' \mathbf{m'}$ .

Suppose now that some single component of  $\mathbf{m}$ , say  $m_i$ , is zero. Then the rank of  $\rho_1$  is m-1 and the possible states of  $\mathcal{R}$ , given that  $\mathcal{RS}$  is in  $|\psi_1\rangle$ , are all the  $|h_l\rangle$ with  $l \neq i$ . The probability that  $\mathcal{R}$  is in  $|h_l\rangle$  is therefore

$$\bar{q}_l = q_l^{(1)} q_1 + q_l^{(2)} q_2, \tag{6}$$

for  $l \neq i$  and

$$\bar{q}_i = q_i^{(2)} q_2.$$
 (7)

We define  $\widehat{\mathbf{m}}_i = (m_1, ..., m_{i-1}, m_{i+1}, ..., m_m)$ . We extend the definition of  $g_m$  (which is defined for all the  $m_j$  different from zero) to a domain  $\widehat{\Delta}_m$  where at most a single  $m_k$  is zero in the following way:

$$\hat{g}_m(\mathbf{m}) = g_m(\mathbf{m}) \qquad \text{for} \qquad \mathbf{m} \in \Delta_m,$$
(8)

$$\hat{g}_{m,k}\left(\mathbf{m}\right) = 0, \quad \hat{g}_{m,i}\left(\mathbf{m}\right) = g_{m-1,i}\left(\mathbf{\hat{m}}_{k}\right) \quad i \neq k \quad \text{when} \quad m_{k} = 0.$$
 (9)

We note that  $\widehat{\Delta}_m$  is obtained from  $\Delta_m$  by adjunction of the subset with nonzero different barycentric coordinates of each face of  $T_m$ . We now prove the following theorem:

**Theorem 7.2.** The mapping  $\hat{g}_m$  satisfies the equation

$$\hat{g}_m \left(\lambda \mathbf{m} + \lambda' \mathbf{m}'\right) = \lambda \hat{g}_m \left(\mathbf{m}\right) + \lambda' \hat{g}_m \left(\mathbf{m}'\right), \tag{10}$$

provided that all the arguments belong to  $\widehat{\Delta}_m$  and that  $\lambda$  and  $\lambda'$  belong to [0,1], that they are different each other and that  $\lambda + \lambda' = 1$ .

*Proof.* Indeed, for  $\lambda = 1$  and  $\lambda' = 1$  we obtain an identity. Otherwise, but when all the arguments belong to  $\Delta_m$  equation (10) coincides with equation (5).

If  $m_i = 0$  for a single *i* and  $\mathbf{m}' \in \Delta_m$ , the argument of  $\hat{g}_m$  in the left side of (10) belongs to  $\Delta_m$ , so that the left side of (10) is the probability distribution of finding  $\mathcal{R}$  in the different states  $|h\rangle$ ; the components of the right side of (10) coincide with the corresponding right sides of (6) for  $l \neq i$  and with the right side of (7) for l = i. Hence (10) is satisfied also in this case.

Exchanging the roles of  $\lambda$ , **m** and  $\lambda'$ , **m'**, we see that (10) is satisfied also when  $\mathbf{m} \in \Delta_m$  and  $m'_i = 0$  for a single *i*. Suppose now that  $m_i = 0$  for a single *i* and  $m'_k = 0$  for a single *k* with  $k \neq i$ . In this case all the states  $|h_l\rangle$  ( $l \neq i, l \neq k$ ) result from both possibilities  $|\psi_1\rangle$  and  $|\psi_2\rangle$ , while the state  $|h_i\rangle$  results only from  $|\psi_2\rangle$  and the state  $|h_k\rangle$  results only from  $|\psi_1\rangle$ . We then have

$$\bar{q}_l = q_l^{(1)} q_1 + q_l^{(2)} q_2 \qquad (l \neq k, l \neq i),$$
(11)

$$\bar{q}_i = q_i^{(2)} q_2,$$
 (12)

$$\bar{q}_k = q_k^{(1)} q_1. \tag{13}$$

As  $\lambda \mathbf{m} + \lambda' \mathbf{m}' \in \Delta_m$ , the left side of (10) is the probability distribution of the states  $|h\rangle$ , while the components of the right side different from *i* and *k* coincide with the corresponding right sides of (11). The components *i* and *k* of the right side of (10) coincide with the right side of (12) and (13) respectively. Hence also in this case (10) is satisfied.

Finally, suppose  $m_i = m'_i = 0$  for a single *i*. In this case the *i*-th component of both sides of (10) is zero. Furthermore the equations for the probabilities are

$$\bar{q}_l = q_l^{(1)} q_1 + q_l^{(2)} q_2 \qquad (l \neq i) \,.$$
 (14)

The other components of the left side of (10) are the corresponding left sides of (14), and the same for the right sides.  $\Box$ 

We are now ready to prove the fundamental result of the above analysis.

**Theorem 7.3.** The unique mapping  $g_m$  expressing the probability law of the states is the identity.

*Proof.* We will prove the theorem by recursion on m. The theorem is true for m = 2 (see sect. 6).

Suppose that the theorem is true for m-1. Let  $\mathbf{m}'' \in \widehat{\Delta}_m$ . If  $m''_i = 0$  for a single i, by virtue of (9) we get  $\widehat{g}_{m,i}(\mathbf{m}'') = 0$  and  $\widehat{g}_{m,l}(\mathbf{m}'') = \widehat{g}_{m-1,l}(\widehat{\mathbf{m}}''_i)$  for  $l \neq i$ . But, for the recursion hypothesis,  $\widehat{g}_{m-1,l}(\widehat{\mathbf{m}}''_i) = \widehat{\mathbf{m}}''_i$ . Hence  $\widehat{g}_m(\mathbf{m}'') = \mathbf{m}''$ .

Suppose now that  $m''_i \neq 0$  for every *i*. We can always choose a segment containing  $\mathbf{m}''$  whose terminal points  $\mathbf{m}$  and  $\mathbf{m}'$  belong to  $\hat{\Delta}_m$  and to two different faces of  $T_m$ , opposite to the vertices *i* and *k* respectively, and such that  $\mathbf{m}''$  is not the middle point. Then

$$\hat{g}_m\left(\mathbf{m}''\right) = \hat{g}_m\left(\lambda\mathbf{m} + \lambda'\mathbf{m}'\right) = \lambda\hat{g}_m\left(\mathbf{m}\right) + \lambda'\hat{g}_m\left(\mathbf{m}'\right).$$
(15)

But we have already shown that, for such points,  $\hat{g}_m(\mathbf{m}) = \mathbf{m}$  and  $\hat{g}_m(\mathbf{m}') = \mathbf{m}'$ , so that

$$\hat{g}_m\left(\mathbf{m}''\right) = \lambda \mathbf{m} + \lambda' \mathbf{m}' = \mathbf{m}''.$$
(16)

Remembering theorem 4.7, i.e. that  $f(\rho_S) = g_m (\delta_{\Xi}(\rho_S) \circ \gamma) \circ \gamma^{-1}$ , we get  $f(\rho_S) = \delta_{\Xi}(\rho_S)$ , that is, if  $\rho_S = \sum p_\alpha |\xi_\alpha\rangle \langle \xi_\alpha|$ ,  $f(\rho_S)(\xi_\alpha) = p_\alpha$ , that is

**Theorem 7.4.** If  $\rho_s$  is a generic density operator, the possible states of the system, considered as isolated, are its non-null eigenstates, and the probability of finding the system in the state  $\xi$  is the correspondent eigenvalue.

We thus recover the standard statistic interpretation of the density operator.

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### Matteo Campanella Curriculum Vitae

Matteo Campanella graduated cum laude in Electronic Engineering at the University of Palermo in May 1972. He has been an Assistant Professor at the same University since 1973. He became an Associate Professor on Fundamentals of Electrical Engineering in 1983 and on Telecommunications in 1992. Since 2002, he has been a Full Professor on Telecommunications at the University of Palermo.

Matteo Campanella has been always a very eclectic researcher, as demonstrated not only by the heterogeneity of his research interests, but also by the variety of subjects that he taught during his career. He started with a class about Synthesis of Passive and Active Circuits in 1973, then he taught Applied Electronics from 1974 to 1978 and Circuit Theory from 1974 to 1991. Although since 1983 he was an Associate Professor on Fundamentals of Electrical Engineering, with the official course on Circuit Theory, in 1980, 1987 and 1988 he taught the course of Electromagnetic fields and circuits, and in 1985-86 he taught again the course of Applied Electronics. In 1991 he taught for the first time the course of Numerical Transmission Systems that he kept during the rest of his career. Since 1997, he also taught the course of Digital Processing for the master program of Telecommunication Engineering and Computer Engineering.

He participated to the Ph.D. course on Communications at the University of Palermo and he was the advisor of several master thesis and Ph.D. thesis dealing with distributed circuits and numerical transmission systems. He devoted his studies to the theory of microwave circuits, optimization techniques for continuous phase modulated systems, evaluation of limit performance of constant envelop channels as well as codes and lattices, convolutional codes over groups and turbo codes. He has been reviewer for several important journals, among which IEEE Transactions on Communications, IEEE Transactions on Information Theory, IEEE Communications Magazine. He also worked on several national research programs, funded by the Italian Minister of University and Research (MIUR).

Matteo Campanella was a very intellectually gifted researcher, but also a very charismatic lecturer. He delighted colleagues and students with his wide knowledge and vibrant passion for ideas as well as the strength of his coherence. Although he was a very reserved and modest person, his mild temperament and strong personality, as well as his way of facing complex problems as a sequence of obvious intuitive steps, provided that good analysis instruments were defined, significantly affected hundreds of students and the whole group of Telecommunications at the University of Palermo.

> Pierluigi Gallo, Giovanni Garbo, Giovanni Mamola, Stefano Mangione, Ilenia Tinnirello

## Ricordo di Matteo Campanella

Ho conosciuto mio cognato Matteo nel lontano 1968, a casa di un comune amico. La sua persona mi colpì molto. Gli occhi erano scuri e vivacissimi, baffoni e capigliatura disordinata, un vocione che sovrastava ogni altro suono mentre una nazionale dopo l'altra si consumava tra le sue dita.

Rividi Matteo qualche tempo dopo a casa di un mio cugino, suo collega. Preparavano insieme non so quale materia. In quelle occasioni la figura di Matteo si delineò con molta precisione. La sua passione per la scienza non era inferiore a quella per la politica. Andava fierissimo della sua militanza, ben diversa da quella salottiera che allora andava di moda, forgiata com'era, molto concretamente, sul terreno delle lotta per l'emancipazione delle classi subalterne. Matteo collezionò così alcune denunce per occupazione abusiva di edifici pubblici e, in altra occasione, per interruzione di pubblico servizio (si era sdraiato insieme ad altri manifestanti) sui binari della Stazione Centrale.

Per molti anni non ebbi sue notizie. Poi un giorno, mia cognata Maria Stella, mi presentò il suo futuro marito e così mi ritrovai davanti i baffoni che già conoscevo corredati dall'immancabile nazionale fumante.

Con Matteo mi trovavo perfettamente a mio agio: anche se, come capita a tutti, non era immune da difetti. Ma se mai vi fu un uomo a cui si potevano perdonare difetti, grandi o piccoli che fossero, questo era Matteo: la sua intelligenza brillante e acuta, la sua cultura, che spaziava dalla musica alla filosofia, superavano largamente gli inevitabili difetti che ogni essere umano porta dentro e fuori di sé. Matteo sapeva anche essere molto generoso. Lo era specialmente verso coloro che riteneva, a torto o ragione, più deboli e indifesi. Era anche, senza saperlo, un poeta. I poeti sanno o cercano di protendersi verso l'infinito. Anche Matteo, con i suoi studi - specie in quelli di fisica quantistica a cui negli ultimi anni della sua vita si era dedicato con fervore ñ sperava forse di sollevare un lembo del manto che nasconde l'Essere, l'Assoluto.

Ma il Tempo è stato con lui inesorabilmente e ingiustamente crudele.

Mario Guarino

## Pensieri

Oggi ci ha lasciato il Prof. Campanella.

Per chi non lo conoscesse, era il docente di teoria delle reti elettriche, trasmissione numerica dei segnali ed elaborazione numerica dei segnali. Ma te lo ritrovavi agli esami di campi elettromagnetici, comunicazioni elettriche, teoria dei segnali...ogni materia che avesse a che fare con le tlc. Era un genio. Uno che sapeva tutto, che aveva una scrivania piena di fogli nel suo ufficio in cui vi erano formule ed equazioni kilometriche. Un giorno chiesi cosa ci fosse in alcuni di quei fogli, e lui mi rispose che stava tentando di risolvere un problema di quantistica.

Il prof. Campanella sapeva spiegarti l'algebra dei campi come se fosse una lezione qualunque, salvo poi parlarti di codici e di tecniche di correzione dell'errore come se ti avesse parlato sempre e solo di quelle. E restavi a bocca aperta...affascinato, sorpreso e meravigliato alla fine di ogni lezione. All'esame si passava solo studiando. Era equo, preciso e inflessibile. Sapeva darti il voto che meritavi...sempre.

Passare una sua materia significava averla capita. E la soddisfazione era infinita.

Ricordo ancora un esame di teoria delle reti in caldo pomeriggio di luglio. Esercizio alla lavagna, e due domande teoriche. Alla seconda dimostrazione eravamo insieme alla lavagna a dimostrare quel teorema, di cui lui scriveva il numeratore di una formula...

Era un grande, amava il suo lavoro e insegnava nel senso letterale del termine. Onesto fino al midollo.

Il corso di tlc ha perso il miglior professore degli ultimi 30 anni...

Possa riposare in pace, e grazie di tutto mitico Prof. Campanella.

#### Luca Scalia

Ci ha lasciato Matteo Campanella, professore ordinario ING-INF/03.

Per quelli come me era il professore di Teoria delle reti elettriche. Ricordo quella sua scrivania con mezzo metro di fogli di carta, pieni di formule e calcoli, stratificati in una sequenza incomprensibile a tutti tranne che a lui.

Ricordo essere chiamato alla lavagna, durante le esercitazioni nei caldi pomeriggi dell'anfiteatro a Ingegneria Elettrica, quando il mio sguardo smarrito tra una maglia e un anello incontrava i suoi baffi sornioni e quegli occhi inquisitori. Senza scampo: "Non si preoccupi di cercare i colleghi", ti diceva a sorpresa, "le dico io tutto quello che deve sapere".

E poi gli esami. Lunghi. Obiettivi. Precisi. Con quel voto che arrivava e ti sembrava un sogno. Perchè lo avevi capito. Lo avevi lasciato soddisfatto del lavoro che aveva fatto con te. Diventati colleghi, non ho mai avuto modo di interagire con lui. Ma il suo ricordo resterà indelebile.

Riposa in pace, caro Matteo. La tua eredità è forte come i tanti semi che germogliano nelle menti e nei cuori di tanti di noi. Grazie.

Antonio Gentile

Grande tristezza per me oggi, se n'è andato uno dei docenti che più stimo e che più ha contribuito alla mia formazione universitaria, il prof. Matteo Campanella.

Aveva grande conoscenza e soprattutto innata capacità di trasferirla.

Lo voglio ricordare con la frase con cui aprì la lezione di Trasmissione Numerica del 25 maggio 1992, giorno dei funerali del giudice Falcone e delle altre vittime della strage: "Io credo che l'unico modo che abbiamo noi per combattere la mafia è diffondere cultura e conoscenza, per formare coscienze libere. Per questo oggi io farò lezione normalmente, nonostante sia un giorno di infinita tristezza".

#### $Salvatore\ Sorce$

Un dispiacere enorme... È stato il mio mentore... Trasmissione Numerica mia ultima materia, alla fine dell'esame con tutto il cuore gli ho detto 'Professore è stato un onore imparare da lei'... Un genio assoluto, a Teoria delle Reti Elettriche ho raggiunto i miei massimi matematici quando spiegò il Fibrato Tangente e io li come un bambino a pendere dalle sua labbra... Che possa riposare in pace.

#### Pietro Corrao

Caro Professore, oggi sono stata in Dipartimento, per fare il mio dovere, come lei ci ha insegnato, con infinita tristezza, ma senza mai mancare agli impegni presi. La pila di fogli è ancora lì, persino l'odore del fumo. E io non riesco ancora a capire, ad accettare, che da oggi saremo più soli, senza la sua guida discreta e il suo vocione imponente e appassionato. Ha lasciato un ricordo indelebile in ciascuno di noi, un desiderio infinito di essere come lei, con la consapevolezza che non ci riuscirà mai.

#### Ilenia Tinnirello

Cari colleghi,

con grandissima tristezza devo comunicarvi la scomparsa improvvisa del Prof. Matteo Campanella avvenuta questa notte. Ho appreso la notizia pochi minuti fa da un collega del DEIM e non ho al momento ulteriori informazioni. Sarà mia cura darvi maggiori informazioni non appena le avrò.

Mi piace però ricordare il Prof. Campanella non come coordinatore o collega ma come suo ex-studente. Il Prof. Campanella aveva la capacità di trasmettere agli studenti, con la estrema chiarezza che lo contraddistingueva, non le semplici nozioni ma i concetti profondi che danno un senso alla materia e alle discipline ingegneristiche in generale.

Non ho difficoltà a scrivere che sarei felice un giorno di riuscire a trasmettere ai miei studenti ciò che lui ha trasmesso a me ma sono anche consapevole di essere molto lontano dall'obiettivo.

Marco La Cascia

#### **En el funeral d'un matemàtic** En la mort de Matteo Campanella

Assisteixo al funeral d'un collega professor, mort inesperadament. El sermó - correcte - ha parlat de Crist i vida eterna.

En acabar, un altre collega ha llegit uns textos brevs d'estudiants i professors en memòria seua: la bellesa de les matemàtiques, la passió per la física, l'espertesa en enginjeria, la curiositat sempre oberta i el saber generosament ofert. Una altra manera de participar en una eternitat, en una transcendència, en una vida en marxa, en una creació humana cap a una creació divina. Suma-li música, comunisme i bona taula i generós acolliment.

De Crist, no en va parlar mai gaire, peró quan ho feu, ser amb respecte. Que la gran Raó divina, d'amor i de saber, l'aculli, tal com el acollia, fent-ne part viva de si mateix, cada teorema, equaciò i amistat que arribava a comprendre.

Palermo, 20 de juny de 2016

David Jou

## Nel funerale di un matematico

Nella morte di Matteo Campanella

Assisto al funerale di un collega professore, morto inaspettatamente. Il sermone - giusto - ha parlato di Cristo e di vita eterna.

Alla fine, un altro collega ha letto alcuni pensieri di studenti e professori in sua memoria: la bellezza delle matematiche, la passione per la fisica, la competenza in ingegneria, la curiosità sempre aperta e il sapere generosamente offerto. Un'altra forma di partecipare in una eternità, in una transcendenza, in una vita sempre dinamica, in una creazione umana verso una creazione divina. Senza dimenticare la musica, il comunismo e la buona tavola, e la generosa ospitalità.

Di Cristo, ne parlò poco, ma rispettosamente. Che la grande Ragione divina, d'amore e di sapienza, l'accolga, come lui accoglieva, facendone parte viva di se stesso, ogni teorema, equazione e amicizia che arrivava ad afferrare.

Palermo, 20 di giugno del 2016

David Jou

## Convergence of the approximate solutions for the equation of coagulation-fragmentation for falling droplets of positive radius type

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#### Abstract

We consider the integro-differential equation, which describes the fall and the coagulation-fragmentation process of the droplets with a positive collision thickness. We construct the approximate solutions by truncation of the coagulation and fragmentation coefficients and prove the convergence in a certain topology of a sequence of approximate solutions whose limit is a locally bounded function.

 $Key\ words:$  Integro-differential equation, Coagulation-fragmentation of droplets, Maximum principle, Weak convergence MSC: 45K05, 35L60 PACS: 02.30.Rz, 92.60.Jq

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## 1 Introduction

In this paper we consider the equation describing the process of coagulation and fragmentation of moving droplets. In [12] Melzak constructed the solution to this equation without move of droplets in the framework of analytic functions. As far as the equation of moving droplets, Dubovskii [7] has shown the existence and uniqueness of the solution. However, it is difficult – it seems to us – to translate the conditions posed in [7] into natural physical conditions (a more precise comment is given in the introduction of [11]). Dubovskii's paper [7] has been preceded by a series of articles of Galkin [8]–[10] on the equation without fragmentation, which give us useful techniques for the study of the equation.

More recently other authors have studied a similar equation (but different, see for example [3]), using techniques inspired by the study of the Boltzmann equation. On the other hand, following the idea of Melzak, in [11] a local solution of this equation has been constructed.

The equation describing the process of coagulation and fragmentation of vertically moving droplets (in a one-dimension domain) can be written in the form

$$\partial_t \sigma(m, z, t) + \partial_z (\sigma(m, z, t)u(m)) =$$

$$= \frac{m}{2} \int_0^m \beta(m - m', m') \sigma(m', z, t) \sigma(m - m', z, t) dm' +$$

$$-m \int_0^\infty \beta(m, m') \sigma(m, z, t) \sigma(m', z, t) dm' - \frac{m}{2} \sigma(m, z, t) \int_0^m \vartheta(m - m', m') dm' +$$

$$+m \int_0^\infty \vartheta(m, m') \sigma(m + m', z, t) dm',$$
(1)

where  $\beta(m_1, m_2)$  is the rate of coagulation of two droplets: one of masse  $m_1$  and one of mass  $m_2$ , while  $\vartheta(m_1, m_2)$  is the rate of fragmentation of a droplet of mass  $m = m_1 + m_2$  into one of mass  $m_1$  and one of mass  $m_2$ ; on the other hand, u(m)denotes the vertical velocity of droplets with mass m.

In the present paper, we introduce the coagulation and fragmentation operator with an enlargement of position z, which may have a similar aspects to collisions of droplets with a strictly positive radius. The introduction of these operators has the effect of regularizing the solution, so that we can obtain a useful estimates to overcome the difficulties encountered in the study of coagulation-fragmentation equation of droplets (1). From the technical point of view, besides the conservation of the mass of the liquid water contained in the droplets, we use the idea of Da Costa [6], Ball and Carr [1] for the estimate of  $m^{\gamma}\sigma(m, \cdot, \cdot)$  as well as the method of Galkin [8] and Dubovskii [7], which is based essentially on the use of the "Maximum Principle" to control the norm in  $L^{\infty}$ 

### 2 Position of the problem

We consider the domain in one-dimension (vertical)

$$\Pi = ] - A, 0[, \tag{2}$$

where A is a strictly positive number. Let us denote by  $\sigma(m, z, t)$  the density of the liquid water contained in the droplets of mass m (density in the sense of the mass in the unit volume of the air in which the droplets are contained) in the position  $z \in \Pi$  and at the moment  $t \geq 0$ .

Let us introduce the coagulation and fragmentation operators defined by the regularization with respect to  $z \in \Pi$  of the function  $\sigma(m, z, t)$ . More precisely, we set

$$\eta_{\varepsilon}(z) = \begin{cases} \frac{1}{\int_{-\varepsilon}^{\varepsilon} \frac{1}{e^{1-(z/\varepsilon)^2}}} & \text{for } -\varepsilon < z < \varepsilon, \\ 0 & \text{for } |z| \ge \varepsilon, \end{cases}$$
(3)

$$\sigma^{\varepsilon}(m, z, t) = \int_{\Pi} \eta_{\varepsilon}(z - z')\sigma(m, z', t)dz', \tag{4}$$
d strictly positive number. Here, the integral of the right-hand side of

where  $\varepsilon$  is a fixed strictly positive number. Here, the integral of the right-hand side of (4) is defined with respect to  $z' \in \Pi$ , so that for  $-\varepsilon < z < 0$  and for  $-A < z < -A + \varepsilon$  we have

$$\sigma^{\varepsilon}(m,z,t) = \int_{z-\varepsilon}^{0} \eta_{\varepsilon}(z-z')\sigma(m,z',t)dz'$$

and

$$\sigma^{\varepsilon}(m,z,t) = \int_{-A}^{-A+\varepsilon} \eta_{\varepsilon}(z-z')\sigma(m,z',t)dz'$$

respectively, even if  $\eta_{\varepsilon}(z-z') > 0$  for some 0 < z' or z' < -A. As we have mentioned above, the introduction of  $\sigma^{\varepsilon}$  is motivated by its behavior similar to droplets with a strictly positive radius in their coagulation.

We define the coagulation and fragmentation operators for  $\sigma^{\varepsilon}$  by the relations

$$K_{t,z}[\sigma^{\varepsilon},\sigma^{\varepsilon}](m) = \frac{m}{2} \int_{0}^{m} \beta(m-m',m')\sigma^{\varepsilon}(m-m',z,t)\sigma^{\varepsilon}(m',z,t)dm' + (5)$$
$$-m \int_{0}^{\infty} \beta(m,m')\sigma^{\varepsilon}(m,z,t)\sigma^{\varepsilon}(m',z,t)dm',$$
$$L_{t,z}[\sigma^{\varepsilon}](m) = -\frac{m}{2} \int_{0}^{m} \vartheta(m-m',m')\sigma^{\varepsilon}(m,z,t)dm' + (6)$$
$$+m \int_{0}^{\infty} \vartheta(m,m')\sigma^{\varepsilon}(m+m',z,t)dm'.$$

So, the equation that we are going to study is written in the form

$$\partial_t \sigma(m, z, t) + \partial_z (\sigma(m, z, t)u(m)) = K_{t,z}[\sigma^\varepsilon, \sigma^\varepsilon](m) + L_{t,z}[\sigma^\varepsilon](m).$$
(7)

This equation will be considered for  $(m, z, t) \in \mathbb{R}_+ \times \Pi \times \mathbb{R}_+$  with the initial condition

$$\sigma(m, z, 0) = \overline{\sigma}_0^*(m, z) \tag{8}$$

and the entry condition

$$\sigma(m,0,t) = \overline{\sigma}_1^*(m,t). \tag{9}$$

We assume that

$$\overline{\sigma}_0^*(\cdot, \cdot) \in L^1(\mathbb{R}_+ \times \Pi), \qquad \overline{\sigma}_1^*(\cdot, \cdot) \in L^1(\mathbb{R}_+ \times \mathbb{R}_+), \qquad \overline{\sigma}_0^*(m, z) \ge 0, \qquad \overline{\sigma}_1^*(m, t) \ge 0.$$
(10)

For the functions  $\beta(m_1, m_2)$  and  $\vartheta(m_1, m_2)$ , according to their physical nature, we assume that

$$\beta(m_1, m_2) \ge 0, \qquad \beta(m_1, m_2) = \beta(m_2, m_1) \quad \forall (m_1, m_2) \in \mathbb{R}_+ \times \mathbb{R}_+,$$
(11)

$$\vartheta(m_1, m_2) \ge 0, \qquad \vartheta(m_1, m_2) = \vartheta(m_2, m_1) \quad \forall (m_1, m_2) \in \mathbb{R}_+ \times \mathbb{R}_+, \tag{12}$$

$$\int_0^m m'\vartheta(m-m',m')dm' \le 1 \qquad \forall m > 0.$$
<sup>(13)</sup>

The nature of the relations (11) and (12) is clear, while the inequality (13) (which is equivalent to the second inequality of  $(H_2)$  of [12]) means that the sum of mass of the droplets produced by the (possible) fragmentation does not exceed the mass of the droplet that eventually breaks up.

In this paper, we assume the following conditions

$$\beta(\cdot, \cdot) \in C(\mathbb{R}_+ \times \mathbb{R}_+), \qquad \vartheta(\cdot, \cdot) \in C(\mathbb{R}_+ \times \mathbb{R}_+), \tag{14}$$

$$\sup_{m,m'>0}\vartheta(m,m') \le C_0,\tag{15}$$

$$(\overline{m} - m')\beta(\overline{m} - m', m') \le \overline{m}\beta(\overline{m}, m') \quad \text{for } 0 < m' < \overline{m}.$$
(16)

We also suppose that there exist constants  $\alpha$ ,  $\mu$ ,  $\gamma$ ,  $r_0$ ,  $K_c$  and  $K_f$  such that

$$\frac{1}{2} < \alpha < 1, \quad \mu > 0, \quad 2\alpha - 1 < \gamma < 1, \quad r_0 \ge 2, \quad K_f > 0,$$
  
$$\beta(m, m') \le K_c (mm')^{\alpha - 1}, \tag{17}$$

$$\int_0^{\frac{r}{2}} m^{\mu+1} \vartheta(m, r-m) dm \ge K_f r^{\gamma+\mu} \qquad \forall r \ge r_0,$$
(18)

and that for each  $\tilde{m}^*$  there exists a constant  $C(\tilde{m}^*)$  dependent on  $\tilde{m}^*$  (increasing as a function of  $\tilde{m}^*$ ) such that

$$\sup_{0 < m, m' \le \widetilde{m}^*} \frac{m}{m'^{\mu}} \beta(m, m') \le C(\widetilde{m}^*).$$
(19)

For the velocity of the droplets u(m) we assume that

$$u(m) < 0 \qquad \forall m > 0. \tag{20}$$

#### **3** Preliminaries

Now we introduce the change of variables: we transform (m, z, t) into  $(\mu, q, \tau)$  by the relations

$$\mu = m, \quad q = z - u(m)t, \quad \tau = t.$$
 (21)

This change of variables transforms the domain  $(m, z, t) \in \mathbb{R}_+ \times \Pi \times \mathbb{R}_+$  into  $\{ (\mu, q, \tau) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}_+ \mid -A - \tau u(\mu) < q < -\tau u(\mu) \}$ . But it will be convenient for us to extend the domain to  $\mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}_+$ , that is, we will also consider the points  $(\mu, q, \tau)$  such that  $q \leq -A - \tau u(\mu)$  or  $q \geq -\tau u(\mu)$ , extending by 0 the function  $\sigma(\mu, q, \tau)$  (and also  $\sigma^{\varepsilon}(\mu, q, \tau)$ ) for  $q \leq -A - \tau u(\mu)$  and for  $q \geq -\tau u(\mu)$ .

We note that in the new coordinates  $(\mu, q, \tau)$  the point  $z \in \Pi$  in which the coagulation and fragmentation can occur at the moment t is transformed into a curve

$$\gamma_z = \{ q = q_z(\mu') \mid \mu' \in \mathbb{R}_+ \}, \qquad q_z(\mu') = z - u(\mu')\tau.$$

Let us also recall the relations between the derivatives

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} - u(m)\frac{\partial}{\partial q}, \qquad \frac{\partial}{\partial z} = \frac{\partial}{\partial q}, \qquad \frac{\partial}{\partial m} = \frac{\partial}{\partial \mu}.$$
(22)

But, to simplify the notation, we will write m instead of  $\mu$  and t instead of  $\tau$ , that is, we will use the change of variables

$$m = m, \quad q = z - u(m)t, \quad t = t,$$
 (23)

with the relations (22) rewritten with (m, q, t).

 $=\frac{m}{2}\int_{0}^{m}\beta$ 

We remark that in the coordinates (m, q, t) the operators  $K_{t,z}[\sigma^{\varepsilon}, \sigma^{\varepsilon}](m)$  and  $L_{t,z}[\sigma^{\varepsilon}](m)$  have the form

$$K_{t,z}[\sigma^{\varepsilon}, \sigma^{\varepsilon}](m) = K_{t,z}[\sigma^{\varepsilon}, \sigma^{\varepsilon}](m,q) =$$

$$(m-m',m')\sigma^{\varepsilon}(m-m',q_{z}(m-m'),t)\sigma^{\varepsilon}(m',q_{z}(m'),t)dm' +$$

$$(24)$$

$$-m \int_{0}^{\infty} \beta(m,m') \sigma^{\varepsilon}(m,q_{z}(m),t) \sigma^{\varepsilon}(m',q_{z}(m'),t) dm' \equiv \equiv K_{t,z} [\sigma^{\varepsilon}(\cdot,q_{z},t),\sigma^{\varepsilon}(\cdot,q_{z},t)](m), L_{t,z} [\sigma^{\varepsilon}](m) = L_{t,z} [\sigma^{\varepsilon}](m,q) = = -\frac{m}{2} \int_{0}^{m} \vartheta(m-m',m') \sigma^{\varepsilon}(m,q_{z}(m),t) dm' + +m \int_{0}^{\infty} \vartheta(m,m') \sigma^{\varepsilon}(m+m',q_{z}(m+m'),t) dm' \equiv L_{t,z} [\sigma^{\varepsilon}(\cdot,q_{z},t)](m),$$

$$(25)$$

where

$$q_z(m') = q + (u(m) - u(m'))t.$$
(26)

808. W. Kaidouchi: Convergence of the approximate solutions for the equation of coagulation-fragmentation (pp. 51 – 73) It is useful to recall that  $q_z(m) = q$ ,

$$q_z(m-m') = q + (u(m) - u(m-m'))t.$$

As for the entry condition (9), in order that we can formulate the equation in  $\mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}_+$ , we will write it in the form of additive term

$$\overline{\sigma}_1^*(m,t)\delta_{-\frac{q}{u(m)}}(t)$$

to the right-hand side of the equation;  $\delta_{-\frac{q}{u(m)}}(t)$  is Dirac's  $\delta$  translated to  $t = -\frac{q}{u(m)}$ . It is clear that the writing with Dirac's  $\delta$  is a convention of writing in a differential form whose exact meaning must be conceived in the integral form; we will also use this convention in the sequel. On the other hand, we translate the fact that we do not consider  $\sigma(m, q, t)$  for  $q \leq -A - u(m)t$  into the additive term

$$-\sigma(m,q,t)\delta_{-\frac{q+A}{n(m)}}(t)$$

which represents the exit of the droplets from  $\Pi$ .

Concerning the initial condition, extending  $\overline{\sigma}_0^*(m, z)$  by 0 outside of  $\Pi$ , we consider the condition

$$\sigma(m,q,0) = \overline{\sigma}_0^*(m,q) \qquad \text{for } (m,q) \in \mathbb{R}_+ \times \mathbb{R}$$
(27)

(we recall that for t = 0 we have q = z).

Thus, in the sequel we will consider, instead of the equation (7), the equation

$$\frac{\partial}{\partial t}\sigma(m,q,t) = K_{t,z}[\sigma^{\varepsilon}(\cdot,q_z,t),\sigma^{\varepsilon}(\cdot,q_z,t)](m) + L_{t,z}[\sigma^{\varepsilon}(\cdot,q_z,t)](m) + (28)$$
$$+\overline{\sigma}_1^*(m,t)\delta_{-\frac{q}{u(m)}}(t) - \sigma(m,q,t)\delta_{-\frac{q+A}{u(m)}}(t), \quad \text{for } (m,q,t) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}_+,$$

which should be considered with the initial condition (27).

We recall a consequence of the change of variables.

**Lemma 3.1.** If  $\sigma(\cdot, \cdot, t) \in L^1(\mathbb{R}_+ \times \mathbb{R})$ ,  $t \in \mathbb{R}_+$ , satisfies the relation  $\sigma(m, q, t) = 0$ for  $q \leq -A - tu(m)$  and for  $q \geq -tu(m)$ , we have

$$\int_{\mathbb{R}\times\mathbb{R}_+} \sigma(m,q,t) dm dq = \int_{-A}^0 dz \int_0^\infty \sigma(m,q_z(m),t) dm.$$

*Proof.* As  $q_z(m) = q = z - u(m)t$  (see (23), (26)) and  $\sigma(m, q, t) = 0$  for  $q \leq -A - tu(m)$  and for  $q \geq -tu(m)$ , we have

$$\int_{\mathbb{R}\times\mathbb{R}_{+}} \sigma(m,q,t) dm dq = \int_{0}^{\infty} \int_{-A}^{0} \sigma(m,q_{z}(m),t) \frac{dq}{dz} dz dm =$$
$$= \int_{-A}^{0} \int_{0}^{\infty} \sigma(m,q_{z}(m),t) dm dz.$$

The lemma is proved.

#### 4 Position of the approximate problem

We will introduce a family of approximate problems. More precisely, we define the functions  $\beta_n(m, m')$  and  $\vartheta_n(m, m')$  by

$$\begin{cases} \beta_n(m, m') = \beta(m, m')\psi^1(m + m' - n), \\ \vartheta_n(m, m') = \vartheta(m, m')\psi^1(m + m' - n), \end{cases}$$
(29)

where  $\psi^1(m)$  is a function of class  $\mathcal{C}^{\infty}(\mathbb{R})$ , decreasing and such that

$$\psi^{1}(r) = \begin{cases} 1 & \text{for } r \le 0, \\ 0 & \text{for } r \ge 1. \end{cases}$$
(30)

Replacing  $\beta(m, m')$  by  $\beta_n(m, m')$  and  $\vartheta(m, m')$  by  $\vartheta_n(m, m')$  in the equation (28) and denoting by  $\sigma_n$  the unknown function instead of  $\sigma$ , we consider the equation

$$\frac{\partial}{\partial t}\sigma_n(m,q,t) = \overline{\sigma}^*_{1n}(m,t)\delta_{-\frac{q}{u(m)}}(t) - \sigma_n(m,q,t)\delta_{-\frac{q+A}{u(m)}}(t) + 
+ K^{[n]}_{t,z}[\sigma^{\varepsilon}_n(\cdot,q_z,t),\sigma^{\varepsilon}_n(\cdot,q_z,t)](m) + L^{[n]}_{t,z}[\sigma^{\varepsilon}_n(\cdot,q_z,t)](m),$$
(31)

where  $K_{t,z}^{[n]}[\cdot,\cdot]$  and  $L_{t,z}^{[n]}[\cdot]$  are defined as in the definition (24)-(25) of  $K_{t,z}[\cdot,\cdot]$  and  $L_{t,z}[\cdot]$  with the replacement of  $\beta(\cdot,\cdot)$  and  $\vartheta(\cdot,\cdot)$  by  $\beta_n(\cdot,\cdot)$  and  $\vartheta_n(\cdot,\cdot)$ , and  $\sigma_n^{\varepsilon}$  is defined as in (4) from  $\sigma_n$ . For the initial condition and the entry condition, we set

$$\sigma_n(m,q,0) = \overline{\sigma}_0^*(m,q)\psi^1(m+m'-n), \qquad (32)$$

$$\overline{\sigma}_{1n}^{*}(m,t)\delta_{-\frac{q}{u(m)}}(t) = \overline{\sigma}_{1}^{*}(m,t)\delta_{-\frac{q}{u(m)}}(t)\psi^{1}(m+m'-n).$$
(33)

We recall that the operators  $K_{t,z}^{[n]}$  and  $L_{t,z}^{[n]}$  conserve the mass.

**Lemma 4.1.** For all  $\sigma(\cdot, q_z(\cdot), t) \in L^1(\mathbb{R}_+)$ , we have

$$\int_{\mathbb{R}_+} K_{t,z}^{[n]}[\sigma(\cdot, q_z(\cdot), t), \sigma(\cdot, q_z(\cdot), t)](m)dm = 0,$$
(34)

$$\int_{\mathbb{R}_{+}} L_{t,z}^{[n]}[\sigma(\cdot, q_{z}(\cdot), t)](m)dm = 0.$$
(35)

Proof. As  $K_{t,z}^{[n]}[\cdot, \cdot]$  and  $L_{t,z}^{[n]}[\cdot]$  are only the particular cases of  $K_{t,z}[\cdot, \cdot]$  and  $L_{t,z}[\cdot]$  in which  $\beta(\cdot, \cdot)$  and  $\vartheta(\cdot, \cdot)$  have the form  $\beta_n(\cdot, \cdot)$  and  $\vartheta_n(\cdot, \cdot)$ , the equalities (34) and (35) are well-known classical results (for the explicite expression of the proof of (34), see for example [2, 13]; the equality (35) is shown in a similar way).

From this lemma results immediately the following property.

**Lemma 4.2.** Let  $\overline{\sigma}_0^*(\cdot, \cdot) \in L^1(\mathbb{R}_+ \times \mathbb{R})$  with  $\overline{\sigma}_0^*(\cdot, \cdot) \geq 0$ . If  $\sigma_n(\cdot, \cdot, t)$  is a solution to the equation (31) with the initial condition (32), then we have

$$\|\sigma_n(\cdot,\cdot,t)\|_{L^1(\mathbb{R}_+\times\mathbb{R})} = \Sigma_0(t) - \int_{\mathbb{R}_+} \int_{-A}^{-A-tu(m)} \sigma_n(m,q,-\frac{q+A}{u(m)}) dq dm, \qquad (36)$$

where

$$\Sigma_0(t) = \|\overline{\sigma}_0^*(\cdot, \cdot)\|_{L^1(\mathbb{R}_+ \times \mathbb{R})} + \int_{\mathbb{R}_+} \int_0^{-tu(m)} \overline{\sigma}_{1n}^*(m, -\frac{q}{u(m)}) dq dm.$$
(37)

*Proof.* We consider the equation (31) expressed in the integral form. By integrating it on  $\mathbb{R} \times \mathbb{R}_+$  with respect to q and m and using the lemmas 3.1 and 4.1, we obtain (36).

**Lemma 4.3.** If  $\sigma_n(\cdot, \cdot, t)$  is a solution to the equation (31) with the initial condition (32) and if  $\sigma_n^{\varepsilon}$  is defined in a similar way as (4), then we have

$$\sup_{-A \le z \le 0} \int_{\mathbb{R}_+} \sigma_n^{\varepsilon}(m, q_z(m), t) dm \le K(t) < \infty$$
(38)

where

$$K(t) = \eta_{\varepsilon}(0)\Sigma_0(t)$$

 $(\eta_{\varepsilon}(\cdot) \text{ and } \Sigma_0(t) \text{ are defined in (3) and (37) respectively}).$ 

*Proof.* According to (4), we have

$$\sigma_n^{\varepsilon}(m,q,t) = \int_{-A}^0 \eta_{\varepsilon}(z_q - z')\sigma_n(m,q_{z'}(m),t)dz' \le \sup_{\zeta' \in \mathbb{R}} \eta_{\varepsilon}(\zeta') \int_{\mathbb{R}} \sigma_n(m,q',t)dq',$$

where  $z_q = q + u(m)t$ . Consequently, taking into account also (3), we have

$$\int_{\mathbb{R}_+} \sigma_n^{\varepsilon}(m, q, t) dm \le \eta_{\varepsilon}(0) \| \sigma_n(\cdot, \cdot, t) \|_{L^1(\mathbb{R}_+ \times \mathbb{R})}$$

This inequality, in virtue of (36), implies (38).

# 5 Existence and uniqueness of the solution of the approximate problem

Now we will show the existence and uniqueness of the solution  $\sigma_n$  of the approximate problem.

**Proposition 5.1.** The equation (31) with the condition (32) admits a unique solution  $\sigma_n \in \mathcal{C}(\mathbb{R}_+; L^1(\mathbb{R}_+ \times \mathbb{R}))$ . Furthermore, we have

$$\sigma_n(m,q,t) = 0 \qquad for \ m \ge n+1. \tag{39}$$

*Proof.* We recall that the condition (10) with the extension of  $\overline{\sigma}_0^*(\cdot, \cdot)$  by 0 outside of  $\Pi$  implies that  $\overline{\sigma}_0^*(\cdot, \cdot) \in L^1(\mathbb{R}_+ \times \mathbb{R})$  and that  $\overline{\sigma}_0^*(m, q) \ge 0$  for all  $(m, q) \in \mathbb{R}_+ \times \mathbb{R}$ . To solve the problem (31)-(32), we consider (31) as an ordinary differential equation with values in the Banach space  $L^1(\mathbb{R}_+ \times \mathbb{R})$ 

$$\frac{d}{dt}\sigma_n(t) = F^{[n]}[\sigma_n^{\varepsilon}(t)] + \Delta_1(t) - \Delta_2(t), \qquad (40)$$

where

$$\begin{split} F^{[n]}[\sigma_n^{\varepsilon}(t)](m,q) &= K_{t,z}^{[n]}[\sigma_n^{\varepsilon}(\cdot,q_z,t),\sigma_n^{\varepsilon}(\cdot,q_z,t)](m) + L_{t,z}^{[n]}[\sigma_n^{\varepsilon}(\cdot,q_z,t)](m),\\ \Delta_1(t)(m,q) &= \overline{\sigma}_{1n}^*(m,t)\delta_{-\frac{q}{u(m)}}(t),\\ \Delta_2(t)(m,q) &= \sigma_n(m,q,t)\delta_{-\frac{q+A}{u(m)}}(t). \end{split}$$

We note that, according to the definition of  $\beta_n$ , there exists a constant  $c_0(n)$  dependent on n such that the inequality

$$\frac{m}{2}\beta_n(m-m',m') \le c_0(n), \qquad \forall m \in \mathbb{R}_+, \forall m' \in ]0, m[\,,$$

holds.

To examine the Lipschitz condition, we consider a bounded set of  $L^1(\mathbb{R}_+ \times \mathbb{R})$ and two functions  $\sigma^{[1]}(m, q_z(m))$  and  $\sigma^{[2]}(m, q_z(m))$  belonging to it. As the definition of  $q_z(m)$  (see (26)) contains implicitly t, temporarily we fix t. It is clear that, if we define the function  $\sigma^{\varepsilon[i]}$  from  $\sigma^{[i]}$  (i = 1, 2) in a similar way as (4), then we have

$$\sup_{-A \le z \le 0} \int_{\mathbb{R}_+} \sigma^{\varepsilon[i]}(m, q_z(m)) dm \le K < \infty, \ i = 1, 2$$

$$\tag{41}$$

(K depends on the bounded set considered). So, using the lemma 3.1, we have

$$\begin{split} \|K_{t,z}^{[n]}[\sigma^{\varepsilon[1]}(\cdot,q_{z}),\sigma^{\varepsilon[1]}(\cdot,q_{z})] - K_{t,z}^{[n]}[\sigma^{\varepsilon[2]}(\cdot,q_{z}),\sigma^{\varepsilon[2]}(\cdot,q_{z})]\|_{L^{1}(\mathbb{R}_{+}\times\mathbb{R})} \leq \\ \leq c_{0}(n) \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{m} \left|\sigma^{\varepsilon[1]}(m',q_{z}(m'))\right| \times \\ \times \left|\sigma^{\varepsilon[1]}(m-m',q_{z}(m-m')) - \sigma^{\varepsilon[2]}(m-m',q_{z}(m-m'))\right| dm' dm + \\ + c_{0}(n) \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{m} \left|\sigma^{\varepsilon[2]}(m-m',q_{z}(m-m'))\right| \times \\ \times \left|\sigma^{\varepsilon[1]}(m',q_{z}(m')) - \sigma^{\varepsilon[2]}(m',q_{z}(m'))\right| dm' dm + \\ + c_{0}(n) \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} \left|\sigma^{\varepsilon[1]}(m,q_{z}(m))\right| \left|\sigma^{\varepsilon[1]}(m',q_{z}(m')) - \sigma^{\varepsilon[2]}(m',q_{z}(m'))\right| dm' dm + \\ + c_{0}(n) \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} \left|\sigma^{\varepsilon[1]}(m,q_{z}(m))\right| \left|\sigma^{\varepsilon[1]}(m',q_{z}(m')) - \sigma^{\varepsilon[2]}(m',q_{z}(m'))\right| dm' dm + \\ + c_{0}(n) \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} \left|\sigma^{\varepsilon[1]}(m,q_{z}(m))\right| \left|\sigma^{\varepsilon[1]}(m',q_{z}(m')) - \sigma^{\varepsilon[2]}(m',q_{z}(m'))\right| dm' dm + \\ + c_{0}(n) \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} \left|\sigma^{\varepsilon[1]}(m,q_{z}(m))\right| \left|\sigma^{\varepsilon[1]}(m',q_{z}(m')) - \sigma^{\varepsilon[2]}(m',q_{z}(m'))\right| dm' dm + \\ - c_{0}(n) \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} \left|\sigma^{\varepsilon[1]}(m,q_{z}(m))\right| \left|\sigma^{\varepsilon[1]}(m',q_{z}(m')) - \sigma^{\varepsilon[2]}(m',q_{z}(m'))\right| dm' dm + \\ - c_{0}(n) \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} \left|\sigma^{\varepsilon[1]}(m,q_{z}(m))\right| d\sigma^{\varepsilon[1]}(m',q_{z}(m')) - \sigma^{\varepsilon[2]}(m',q_{z}(m'))\right| dm' dm + \\ - c_{0}(n) \int_{0}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} \left|\sigma^{\varepsilon[1]}(m,q_{z}(m))\right| d\sigma^{\varepsilon[1]}(m',q_{z}(m')) dm' dm + \\ - c_{0}(n) \int_{0}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} \left|\sigma^{\varepsilon[1]}(m,q_{z}(m))\right| d\sigma^{\varepsilon[1]}(m',q_{z}(m')) dm' dm + \\ - c_{0}(n) \int_{0}^{\infty} dz \int_{0}^{\infty} \int_{0}^{\infty} dz \int_{0$$

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$$+c_{0}(n)\int_{-A}^{0}dz\int_{0}^{\infty}\int_{0}^{\infty}\left|\sigma^{\varepsilon[2]}(m',q_{z}(m'))\right|\left|\sigma^{\varepsilon[1]}(m,q_{z}(m))-\sigma^{\varepsilon[2]}(m,q_{z}(m))\right|dm'dm.$$

Concerning the term of fragmentation (see the definition (25)), we note that, with the change of variables m'' = m + m', we have

$$\int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{\infty} m\vartheta(m,m')\sigma^{\varepsilon}(m+m',q_{z}(m+m'))dm'dm =$$
$$= \int_{-A}^{0} dz \int_{0}^{\infty} \int_{0}^{m} (m-m')\vartheta(m-m',m')\sigma^{\varepsilon}(m,q_{z}(m))dm'dm.$$

Therefore, taking into account the condition (13), we deduce that

$$\begin{split} \|L_{t,z}^{[n]}[\sigma^{\varepsilon[1]}(\cdot,q_z)] - L_{t,z}^{[n]}[\sigma^{\varepsilon[2]}(\cdot,q_z)]\|_{L^1(\mathbb{R}_+\times\mathbb{R})} &\leq \\ &\leq 2\int_{-A}^0 dz \int_0^\infty \left|\sigma^{\varepsilon[1]}(m,q_z(m)) - \sigma^{\varepsilon[2]}(m,q_z(m))\right| dm. \end{split}$$

By virtue of the inequality (41) and the inequality

$$\|\sigma^{\varepsilon[1]} - \sigma^{\varepsilon[2]}\|_{L^1(\mathbb{R}_+ \times \mathbb{R})} \le \|\sigma^{[1]} - \sigma^{[2]}\|_{L^1(\mathbb{R}_+ \times \mathbb{R})},$$

we deduce that

$$\begin{split} \|K_{t,z}^{[n]}[\sigma^{\varepsilon[1]}(\cdot,q_z),\sigma^{\varepsilon[1]}(\cdot,q_z)] - K_{t,z}^{[n]}[\sigma^{\varepsilon[2]}(\cdot,q_z),\sigma^{\varepsilon[2]}(\cdot,q_z)]\|_{L^1(\mathbb{R}_+\times\mathbb{R})} \leq \\ \leq 4Kc_0(n)\|\sigma^{[1]} - \sigma_n^{[2]}\|_{L^1(\mathbb{R}_+\times\mathbb{R})}, \end{split}$$

$$\|L_{t,z}^{[n]}[\sigma^{\varepsilon[1]}(\cdot,q_z)] - L_{t,z}^{[n]}[\sigma^{\varepsilon[2]}(\cdot,q_z)]\|_{L^1(\mathbb{R}_+\times\mathbb{R})} \le 2\|\sigma^{[1]} - \sigma^{[2]}\|_{L^1(\mathbb{R}_+\times\mathbb{R})}.$$

As the coefficients of these inequalities do not depend on t, from these inequalities we deduce that  $F^{[n]}[\sigma^{\varepsilon}]$  verify locally the Lipschitz condition in the topology of  $L^1(\mathbb{R}_+ \times \mathbb{R})$  for each  $t \in \mathbb{R}_+$ . The local Lipschitz condition for each t being proved, by using (38) and the reasoning for (41), we can extend the solution (by repeating the application of the local Lipschitz condition) for all  $t \in \mathbb{R}_+$ , that is, we have shown that the equation (31) with the condition (32) admits a unique solution  $\sigma_n(\cdot, \cdot, t) \in L^1(\mathbb{R}_+ \times \mathbb{R}), t \geq 0$ ; the continuity in t in the topology of  $L^1(\mathbb{R}_+ \times \mathbb{R})$ results from (40).

Finally, we note that, in virtue of the conditions (29), (32) and (33), for  $m \ge n+1$  the equation (31) is reduced to

$$\frac{\partial}{\partial t}\sigma_n(m,q,t) = -\sigma_n(m,q,t)\delta_{-\frac{q+A}{u(m)}}(t),$$

which gives us (39).

## 6 Estimate of $\mu$ -moment of the approximate solutions

Now, using the idea of [1, 6], we are going to prove that the moment of order  $\mu > 0$  of the approximate solutions is bounded. First we define the moment of order  $\mu$  (or, simply,  $\mu$ -moment) of  $\sigma = \sigma(m, q_z, t)$  by

$$\int_{-A}^0 \|\sigma_z(t)\|_\mu dz,$$

where

$$\|\sigma_z(t)\|_{\mu} = \|\sigma_z\|_{\mu} = \int_0^\infty m^{\mu} \sigma(m, q_z(m), t) dm \qquad (q_z(m) = z - u(m)t).$$

Before giving the estimate of  $\mu$ -moment, we recall some preliminary properties. Consider  $\sigma \in L^1(\mathbb{R}_+)$  such that  $\sigma(m) \ge 0$  for all  $m \in \mathbb{R}_+$ . For  $\lambda \ge 0$ , we define

$$\|\sigma\|_{\lambda} = \int_0^\infty m^{\lambda} \sigma(m) dm$$

**Lemma 6.1.** For all  $\lambda < \beta < \delta$ , we have

$$\|\sigma\|_{\beta}^{\delta-\lambda} \le \|\sigma\|_{\lambda}^{\delta-\beta} \|\sigma\|_{\delta}^{\beta-\lambda}.$$
(42)

For the proof, see [5].

**Lemma 6.2.** *Let*  $\nu \ge 1$ *.* 

i) There exists a constant  $C_{\nu} > 0$  such that

$$(m+m')[(m+m')^{\nu} - m^{\nu} - m'^{\nu}] \le C_{\nu}(m^{\nu}m' + mm'^{\nu}).$$
(43)

ii) For  $1 \le m \le \frac{r}{2}$ ,  $r \ge r_0 \ge 2$ , we have

$$r^{\nu} - m^{\nu} - (r - m)^{\nu} \ge (2^{\nu} - 2)m^{\nu}.$$
(44)

For the proof, see [4].

**Lemma 6.3.** Let  $\sigma_n$  be the solution to the equation (31) with the condition (32). Then we have

$$\int_{0}^{n+1} m^{\mu} \frac{\partial}{\partial t} \sigma_{n}(m,q,t) dm = \frac{1}{2} \int_{m+m' \le n+1} \left( (m+m')^{\mu+1} - m^{\mu+1} - m'^{\mu+1} \right) \times (45)$$

$$\times \left( \beta_{n}(m,m') \sigma_{n}^{\varepsilon}(m,q_{z}(m),t) \sigma_{n}^{\varepsilon}(m',q_{z}(m'),t) + -\vartheta_{n}(m,m') \sigma_{n}^{\varepsilon}(m+m',q_{z}(m+m'),t) \right) dm' dm + \int_{0}^{n+1} m^{\mu} \overline{\sigma}_{1n}^{*}(m,t) \delta_{-\frac{q}{u(m)}}(t) dm - \int_{0}^{n+1} m^{\mu} \sigma_{n}(m,q,t) \delta_{-\frac{q+A}{u(m)}}(t) dm.$$

Proof. We consider

$$\int_{0}^{n+1} m^{\mu} K_{t,z}^{[n]} [\sigma_{n}^{\varepsilon}(\cdot, q_{z}, t), \sigma_{n}^{\varepsilon}(\cdot, q_{z}, t)](m) dm + \int_{0}^{n+1} m^{\mu} L_{t,z}^{[n]} [\sigma_{n}^{\varepsilon}(\cdot, q_{z}, t)](m) dm =$$

$$= I_{1} - I_{2} - J_{1} + J_{2},$$
(46)

where

$$\begin{split} I_{1} &= \int_{0}^{n+1} m^{\mu} \frac{m}{2} \int_{0}^{m} \beta_{n} (m-m',m') \sigma_{n}^{\varepsilon} (m-m',q_{z}(m-m'),t) \sigma_{n}^{\varepsilon} (m',q_{z}(m'),t) dm' dm, \\ I_{2} &= \int_{0}^{n+1} m^{\mu} m \int_{0}^{n-m+1} \beta_{n} (m,m') \sigma_{n}^{\varepsilon} (m,q_{z}(m),t) \sigma_{n}^{\varepsilon} (m',q_{z}(m'),t) dm' dm, \\ J_{1} &= \int_{0}^{n+1} m^{\mu} \frac{m}{2} \int_{0}^{m} \vartheta_{n} (m-m',m') \sigma_{n}^{\varepsilon} (m,q,t) dm' dm, \\ J_{2} &= \int_{0}^{n+1} m^{\mu} m \int_{0}^{n-m+1} \vartheta_{n} (m,m') \sigma_{n}^{\varepsilon} (m+m',q_{z}(m+m'),t) dm' dm. \end{split}$$

We note that, if we use the change of variables m'' = m - m',  $I_1$  and  $J_1$  are transformed into

$$I_{1} = \int_{0 \le m' + m'' \le n+1} (m' + m'')^{\mu} \frac{m' + m''}{2} \times \\ \times \beta_{n}(m', m'') \sigma_{n}^{\varepsilon}(m', q_{z}(m'), t) \sigma_{n}^{\varepsilon}(m'', q_{z}(m''), t) dm' dm'',$$

$$J_{1} = \int_{0 \le m' + m'' \le n+1} (m' + m'')^{\mu} \frac{m' + m''}{2} \vartheta_{n}(m', m'') \sigma_{n}^{\varepsilon}(m' + m'', q_{z}(m' + m''), t) dm' dm''.$$

By summing  $I_1 - I_2 - J_1 + J_2$  and recalling (46) and (31), we obtain (45).

**Lemma 6.4.** There exists an increasing function  $K_1(t)$  independent of n such that for all t > 0 we have

$$\int_{-A}^{0} \|\sigma_{n,z}(t)\|_{\mu} dz \le K_1(t).$$
(47)

*Proof.* Let us recall that, if the conditions (17) and (18) are satisfied, then the relations (29) imply that

$$\beta_n(m,m') \le K_c(mm')^{\alpha-1},\tag{48}$$

$$\int_{0}^{\frac{1}{2}} m^{\mu+1} \vartheta_{n}(m, r-m) dm \ge K_{f}(r-1)^{\gamma+\mu} \qquad \forall r_{0} \le r \le n+1.$$
(49)

According to the lemma 6.3, we have

$$\frac{d}{dt} \int_{-A}^{0} \|\sigma_{n,z}\|_{\mu} dz =$$
 (50)

$$= \int_{-A}^{0} \frac{1}{2} \int_{m+m' \le n+1} (Q_1 - Q_2) dm' dm dz + \int_{0}^{n+1} \int_{0}^{-tu(m)} m^{\mu} \overline{\sigma}_{1n}^*(m, -\frac{q}{u(m)}) dq dm + \int_{0}^{n+1} \int_{-A}^{-A-tu(m)} m^{\mu} \sigma_n(m, q, -\frac{q+A}{u(m)}) dq dm,$$

where

$$Q_{1} = \left( (m+m')^{\mu+1} - m^{\mu+1} - m'^{\mu+1} \right) \beta_{n}(m,m') \sigma_{n}^{\varepsilon}(m,q_{z}(m),t) \sigma_{n}^{\varepsilon}(m',q_{z}(m'),t)$$
$$Q_{2} = \left( (m+m')^{\mu+1} - m^{\mu+1} - m'^{\mu+1} \right) \vartheta_{n}(m,m') \sigma_{n}^{\varepsilon}(m+m',q_{z}(m+m'),t).$$

We note that, by virtue of (43) and (48), there exists a constant  $\widetilde{C}$  such that

$$\left((m+m')^{\mu+1} - m^{\mu+1} - m'^{\mu+1}\right)\beta_n(m,m') \le \frac{\tilde{C}}{2}\left(m^{\mu+\alpha-1}m'^{\alpha} + m^{\alpha}m'^{\mu+\alpha-1}\right).$$

Therefore, taking into account the symmetry between m and m', we have

$$\int_{-A}^{0} \frac{1}{2} \int_{m+m' \le n+1} Q_1 dm' dm dz \le$$

$$\tag{51}$$

$$\leq \int_{-A}^{0} \widetilde{C} \int_{m+m' \leq n+1} m^{\mu+\alpha-1} m'^{\alpha} \sigma_{n}^{\varepsilon}(m, q_{z}(m), t) \sigma_{n}^{\varepsilon}(m', q_{z}(m'), t) dm' dm dz \leq \\ \leq \widetilde{C} \int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\alpha} \|\sigma_{n,z}^{\varepsilon}\|_{\mu+\alpha-1} dz.$$

According to the lemma 6.1, for  $\mu > \alpha$  we have

$$\|\sigma_{n,z}^{\varepsilon}\|_{\alpha} \leq \|\sigma_{n,z}^{\varepsilon}\|_{0}^{\frac{\mu-\alpha}{\mu}} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\frac{\alpha}{\mu}}, \qquad \|\sigma_{n,z}^{\varepsilon}\|_{\mu+\alpha-1} \leq \|\sigma_{n,z}^{\varepsilon}\|_{0}^{\frac{1-\alpha}{\mu}} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\frac{\mu+\alpha-1}{\mu}}.$$

On the other hand, by virtue of the lemma 4.3, we have

$$\|\sigma_{n,z}^{\varepsilon}\|_{0} \leq K(t) \qquad \forall z \in [-A,0], \ \forall n \in \mathbb{N}.$$

Therefore we have

$$\int_{-A}^{0} \frac{1}{2} \int_{m+m' \le n+1} Q_1 dm' dm dz \le C_1(t) \int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_1} dz,$$
(52)

where  $C_1(t) = \tilde{C}(K(t))^{1 - \frac{2\alpha - 1}{\mu}}, \, \alpha_1 = 1 + \frac{2\alpha - 1}{\mu}.$ 

Let us now turn to the study of the integral of  $Q_2$ . Using the inequalities (44), (49) and the change of variables r = m + m' we have

$$\int_{-A}^0 \frac{1}{2} \int_{m+m' \le n+1} Q_2 dm' dm dz \ge$$

$$\geq \int_{-A}^{0} \frac{1}{2} \int_{2}^{n+1} \int_{0}^{r-m} (r^{\mu+1} - m^{\mu+1} - (r-m)^{\mu+1}) \vartheta_{n}(m, r-m) \sigma_{n}^{\varepsilon}(r, q_{z}(r), t)) dr dm dz$$

$$\geq \int_{-A}^{0} \frac{1}{2} \int_{2}^{n+1} \int_{0}^{\frac{r}{2}} (2^{\mu+1} - 2) m^{\mu+1} \vartheta_{n}(m, r-m) \sigma_{n}^{\varepsilon}(r, q_{z}(r), t) dr dm dz$$

$$\geq \int_{-A}^{0} (2^{\mu} - 1) K_{f}(\mu) \int_{2}^{n+1} (r-1)^{\gamma+\mu} \sigma_{n}^{\varepsilon}(r, q_{z}(r), t) dr dz$$

$$\geq \frac{(2^{\mu} - 1) K_{f}(\mu)}{2^{\gamma+\mu}} \Big[ \int_{-A}^{0} \int_{0}^{n+1} r^{\gamma+\mu} \sigma_{n}^{\varepsilon}(r, q_{z}(r), t) dr dz - \int_{-A}^{0} \int_{0}^{2} r^{\gamma+\mu} \sigma_{n}^{\varepsilon}(r, q_{z}(r), t) dr dz \Big]$$

$$\geq \frac{(2^{\mu} - 1) K_{f}(\mu)}{2^{\gamma+\mu}} \Big[ \int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\gamma+\mu} dz - 2^{\gamma+\mu} K(t) A \Big] =$$

$$= \frac{(2^{\mu} - 1) K_{f}(\mu)}{2^{\gamma+\mu} \overline{C}} \int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\gamma+\mu} \overline{C} dz - (2^{\mu} - 1) K_{f}(\mu) K(t) A.$$

So, taking into account the lemma 6.1, we have

$$\int_{-A}^{0} \frac{1}{2} \int_{m+m' \le n+1} Q_2 dm' dm dz \ge C_3 \int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_2} dz - C_2,$$
(53)

where  $C_3 = \frac{(2^{\mu}-1)K_f(\mu)}{2^{\gamma+\mu}\overline{C}}$ ,  $\alpha_2 = 1 + \frac{\gamma}{\mu}$  and  $C_2(t) = (2^{\mu}-1)K_f(\mu)K(t)A$ . By substituting (52) and (53) into (50), we obtain for  $\mu > \alpha$ 

$$\frac{d}{dt} \int_{-A}^{0} \|\sigma_{n,z}\|_{\mu} dz \le C_1(t) \int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_1} dz +$$
(54)

$$\begin{split} -C_3 \int_{-A}^0 \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_2} dz + C_2(t) + \int_0^{n+1} \int_0^{-tu(m)} m^{\mu} \overline{\sigma}_{1n}^*(m, -\frac{q}{u(m)}) dq dm + \\ &- \int_0^{n+1} \int_{-A}^{-A-tu(m)} m^{\mu} \sigma_n(m, q, -\frac{q+A}{u(m)}) dq dm. \end{split}$$

As  $0 < \alpha_1 < \alpha_2$ , we have

$$\int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_{1}} dz \leq \left(\int_{-A}^{0} (\|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_{1}})^{\frac{\alpha_{2}}{\alpha_{1}}} dz\right)^{\frac{\alpha_{1}}{\alpha_{2}}} \left(\int_{-A}^{0} 1 dz\right)^{\frac{\alpha_{2}-\alpha_{1}}{\alpha_{2}}} = A^{\frac{\alpha_{2}-\alpha_{1}}{\alpha_{2}}} \left(\int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_{2}} dz\right)^{\frac{\alpha_{1}}{\alpha_{2}}},$$

and therefore

$$\left(\int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_{1}} dz\right)^{\frac{\alpha_{2}}{\alpha_{1}}} \leq A^{\frac{\alpha_{2}-\alpha_{1}}{\alpha_{1}}} \int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_{2}} dz$$

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Consequently, we have

$$\frac{d}{dt} \int_{-A}^{0} \|\sigma_{n,z}\|_{\mu} dz \leq C_{1}(t) \int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_{1}} dz - \frac{C_{3}}{A^{\frac{\alpha_{2}-\alpha_{1}}{\alpha_{1}}}} (\int_{-A}^{0} \|\sigma_{n,z}^{\varepsilon}\|_{\mu}^{\alpha_{1}} dz)^{\frac{\alpha_{2}}{\alpha_{1}}} + (55) \\
+ C_{2}(t) + \int_{0}^{n+1} \int_{0}^{-tu(m)} m^{\mu} \overline{\sigma}_{1n}^{*}(m, -\frac{q}{u(m)}) dq dm + \\
- \int_{0}^{n+1} \int_{-A}^{-A-tu(m)} m^{\mu} \sigma_{n}(m, q, -\frac{q+A}{u(m)}) dq dm.$$

We note that  $\frac{\alpha_2}{\alpha_1} > 1$  and so that

$$\sup_{r>0} \left[ C_1(t)r - \frac{C_3}{A^{\frac{\alpha_2 - \alpha_1}{\alpha_1}}} r^{\frac{\alpha_2}{\alpha_1}} \right] \equiv C_4(t) < \infty.$$

Therefore, if we put

$$K_1(t) = \int_{-A}^0 \|\sigma_{n,z}(0)\|_{\mu} dz + \int_0^t [G(t') + C_4(t')] dt'$$
(56)

with

$$G(t) = C_2(t) + \int_0^{n+1} \int_0^{-tu(m)} m^{\mu} \overline{\sigma}_{1n}^*(m, -\frac{q}{u(m)}) dq dm,$$

then from the inequality (55) we deduce immediately that the function  $K_1(t)$  satisfies the inequality (47).

From the lemmas 4.3 and 6.4 results immediately the following lemma.

**Lemma 6.5.** If  $\sigma_n(\cdot, \cdot, t)$  is a solution to the equation (31) with the initial condition (32) and if  $\sigma_n^{\varepsilon}$  is defined in a similar way as (4), then we have

$$\sup_{zA \le z \le 0} \int_{\mathbb{R}_+} m^{\mu} \sigma_n^{\varepsilon}(m, q_z(m), t) dm \le K_0(t) < \infty,$$
(57)

where

$$K_0(t) = \eta_{\varepsilon}(0) \int_{-A}^0 \|\sigma_{n,z}(t)\|_{\mu} dz = \eta_{\varepsilon}(0) K_1(t)$$

 $(\eta_{\varepsilon}(\cdot) \text{ and } K_1(t) \text{ are defined in (3) and (56) respectively}).$ 

*Proof.* The lemma can be proved in a similar way to the lemma 4.3. More precisely, we multiply (4) by  $m^{\mu}$  and integrate it on  $\mathbb{R}_+$  with respect to m, so that, using the lemma 6.4, we obtain (57).

# 7 $L^{\infty}$ estimate of the approximate solutions

In order to estimate the approximate solutions in the norm of  $L^{\infty}(\mathbb{R}_+ \times \mathbb{R})$ , we adopt the idea of the maximum principle used by Galkin [8] and Dubovskii [7], generalizing it slightly. We have the following lemma.

**Lemma 7.1.** Let  $\Omega$  be an open set of  $\mathbb{R}^n$ . Let u(x,t) be a non-negative function, continuous in  $\Omega \times [0,t_1]$  and admitting the partial derivative  $\partial_t u(x,t)$  for all  $(x,t) \in \Omega \times ]0,t_1[$ . We assume that for every  $t \in [0,t_1]$  there exists at least a point  $\overline{x} \in \Omega$  such that

$$u(\overline{x},t) \ge u(x,t) \qquad \forall x \in \Omega, \tag{58}$$

and that for all  $t \in [0, t_1]$ , at the point  $\overline{x}$  we have

$$\partial_t u(\overline{x}, t) \le b(t) + k u(\overline{x}, t) \qquad (b(t) \ge 0).$$
(59)

Then we have

$$u(x,t) \le a \exp(kt) + \int_0^t b(s) \exp k(t-s) ds \equiv A(t) \qquad \forall (x,t) \in \Omega \times ]0, t_1[, \quad (60)$$

where

$$a = \max_{x \in \Omega} u(x, 0).$$

*Proof.* We use the idea of Galkin, which proves the lemma in the case where b(t) = 0 and k = 0.

We will prove (60) by absurdity. To do this, for each  $\varepsilon > 0$  we put

$$a_{\varepsilon} = \max_{x \in \Omega} u(x, 0) + \varepsilon = a + \varepsilon,$$
$$A_{\varepsilon}(t) = a_{\varepsilon} \exp((k + \varepsilon)t) + \int_{0}^{t} b(s) \exp((k + \varepsilon)(t - s))ds,$$
$$U_{\varepsilon}(x, t) = \frac{u(x, t)}{A_{\varepsilon}(t)}.$$

We suppose that there exists  $(x,t) \in \Omega \times [0,t_1]$  such that  $u(x,t) > A_{\varepsilon}(t)$ . Then there exists an  $\tilde{t} \in [0,t_1]$  such that

$$\widetilde{t} = \min\{t > 0 \mid \max_{x \in \Omega} U_{\varepsilon}(x, t) \ge 1\}.$$
(61)

According to our hypothesis (see (58)) there exists a point  $\overline{x} \in \Omega$  such that

$$u(\overline{x}, \widetilde{t}) \ge u(x, \widetilde{t}), \qquad \forall x \in \Omega.$$

We have obviously

$$U_{\varepsilon}(\overline{x}, \widetilde{t}) \ge U_{\varepsilon}(x, \widetilde{t}) \qquad \forall x \in \Omega.$$

From the definition of  $U_{\varepsilon}(\overline{x}, \widetilde{t}), A_{\varepsilon}$  and the hypothesis (59) we have

$$\partial_t U_{\varepsilon}(\overline{x}, \widetilde{t}) = \frac{1}{(A_{\varepsilon}(\widetilde{t}))^2} \Big[ \partial_{\widetilde{t}} u(\overline{x}, \widetilde{t}) A_{\varepsilon}(\widetilde{t}) - u(\overline{x}, \widetilde{t}) \partial_{\widetilde{t}} A_{\varepsilon}(\widetilde{t}) \Big] \le \frac{1}{(A_{\varepsilon}(\widetilde{t}))^2} [(b(\widetilde{t}) + ku(\overline{x}, \widetilde{t})) A_{\varepsilon}(\widetilde{t}) - u(\overline{x}, \widetilde{t})((k+\varepsilon)A_{\varepsilon}(\widetilde{t}) + b(\widetilde{t}))].$$

As  $U_{\varepsilon}(\overline{x}, \widetilde{t}) = \frac{u(\overline{x}, \widetilde{t})}{A_{\varepsilon}(\widetilde{t})} = 1$ , we obtain

$$\begin{split} \partial_t U_{\varepsilon}(\overline{x},\widetilde{t}) &\leq \frac{1}{(A_{\varepsilon}(\widetilde{t}))^2} \big[ b(\widetilde{t}) A_{\varepsilon}(\widetilde{t}) + ku(\overline{x},\widetilde{t}) A_{\varepsilon}(\widetilde{t}) - ku(\overline{x},\widetilde{t}) A_{\varepsilon}(\widetilde{t}) + \\ &-\varepsilon u(\overline{x},\widetilde{t}) A_{\varepsilon}(\widetilde{t}) - b(\widetilde{t}) u(\overline{x},\widetilde{t}) \big] = \\ &= \frac{1}{(A_{\varepsilon}(\widetilde{t}))^2} \big[ b(\widetilde{t}) A_{\varepsilon}(\widetilde{t}) + kA_{\varepsilon}(\widetilde{t})^2 - kA_{\varepsilon}(\widetilde{t})^2 - \varepsilon A_{\varepsilon}(\widetilde{t})^2 - b(\widetilde{t}) A_{\varepsilon}(\widetilde{t}) \big] \\ &= \frac{1}{(A_{\varepsilon}(\widetilde{t}))^2} \big( -\varepsilon A_{\varepsilon}(\widetilde{t})^2 \big) = -\varepsilon < 0. \end{split}$$

So there exists a point  $(\overline{x}, \widetilde{t}') \in \Omega \times ]0, \widetilde{t}[$  (that is,  $\widetilde{t}' < \widetilde{t}$ ) such that

 $U_{\varepsilon}(\overline{x}, \widetilde{t}') > 1,$ 

which contradicts the definition (61) of  $\tilde{t}$ , that is,  $\tilde{t}$  does not exist. Therefore, we have

 $U_{\varepsilon}(x,t) \leq 1 \qquad \forall (x,t) \in \Omega \times [0,t_1].$ 

Consequently, we have

$$u(x,t) \le A_{\varepsilon}(t).$$

Since this inequality is valid for all  $\varepsilon > 0$ , passing to the limit for  $\varepsilon \to 0$ , we obtain the inequality

$$u(x,t) \le A(t)$$
  $\forall (x,t) \in \Omega \times ]0, t_1[.$ 

The lemma is proved.

Now we are going to show that  $\sigma_n(m, q, t)$  is locally bounded.

**Lemma 7.2.** There exists a continuous function  $C(\tilde{m}^*;t)$  defined in  $(\tilde{m}^*,t) \in \mathbb{R}_+ \times \mathbb{R}_+$  and satisfying the relation

$$\sup_{0 < m \le \widetilde{m}^*, q \in \mathbb{R}} \sigma_n(m, q, t) \le C(\widetilde{m}^*; t)$$
(62)

for all  $n \geq \tilde{m}^*$ , where  $\sigma_n(m, q, t)$  is the solution to the equation (31) (with (33)) with the initial condition (32).

*Proof.* For each  $\widetilde{m}^* > 0$  we define the function  $\psi_{\widetilde{m}^*}(m)$  by

$$\psi_{\widetilde{m}^*}(m) = \psi^1(m - \widetilde{m}^*)$$

with the function  $\psi^1(\cdot)$  which we have used for the definition of  $\beta_n$  and  $\vartheta_n$  (see (29)-(30)).

Let  $(\overline{m}, \overline{q})$  be the maximum point of the function  $\psi_{\widetilde{m}^*}(m) \frac{\sigma_n(m,q_z,t)}{m}$  at time  $t \ge 0$ and for  $n \ge \widetilde{m}^*$ , that is,

$$\psi_{\widetilde{m}^*}(\overline{m})\frac{\sigma_n(\overline{m},\overline{q}_z,t)}{\overline{m}} = \max_{0 < m \le \widetilde{m}^*, q \in \mathbb{R}} \psi_{\widetilde{m}^*}(m)\frac{\sigma_n(m,q_z,t)}{m}.$$
(63)

Recalling the definitions of the coagulation and fragmentation operators (see (24) and (25)), we have  $2 = (\overline{x}, \overline{z}, t)$ 

$$\psi_{\widetilde{m}^{*}}(\overline{m})\frac{\partial}{\partial t}\frac{\sigma_{n}(m,q,t)}{\overline{m}} \leq$$

$$\leq \frac{1}{2}\int_{0}^{\overline{m}} \left[\beta_{n}(\overline{m}-m',m')\psi_{\widetilde{m}^{*}}(\overline{m})\sigma_{n}^{\varepsilon}(\overline{m}-m',\overline{q}_{z}(\overline{m}-m'),t)+\right.\\\left.\left.-\beta_{n}(\overline{m},m')\psi_{\widetilde{m}^{*}}(\overline{m})\sigma_{n}^{\varepsilon}(\overline{m},\overline{q}_{z}(\overline{m}),t)\right]\sigma_{n}^{\varepsilon}(m',q_{z}(m'),t)dm'+\right.\\\left.\left.-\frac{1}{2}\int_{\overline{m}}^{\widetilde{m}^{*}}\beta_{n}(\overline{m},m')\psi_{\widetilde{m}^{*}}(\overline{m})\sigma_{n}^{\varepsilon}(\overline{m},\overline{q}_{z}(\overline{m}),t)\sigma_{n}^{\varepsilon}(m',q_{z}(m'),t)dm'+\right.\\\left.\left.+\int_{0}^{\widetilde{m}^{*}}\vartheta_{n}(\overline{m},m')\psi_{\widetilde{m}^{*}}(\overline{m})\sigma_{n}^{\varepsilon}(\overline{m}+m',\overline{q}_{z}(\overline{m}+m'),t)dm'+\right.\\\left.\left.-\int_{0}^{\overline{m}}\vartheta_{n}(\overline{m}-m',m')\psi_{\widetilde{m}^{*}}(\overline{m})\sigma_{n}^{\varepsilon}(\overline{m},\overline{q}_{z}(\overline{m}),t)dm'+\right.\\\left.\left.+\psi_{\widetilde{m}^{*}}(\overline{m})\frac{\overline{\sigma}_{1n}^{*}(\overline{m},t)}{\overline{m}}\delta_{-\frac{q}{u(m)}}(t)-\psi_{\widetilde{m}^{*}}(\overline{m})\frac{\sigma_{n}(\overline{m},\overline{q},t)}{\overline{m}}\delta_{-\frac{q+A}{u(m)}}(t).\right.$$

Let us examine the sign of the term

$$\begin{split} D &= \frac{1}{2} \int_0^{\overline{m}} \Big[ \beta_n(\overline{m} - m', m') \psi_{\widetilde{m}^*}(\overline{m}) \sigma_n^{\varepsilon}(\overline{m} - m', \overline{q}_z(\overline{m} - m'), t) + \\ &- \beta_n(\overline{m}, m') \psi_{\widetilde{m}^*}(\overline{m}) \sigma_n^{\varepsilon}(\overline{m}, \overline{q}_z(\overline{m}), t) \Big] \sigma_n^{\varepsilon}(m', q_z(m'), t) dm'. \end{split}$$

We first note that D can be written in the form

$$D = \frac{1}{2} \int_0^{\overline{m}} \left[ (\overline{m} - m')\beta_n(\overline{m} - m', m')\psi_{\widetilde{m}^*}(\overline{m}) \frac{\sigma_n^{\varepsilon}(\overline{m} - m', \overline{q}_z(\overline{m} - m'), t)}{\overline{m} - m'} + \right]$$

$$\begin{split} & -\overline{m}\beta_{n}(\overline{m},m')\psi_{\widetilde{m}^{*}}(\overline{m})\frac{\sigma_{n}^{\varepsilon}(\overline{m},\overline{q}_{z}(\overline{m}),t)}{\overline{m}}\Big]\sigma_{n}^{\varepsilon}(m',q_{z}(m'),t)dm' = \\ & = \frac{1}{2}\int_{0}^{\overline{m}}\Big[(\overline{m}-m')\beta_{n}(\overline{m}-m',m')\psi_{\widetilde{m}^{*}}(\overline{m})\frac{\sigma_{n}^{\varepsilon}(\overline{m}-m',\overline{q}_{z}(\overline{m}-m'),t)}{\overline{m}-m'} + \\ & -\overline{m}\beta_{n}(\overline{m},m')\psi_{\widetilde{m}^{*}}(\overline{m})\frac{\sigma_{n}(\overline{m},\overline{q}_{z}(\overline{m}),t)}{\overline{m}}\Big]\sigma_{n}^{\varepsilon}(m',\overline{q}_{z}(m'),t)dm' + \\ & +\frac{1}{2}\int_{0}^{\overline{m}}\overline{m}\beta_{n}(\overline{m},m')\psi_{\widetilde{m}^{*}}(\overline{m})\Big[\frac{\sigma_{n}(\overline{m},\overline{q}_{z}(\overline{m}),t)}{\overline{m}} - \frac{\sigma_{n}^{\varepsilon}(\overline{m},\overline{q}_{z}(\overline{m}),t)}{\overline{m}}\Big]\sigma_{n}^{\varepsilon}(m',q_{z}(m'),t)dm'. \end{split}$$

From this expression of D, by using the relation (16), the definition (4), and the inequality

$$\frac{\sigma_n(\overline{m} - m', \overline{q}_z(\overline{m} - m'), t)}{\overline{m} - m'} \le \frac{\sigma_n(\overline{m}, \overline{q}_z(\overline{m}), t)}{\overline{m}} \qquad \text{pour } 0 \le m' \le \overline{m} \le \widetilde{m}^*, \overline{q} \in \mathbb{R},$$
(65)

we obtain

$$D \leq \frac{1}{2} \int_0^{\overline{m}} \overline{m} \beta_n(\overline{m}, m') \psi_{\widetilde{m}^*}(\overline{m}) \Big[ \frac{\sigma_n(\overline{m}, \overline{q}_z(\overline{m}), t)}{\overline{m}} - \frac{\sigma_n^{\varepsilon}(\overline{m}, \overline{q}_z(\overline{m}), t)}{\overline{m}} \Big] \sigma_n^{\varepsilon}(m', q_z(m'), t) dm'.$$

Using this last relation, neglecting the negative terms in (64), we obtain

$$\begin{split} \psi_{\widetilde{m}^*}(\overline{m}) \frac{\partial}{\partial t} \frac{\sigma_n(\overline{m},\overline{q},t)}{\overline{m}} \leq \\ \leq \frac{1}{2} \int_0^{\overline{m}} \overline{m} \beta_n(\overline{m},m') \psi_{\widetilde{m}^*}(\overline{m}) \frac{\sigma_n(\overline{m},\overline{q}_z(\overline{m}),t)}{\overline{m}} \sigma_n^{\varepsilon}(m',q_z(m'),t) dm' + \\ + \int_0^{\widetilde{m}^*} \vartheta_n(\overline{m},m') \sigma_n^{\varepsilon}(\overline{m}+m',\overline{q}_z(\overline{m}+m'),t) dm' + \psi_{\widetilde{m}^*}(\overline{m}) \frac{\overline{\sigma}_{1n}^*(\overline{m},t)}{\overline{m}} \delta_{-\frac{q}{u(m)}}(t) = \\ = \frac{1}{2} \int_0^{\overline{m}} \frac{\overline{m}}{m'^{\mu}} \beta_n(\overline{m},m') \psi_{\widetilde{m}^*}(\overline{m}) \frac{\sigma_n(\overline{m},\overline{q}_z(\overline{m}),t)}{\overline{m}} m'^{\mu} \sigma_n^{\varepsilon}(m',q_z(m'),t) dm' + \\ + \int_0^{\widetilde{m}^*} \vartheta_n(\overline{m},m') \sigma_n^{\varepsilon}(\overline{m}+m',\overline{q}_z(\overline{m}+m'),t) dm' + \psi_{\widetilde{m}^*}(\overline{m}) \frac{\overline{\sigma}_{1n}^*(\overline{m},t)}{\overline{m}} \delta_{-\frac{q}{u(m)}}(t). \end{split}$$

From this inequality, by using the relations (19), (15), (38), and (57), we deduce that

$$\psi_{\widetilde{m}^*}(\overline{m})\frac{\partial}{\partial t}\frac{\sigma_n(\overline{m},\overline{q},t)}{\overline{m}} \leq \leq (C_0K(t) + \psi_{\widetilde{m}^*}(\overline{m})\frac{\overline{\sigma}_{1n}^*(\overline{m},t)}{\overline{m}}\delta_{-\frac{q}{u(m)}}(t)) + \frac{C(\widetilde{m}^*)}{2}K_0(t)\psi_{\widetilde{m}^*}(\overline{m})\frac{\sigma_n(\overline{m},\overline{q},t)}{\overline{m}}.$$

Therefore, according to the lemma of the maximum principle cited above (Lemma 7.1), we have

$$\frac{\sigma_n(m,q,t)}{m} \le \max_{m',q} \frac{\overline{\sigma}_0^*(m',q)}{m'} e^{\frac{C(\widetilde{m}^*)}{2} \sup_t K_0(t)t} +$$
(66)

$$+ \int_{0}^{t} (C_0 K(s) + \sup_{m'} \frac{\overline{\sigma}_{1n}^*(m',t)}{m'} \delta_{-\frac{q}{u(m)}}(s)) e^{\frac{C(\widetilde{m}^*)}{2} \sup_{t} K_0(t)(t-s)} ds.$$

As the right-hand side of (66) depends only on  $\tilde{m}^*$  and t, we can write it  $\frac{C(\tilde{m}^*;t)}{\tilde{m}^*}$ , which implies (62). The lemma is proved.

## 8 Weak convergence of the approximate solutions

First let us prove an additional property of the mass conservation.

**Lemma 8.1.** For each  $\varepsilon > 0$ , there exists an increasing function  $m_{\varepsilon}^{*}(t)$  independent of n such that we have

$$\int_{-A}^{0} \int_{0}^{\infty} \widetilde{\psi}_{m_{\varepsilon}^{*}(t)}(m) \sigma_{n}(m, q_{z}, t) dm dz \geq$$

$$\geq \Sigma_{0}(t) - \int_{\mathbb{R}_{+}} \int_{-A}^{-A - tu(m)} \sigma_{n}(m, q, -\frac{q + A}{u(m)}) dq dm - \varepsilon,$$

$$(67)$$

where  $\Sigma_0(t)$  is the function defined in (37) and  $\widetilde{\psi}_{m_e^*(t)}(\cdot)$  is the function defined by

$$\widetilde{\psi}_{m_{\varepsilon}^*(t)}(m) = \psi^1(m - m_{\varepsilon}^*(t)),$$

 $\psi^1(\cdot)$  being the function introduced in (29)–(30).

Proof. We put

$$\Sigma_n(m^*, z) = \int_{-A}^0 \int_{m^*}^\infty \sigma_n(m, q_z, t) dm dz.$$
 (68)

Then, using the function  $K_1(t)$  introduced in the lemma 6.4, we have

$$K_1(t) \ge \int_{-A}^0 \|\sigma_{n,z}(t)\|_{\mu} dz \ge \int_{-A}^0 \int_{m^*}^\infty m^{\mu} \sigma_n(m, q_z, t) dm dz \ge m^{*\mu} \Sigma_n(m^*, z);$$

therefore we have

$$\Sigma_n(m^*, z) \le \frac{K_1(t)}{m^{*\mu}}$$

Taking  $m_{\varepsilon}^{*}(t) = (\frac{K_{1}(t)}{\varepsilon})^{\frac{1}{\mu}}$ , we have

$$\varepsilon = \frac{K_1(t)}{(m_{\varepsilon}^*(t))^{\mu}} \ge \Sigma_n(m^*, z).$$
(69)

We recall that  $K_1(t)$  is an inceasing function (see the lemma 6.4). From (69), taking into account (68), we deduce the inequality (67).

Finally we obtain the convergence of a subsequence of the approximate solutions.

**Proposition 8.1.** Let  $\{\sigma_n\}_{n=1}^{\infty}$  be the sequence of the solutions of the approximate equations (31) (with (33)) with the initial condition (32). Under the conditions mentioned in Section 2, there exist a subsequence  $\{\sigma_{n_k}\}_{k=1}^{\infty}$  of  $\{\sigma_n\}_{n=1}^{\infty}$  and a function  $\sigma \in L_{loc}^{\infty}(\mathbb{R}_+, L^1(\mathbb{R}_+ \times \Pi))$  such that

1) for all 
$$\bar{t} > 0$$
,  $\sigma_{n_k} \rightharpoonup \sigma$  in  $L^1(\mathbb{R}_+ \times \Pi \times ]0, \bar{t}[)$ ,

2) for all 
$$\overline{t} > 0$$
,  $\|\sigma_{n_k}(\cdot, \cdot, t)\|_{L^1(\mathbb{R}_+ \times \Pi)} \rightharpoonup^* \|\sigma(\cdot, \cdot, t)\|_{L^1(\mathbb{R}_+ \times \Pi)}$  in  $L^\infty(0, \overline{t})$ ,

3) for all  $m^* > 0$  and for all  $\bar{t} > 0$ ,  $\sigma_{n_k} \rightharpoonup^* \sigma$  in  $L^{\infty}(]0, m^*[\times \Pi \times ]0, \bar{t}[),$ 

4) for all  $\varepsilon > 0$  there exists a function  $m_{\varepsilon}^*(\bar{t})$  which is increasing in  $\bar{t} \in [0, \infty[$  and such that for every  $\bar{t} > 0$  the inequality

$$\int_{-A}^{0} \int_{0}^{\infty} \widetilde{\psi}_{m_{\varepsilon}^{*}(t)}(m) \sigma(m, q_{z}, t) dm dz \ge \|\sigma(\cdot, \cdot, t)\|_{L^{1}(\mathbb{R}_{+} \times \Pi)} - \varepsilon$$
(70)

holds for almost all  $t \in [0, \bar{t}]$  (the function  $\tilde{\psi}_{m_{\varepsilon}^*(t)}(m)$  is defined as in the lemma 8.1).

*Proof.* Let us denote by  $\{\sigma_{n'}\}_{n'=1}^{\infty}$  a generic subsequence of  $\{\sigma_n\}_{n=1}^{\infty}$ .

First of all, the lemma 7.2 implies that there exists a subsequence of  $\{\sigma_{n'}\}_{n'=1}^{\infty}$  which converges weakly-\* in  $L^{\infty}(]0, m^*[\times \Pi \times ]0, \bar{t}[)$  for all  $m^* > 0$  and for all  $\bar{t} > 0$ .

Secondly, we recall that according to the lemma 4.2 the norm in  $L^{\infty}(0, \bar{t}; L^1(\mathbb{R}_+ \times \Pi))$  of the functions  $\sigma_n$  is uniformly bounded. Therefore, using the lemma 7.2 and the inequality (69), we can extract from  $\{\sigma_{n'}\}_{n'=1}^{\infty}$  a subsequence  $\{\sigma_{n'_k}\}_{k=1}^{\infty}$  such that it converges weakly in  $L^1(\mathbb{R}_+ \times \Pi \times ]0, \bar{t}[)$  to a function belonging to  $L^1(\mathbb{R}_+ \times \Pi \times ]0, \bar{t}[)$  and  $\|\sigma_{n'_k}(\cdot, \cdot, t)\|_{L^1(\mathbb{R}_+ \times \Pi)}$  converge weakly-\* in  $L^{\infty}(0, \bar{t})$ .

To prove the property 4), we take a  $\bar{t} > 0$  and, remembering (36), rewrite (67) in the form

$$\int_{-A}^{0} \int_{0}^{\infty} \widetilde{\psi}_{m_{\varepsilon}^{*}(t)}(m) \sigma_{n}(m, q_{z}, t) dm dz \geq \|\sigma_{n}(\cdot, \cdot, t)\|_{L^{1}(\mathbb{R}_{+} \times \mathbb{R})} - \varepsilon.$$

As the left-hand side of this inequality is uniformly bounded with respect to  $t \in [0, \bar{t}]$ and to  $n \in \mathbb{N}$ , we can extract from  $\{\sigma_{n'}\}_{n'=1}^{\infty}$  a subsequence  $\{\sigma_{n'_k}\}_{k=1}^{\infty}$  such that the left-hand side of the latter inequality converges weakly-\* in  $L^{\infty}(0, \bar{t})$ , so that (see also the property 2)) (70) holds for almost all  $t \in [0, \bar{t}]$ .

In a usual way, from these extraction processes of a convergent subsequence, we can construct a subsequence  $\{\sigma_{n_k}\}_{k=1}^{\infty}$  of  $\{\sigma_n\}_{n=1}^{\infty}$  and  $\sigma \in L^{\infty}_{loc}(\mathbb{R}_+, L^1(\mathbb{R}_+ \times \Pi))$  which satisfy the conditions 1), 2), 3), and 4). The proposition 8.1 is proved.  $\Box$ 

We note that, if we interpret  $\Sigma_0(t) - \|\sigma(\cdot, \cdot, t)\|_{L^1(\mathbb{R}_+ \times \Pi)}$  as the exit of the liquid water from  $\Pi$ , which might be represented by

$$\int_{\mathbb{R}_+} \int_{-A}^{-A-tu(m)} \sigma(m,q,-\frac{q+A}{u(m)}) dq dm,$$

the inequality (70) is a weak form of the inequality

$$\int_{-A}^0 \int_0^\infty \widetilde{\psi}_{m_\varepsilon^*}(m) \sigma(m,q_z,t) dm dz \geq \Sigma_0(t) - \int_{\mathbb{R}_+} \int_{-A}^{-A-tu(m)} \sigma(m,q,-\frac{q+A}{u(m)}) dq dm - \varepsilon dt dm dz$$

and can be interpreted as absence of escape of the mass to infinity in a finite time.

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# On the 2-(25, 5, $\lambda$ ) design of zero-sum 5-sets in the Galois field GF(25)

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#### Abstract

In this paper we consider the incidence structure  $\mathcal{D} = (\mathcal{F}, \mathcal{B}_5^0)$ , where  $\mathcal{F}$  is the Galois field with 25 elements, and  $\mathcal{B}_5^0$  is the family of all 5-subsets of  $\mathcal{F}$ whose elements sum up to zero. It is known that  $\mathcal{D}$  is a 2-(25, 5, 71) design. Here we provide two alternative, direct proofs of this result and, moreover, we prove that  $\mathcal{D}$  is not a 3-design. Furthermore, if  $\mathcal{B}_5^x$  denotes the family of all 5subsets of  $\mathcal{F}$  whose elements sum up to a given element  $x \in \mathcal{F}$ , we also provide an alternative, direct proof that  $(\mathcal{F}, \mathcal{B}_5^x)$  is not a 2-design for  $x \neq 0$ . If  $\mathcal{B}_5^{x,*}$ denotes the family of all 5-subsets of  $\mathcal{F} \setminus \{0\}$  whose elements sum up to x, this also provides an alternative proof that the incidence structure  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_5^{x,*})$  is a 1-(24, 5, r) design if and only if x = 0.

Key words: Block designs, 2-designs, zero sums. AMS MSC 2010: 05B05, 11B75, 11P99.

### Contents

- 1 Introduction
- 2 The main results

### 1 Introduction

We recall that a t- $(v, k, \lambda_t)$  block design  $\mathcal{D} = (\mathcal{P}, \mathcal{B})$  is defined by a finite set  $\mathcal{P}$ with  $|\mathcal{P}| = v$ , the elements of which are called *points*, together with a family  $\mathcal{B}$  of subsets of  $\mathcal{P}$ , called *blocks*, such that each block contains exactly k points and any tdistinct points are contained exactly in  $\lambda_t$  common blocks (see [1], [6]). By letting  $b = |\mathcal{B}|$ , one finds the basic relation vr = bk in all 1-(v, k, r) designs. Moreover, it is well-known that, for any s < t, a t- $(v, k, \lambda_t)$  design is also a s- $(v, k, \lambda_s)$  design, with

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 $\lambda_s \binom{k-s}{t-s} = \lambda_t \binom{v-s}{t-s}$ . In particular, a 2- $(v, k, \lambda)$  design is also a 1-(v, k, r) design, with  $r(k-1) = \lambda(v-1)$ .

Examples of 2-designs can be easily constructed as follows. If  $\mathcal{F} = GF(9)$  is the Galois fields with 9 elements, and if  $\mathcal{B}_3^0$  denotes the family of all the 3-subsets of  $\mathcal{F}$  whose elements sum up to zero, then  $(\mathcal{F}, \mathcal{B}_0^3)$  is a 2-(9, 3, 1) design (that is, a *Steiner triple system* with 9 points). Similarly, if  $\mathcal{F} = GF(8)$  is the Galois fields with 8 elements, and if  $\mathcal{B}_3^{0,*}$  is the family of all the 3-subsets of  $\mathcal{F}^* = GF(8) \setminus \{0\}$  whose elements sum up to zero, then  $(\mathcal{F}^*, \mathcal{B}_3^{0,*})$  is a 2-(7, 3, 1) design (that is, a Steiner triple system with 7 points).

It is natural to ask what could be the possible generalizations of these two basic examples. On the one hand, one may ask what 2-designs  $\mathcal{D} = (\mathcal{P}, \mathcal{B})$  are additive, that is, can be embedded in a finite (additive) commutative group in such a way that the sum of the elements in every block is zero. In [4] and [5] we show that symmetric and affine 2-designs are all additive (up to trivial exceptions), and, moreover, we characterize the class of additive Steiner triple systems.

On the other hand, one may ask whether the family  $\mathcal{B}_k^0$  of all k-sets of elements, summing to zero in a finite (additive) commutative group G with v elements, is the family of blocks of a (necessarily additive) 2- $(v, k, \lambda)$  design. If this is the case, then one may also ask whether  $(G, \mathcal{B}_k^0)$  is also a 3-design. In [2] it is shown that if G is an elementary abelian 2-group, then  $(G, \mathcal{B}_4^0)$  is a 2- $(v, 4, \lambda)$  design with  $\lambda = \frac{v-2}{2}$ , and that, moreover,  $(G, \mathcal{B}_4^0)$  is a 3-(v, 4, 1) design with  $\frac{1}{4} {v \choose 3}$  blocks. In [3] it is shown that if G is an elementary abelian 5-group, then  $(G, \mathcal{B}_5^0)$  is a 2- $(v, 5, \lambda)$  design with

$$\lambda = \frac{v-3}{2} + \frac{(v-7)(v-5)}{6} \,.$$

In the special case where v = 25, this gives  $\lambda = 71$ . Finally, in [7] it is shown that if  $\mathcal{F}$  is a Galois field with  $v = p^d$  elements, where p is an odd prime, then  $(\mathcal{F}, \mathcal{B}_k^0)$  is a 2- $(v, k, \lambda)$  design for any k = mp, with

$$\lambda = \frac{1}{p^d} \binom{p^d - 2}{k - 2} + \frac{k - 1}{p^d} \binom{p^{d - 1} - 1}{m - 1}.$$

Again, in the case where  $p^d = 25$  and k = 5, the formula gives  $\lambda = 71$ .

In [3] the elementary abelian 5-group G is regarded as a vector space over GF(5), and it is noted that the affine group Aff(G) acts 2-homogeneously on G, which allows one to conclude that  $(G, \mathcal{B}_5^0)$  is a 2-design by Proposition 4.6 in [1, III, p. 175]. In [7] it is shown that  $(\mathcal{F}, \mathcal{B}_k^0)$  is a 2-design, for any k multiple of p, as a consequence of the fact that  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_k^{0,*})$  is a 1-design (see Lemma 3.3 and Theorem 3.5), where  $\mathcal{B}_k^{0,*}$ is the family of all the k-subsets of  $\mathcal{F}^* = \mathcal{F} \setminus \{0\}$  whose elements sum up to zero. In both cases, the authors resort to an indirect proof to show that the considered incidence structure is a 2-design.

In this paper we give two direct proofs that  $(\mathcal{F}, \mathcal{B}_5^0)$  is a 2-(25, 5, 71) design, where  $\mathcal{F}$  is the Galois field GF(25). We also prove that  $(\mathcal{F}, \mathcal{B}_5^0)$  is not a 3-design. Moreover,

if we denote by  $\mathcal{B}_5^x$  the family of all 5-subsets of  $\mathcal{F}$  whose elements sum up to a given element  $x \in \mathcal{F}$ , we also provide an alternative, direct proof that  $(\mathcal{F}, \mathcal{B}_5^x)$  is a 2-design if and only if x = 0 (see [7, Theorem 3.7]), by giving an explicit formula, for any distinct  $y, z \in \mathcal{F}$ , of the number of 5-sets in  $\mathcal{B}_5^x$  containing y and z.

#### 2 The main results

Let  $\mathcal{F}$  be the Galois field GF(25) with 25 elements. Also, let  $\mathcal{F}^* = \mathcal{F} \setminus \{0\}$ .

**Definition 2.1.** For any  $1 \le k \le 5$ , and for any  $x \in \mathcal{F}$ , let  $\mathcal{B}_k^x$  (respectively,  $\mathcal{B}_k^{x,*}$ ) be the family of all the k-subsets of  $\mathcal{F}$  (respectively, of  $\mathcal{F}^*$ ) whose elements sum up to x. For any  $x \in \mathcal{F}$ , and for any distinct  $y, z \in \mathcal{F}$ , let  $r_5^x(y, z)$  be the number of 5-sets in  $\mathcal{B}_5^x$  containing y and z.

**Theorem 2.1.** Let  $\mathcal{F}$  be the Galois field GF(25). Then the incidence structure  $(\mathcal{F}, \mathcal{B}_5^0)$  is a 2-(25, 5, 71) design with 2130 blocks and replication number 426. Equivalently, the incidence structure  $(\mathcal{F}\setminus\{0\}, \mathcal{B}_4^{0,*})$  is a 1-(24, 4, 71) design with 426 blocks.

*Proof.* Let y, z be any two elements of  $\mathcal{F}$  with  $y \neq z$ . We claim that the number  $r_5^0(y, z)$  of 5-sets in  $\mathcal{B}_5^0$  containing y and z is equal exactly to 71.

First proof. Note that the map

$$\{y, z, x_1, x_2, x_3\} \mapsto \{y - z, 0, x_1 - z, x_2 - z, x_3 - z\}$$

is a one-to-one correspondence between the 5-sets in  $\mathcal{B}_5^0$  containing y and z and the 5-sets in  $\mathcal{B}_5^0$  containing y - z and 0. Hence we may assume that z = 0, thus it suffices to show that, for any nonzero y in  $\mathcal{F}$ , there exist exactly 71 5-sets in  $\mathcal{B}_5^0$  containing y and 0. This is the same as showing that, for any y in  $\mathcal{F} \setminus \{0\}$ , there exist exactly 71 4-sets in  $\mathcal{B}_4^{0,*}$  containing y, which, in turn, is equivalent to saying that  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_4^{0,*})$  is a 1-(24, 4, 71) design.

Now let y be a fixed element in  $\mathcal{F} \setminus \{0\}$ . Then the 4-sets in  $\mathcal{B}_4^{0,*}$  containing y are precisely all the sets of the form

$$\{y, a, b, -y - a - b\},\$$

where a and b are two distinct elements in  $\mathcal{F} \setminus \{0, y\}$ , and where

$$-y - a - b \notin \{0, y, a, b\}.$$
 (1)

By solving the equations -y - a - b = 0, -y - a - b = y, -y - a - b = a, and -y - a - b = b, one finds, respectively, b = -y - a, b = -2y - a, b = -y - 2a, and  $b = \frac{1}{2}(-y - a) = 3(-y - a) = 2y + 2a$ . Hence condition (1) is equivalent to

$$b \notin \{-y-a, -2y-a, -y-2a, 2y+2a\}.$$

Therefore the set  $\{y, a, b, -y - a - b\}$  is in  $\mathcal{B}_4^{0,*}$  if and only if a is an element of  $\mathcal{F} \setminus \{0\}$  such that  $a \neq y$  (which gives precisely 23 possible choices for a) and b is an element of  $\mathcal{F} \setminus \{0\}$  such that

$$b \notin A_a = \{y, a, -y - a, -2y - a, -y - 2a, 2y + 2a\}.$$
(2)

Hence the number of 4-sets in  $\mathcal{B}_4^{0,*}$  containing y depends on the cardinalities of the sets  $A_a$  defined in (2). Given a in  $\mathcal{F} \setminus \{0, y\}$ , it is immediate that if either  $0 \in A_a$  or  $|A_a| < 6$ , then a is necessarily a multiple of y, that is,  $a \in \{2y, 3y, 4y\}$  (for example, -y - 2a = 0 if and only if a = 2y, and -y - a = y if and only if a = 3y). Therefore,  $A_a \subseteq \mathcal{F} \setminus \{0\}$  and  $|A_a| = 6$  for all a in  $\mathcal{F} \setminus \{0, y, 2y, 3y, 4y\}$ . This happens for 20 possible choices of a, each of which gives in turn 18 possible choices for b. On the other hand, one easily finds by direct inspection that

$$(\forall a \in \{2y, 3y, 4y\}) \quad A_a = \{0, y, a\}.$$

For instance, for a = 2y, it is immediate that  $A_a = \{0, y, 2y\}$ . This adds another 3 possible choices of a, each of which gives in turn 22 possible choices for b. This shows that the number of 4-sets in  $\mathcal{B}_4^{0,*}$  containing y is equal to

$$\frac{20\cdot 18 + 3\cdot 22}{3!} = 71,$$

as claimed. Hence  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_4^{0,*})$  is a 1-(24, 4, 71) design, and  $(\mathcal{F}, \mathcal{B}_5^0)$  is a 2- $(v, k, \lambda)$  design with v = 25, k = 5, and  $\lambda = 71$ .

Second proof. Note that  $r_5^0(y, z)$  is equal to the number of 3-sets in  $\mathcal{B}_3^{-y-z}$  that contain neither y nor z. If we denote by  $\mathcal{B}_3^{-y-z}(y)$  (resp.  $\mathcal{B}_3^{-y-z}(z)$ , resp.  $\mathcal{B}_3^{-y-z}(y, z)$ ) the family of all 3-sets in  $\mathcal{B}_3^{-y-z}$  that contain y (resp. z, resp. y and z), then, by the inclusion-exclusion principle,

$$r_5^0(y,z) = |\mathcal{B}_3^{-y-z}| - |\mathcal{B}_3^{-y-z}(y)| - |\mathcal{B}_3^{-y-z}(z)| + |\mathcal{B}_3^{-y-z}(y,z)|.$$

Now, by formula (3) in [7],

$$|\mathcal{B}_3^{-y-z}| = \frac{1}{25} \binom{25}{3} = 92.$$

Moreover,  $|\mathcal{B}_3^{-y-z}(y)|$  is equal to the number of all (unordered) triples of the form  $\{y, a, -2y - z - a\}$  whose elements are mutually distinct. This happens if and only if  $a \in \mathcal{F} \setminus \{y, 2y - z, 2z - y\}$ , where  $\{y, 2y - z, 2z - y\}$  is a 3-subset of  $\mathcal{F}$ , since  $y \neq z$ . Hence

$$|\mathcal{B}_3^{-y-z}(y)| = \frac{25-3}{2} = 11.$$

Similarly,  $|\mathcal{B}_3^{-y-z}(z)| = 11$ . Finally,  $\{y, z, -2y - 2z\}$  is a 3-subset of  $\mathcal{F}$ , as well, since  $y \neq z$ . Hence

$$|\mathcal{B}_3^{-y-z}(y,z)| = |\{\{y, z, -2y - 2z\}\}| = 1.$$

Therefore

$$r_5^0(y,z) = 92 - 11 - 11 + 1 = 71,$$

as claimed.

If r and b denote, respectively, the replication number and the number of blocks of  $(\mathcal{F}, \mathcal{B}_5^0)$ , then it follows from the basic relations  $\lambda(v-1) = r(k-1)$  and bk = rv that r = 426 and b = 2130. Similarly, the latter basic relation also shows that there are precisely 426 blocks in  $(\mathcal{F}\setminus\{0\}, \mathcal{B}_4^{0,*})$ . This can also be deduced from the fact that  $(\mathcal{F}\setminus\{0\}, \mathcal{B}_4^{0,*})$  is precisely the derived design at 0 of  $(\mathcal{F}, \mathcal{B}_5^0)$ , whose replication number is equal to 426.

This completes the proof of the Theorem.

**Corollary 2.1.** The incidence structure  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_5^{0,*})$  is a 1-(24, 5, 355) design with 1704 blocks.

*Proof.* By the Theorem above,  $(\mathcal{F}, \mathcal{B}_5^0)$  is a 2-(25, 5,  $\lambda$ ) design with  $\lambda = 71$  and replication number r = 426. Hence, by Lemma 3.3 in [7],  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_5^{0,*})$  is a 1-(24, 5,  $r^*$ ) design with  $r^* = r - \lambda = 355$ . If  $b^*$  is the number of blocks in  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_5^{0,*})$ , then the basic relation  $b^*5 = r^*24$  yields  $b^* = 1704$ . Alternatively, the value of  $b^*$  may be computed directly by means of formula (6) in [7].

**Proposition 2.1.** The 2-design  $(\mathcal{F}, \mathcal{B}_5^0)$  is not a 3-design. Moreover, the 1-designs  $(\mathcal{F}\setminus\{0\}, \mathcal{B}_4^{0,*})$  and  $(\mathcal{F}\setminus\{0\}, \mathcal{B}_5^{0,*})$  are not 2-designs.

*Proof.* Let y be a fixed element in  $\mathcal{F}\setminus\{0\}$ . We first wish to count the number of 5-sets in  $\mathcal{B}_5^0$  containing 0, y, and -y. If  $\{0, y, -y, a, b\}$  is any such 5-set, then  $\{a, b\}$  is a pair of opposite elements in  $\mathcal{F}\setminus\{0, y, -y\}$ , and conversely. Hence the number of 5-sets in  $\mathcal{B}_5^0$  containing 0, y, and -y is equal to  $\frac{25-3}{2} = 11$ .

Now let z be any element in  $\mathcal{F}\setminus\{0, y, 2y, 3y, 4y\}$ . Any 5-sets in  $\mathcal{B}_5^0$  containing 0, y, and z is of the form  $\{0, y, z, a, b\}$ , with a+b=-y-z, hence  $a \notin \{-y-z, \frac{1}{2}(-y-z)\}$ . Since -y-z and  $\frac{1}{2}(-y-z)$  are two distinct elements in  $\mathcal{F}\setminus\{0, y, z\}$ , the number of 5-sets in  $\mathcal{B}_5^0$  containing 0, y, and z is equal at most to  $\frac{25-5}{2} = 10$ . Hence, by definition,  $(\mathcal{F}, \mathcal{B}_5^0)$  is not a 3-design.

It follows immediately that  $(\mathcal{F}\setminus\{0\}, \mathcal{B}_4^{0,*})$  is not a 2-design, since for any pair of distinct elements y and z in  $\mathcal{F}\setminus\{0\}$ , the number of 4-sets in  $\mathcal{B}_4^{0,*}$  containing y and z is equal to the number of 5-sets in  $\mathcal{B}_5^0$  containing 0, y, and z. Similarly,  $(\mathcal{F}\setminus\{0\}, \mathcal{B}_5^{0,*})$  is not a 2-design, since for any pair of distinct elements y and z in  $\mathcal{F}\setminus\{0\}$ , the number of 5-sets in  $\mathcal{B}_5^{0,*}$  containing y and z is equal to the number of 5-sets in  $\mathcal{B}_5^0$  containing y and z is equal to the number of 5-sets in  $\mathcal{B}_5^0$  containing y and z is equal to the number of 5-sets in  $\mathcal{B}_5^0$  containing y and z.

Alternatively, all these results can be proved by showing that the designs involved do not satisfy the necessary conditions on the parameters. For instance, if the 2- $(v, k, \lambda)$  design  $(\mathcal{F}, \mathcal{B}_5^0)$  were also a 3- $(v, k, \lambda_3)$  design, then it would satisfy the basic relation  $\lambda(k-2) = \lambda_3(v-2)$ , but for v = 25, k = 5, and  $\lambda = 71$  there exists no positive integer  $\lambda_3$  satisfying the equality. The cases of  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_4^{0,*})$  and  $(\mathcal{F} \setminus \{0\}, \mathcal{B}_5^{0,*})$  are dealt with similarly.

**Proposition 2.2.** Let  $\mathcal{F}$  be the Galois field GF(25). Then, for any  $x \in \mathcal{F} \setminus \{0\}$ , the incidence structure  $(\mathcal{F}, \mathcal{B}_5^x)$  is a 1-design but not a 2-design. More precisely, for any  $x \in \mathcal{F} \setminus \{0\}$ , and for any y, z distinct elements of  $\mathcal{F}$ ,

$$r_5^x(y,z) = \begin{cases} 70 & \text{if } z \in \{y+x, y+2x, y+3x, y+4x\} \\ \\ 71 & \text{if } z \in \mathcal{F} \setminus \{y+x, y+2x, y+3x, y+4x\}. \end{cases}$$

*Proof.* Let x be a given element in  $\mathcal{F} \setminus \{0\}$ . For any y in  $\mathcal{F}$ , the map

 $\{y, x_1, x_2, x_3, x_4\} \mapsto \{0, x_1 - y, x_2 - y, x_3 - y, x_4 - y\}$ 

is a one-to-one correspondence between the 5-sets in  $\mathcal{B}_5^x$  containing y and the 5-sets in  $\mathcal{B}_5^x$  containing 0. Hence the number of 5-sets in  $\mathcal{B}_5^x$  containing y is constant in y, that is, by definition,  $(\mathcal{F}, \mathcal{B}_5^x)$  is a 1-design.

Let y, z be two given distinct elements in  $\mathcal{F}$ . The number  $r_5^x(y, z)$  of 5-sets in  $\mathcal{B}_5^x$  containing y and z is equal to the number of 3-sets in  $\mathcal{B}_3^{x^{-y-z}}$  that contain neither y nor z. If we denote by  $\mathcal{B}_3^{x^{-y-z}}(y)$  (resp.  $\mathcal{B}_3^{x^{-y-z}}(z)$ , resp.  $\mathcal{B}_3^{x^{-y-z}}(y, z)$ ) the family of all 3-sets in  $\mathcal{B}_3^{x^{-y-z}}$  that contain y (resp. z, resp. y and z), then, by the inclusion-exclusion principle,

$$r_5^x(y,z) = |\mathcal{B}_3^{x-y-z}| - |\mathcal{B}_3^{x-y-z}(y)| - |\mathcal{B}_3^{x-y-z}(z)| + |\mathcal{B}_3^{x-y-z}(y,z)|.$$
(3)

Now, by formula (3) in [7],

$$|\mathcal{B}_3^{x-y-z}| = \frac{1}{25} \binom{25}{3} = 92.$$

Moreover,  $|\mathcal{B}_3^{x-y-z}(y)|$  is equal to the number of all (unordered) triples of the form  $\{y, a, x-2y-z-a\}$  whose elements are mutually distinct. This happens if and only if  $a \in \mathcal{F} \setminus \{y, x+2y-z, 3x+2z-y\}$ . Now

$$\{y, x + 2y - z, 3x + 2z - y\} = \begin{cases} 1 & \text{if } z = y + x \\ 3 & \text{if } z \neq y + x. \end{cases}$$

Hence

$$|\mathcal{B}_{3}^{x-y-z}(y)| = \begin{cases} \frac{25-1}{2} = 12 & \text{if } z = y+x \\ \frac{25-3}{2} = 11 & \text{if } z \neq y+x. \end{cases}$$

Similarly,

$$|\mathcal{B}_{3}^{x-y-z}(z)| = \begin{cases} 12 & \text{if } z = y - x \ (= y + 4x) \\ 11 & \text{if } z \neq y - x \ (= y + 4x). \end{cases}$$

Finally, the (unordered) triple  $\{y, z, x-2y-2z\}$  (containing y and z and summing up to x - y - z) is a 3-set if and only if  $z \in \mathcal{F} \setminus \{y + 2x, y + 3x\}$ , hence

$$|\mathcal{B}_{3}^{x-y-z}(y,z)| = \begin{cases} 0 & \text{if } z \in \{y+2x, y+3x\} \\ 1 & \text{if } z \in \mathcal{F} \setminus \{y+2x, y+3x\} \end{cases}$$

Therefore, by (3),

$$r_5^x(y,z) = \begin{cases} 92 - 11 - 12 + 1 = 70 & \text{if } z \in \{y + x, y + 4x\} \\ 92 - 11 - 11 + 0 = 70 & \text{if } z \in \{y + 2x, y + 3x\} \\ 92 - 11 - 11 + 1 = 71 & \text{if } z \in \mathcal{F} \setminus \{y + x, y + 2x, y + 3x, y + 4x\}. \end{cases}$$

This completes the proof of the Proposition.

**Remark 2.1.** Let x be a given element in  $\mathcal{F}\setminus\{0\}$ . Then  $(\mathcal{F}, \mathcal{B}_5^x)$  is not a 2-design by Proposition 2.2, but we may write a formula that is analogous to the basic relation

$$\lambda(v-1) = r(k-1)$$

valid for 2-designs. Indeed, by Theorem 3.1 and formula (5) in [7],  $(\mathcal{F}, \mathcal{B}_5^x)$  is a 1-(v, k, r) design with v = 25, k = 5, and r = 425. In particular, the relation  $\lambda(v-1) = r(k-1)$ , that is,  $\lambda \cdot 24 = 425 \cdot 4$ , cannot be satisfied by any positive integer  $\lambda$ , thereby giving another proof that  $(\mathcal{F}, \mathcal{B}_5^x)$  is not a 2-design.

Moreover, let y be a given element in  $\mathcal{F}$ . With a double-counting argument, we wish to count, with repetition, the points in  $\mathcal{F} \setminus \{y\}$  that lie in the r blocks in  $\mathcal{B}_5^x$  containing y. On the one hand, such number is equal to the number of blocks times the number of points different from y in each block, that is,  $r \cdot (k-1)$ . On the other hand, by Proposition 2.2 above, each element z in  $\{y + x, y + 2x, y + 3x, y + 4x\}$  belongs to precisely  $\lambda_1 = 70$  blocks containing y, whereas each element z in  $\mathcal{F} \setminus \{y, y + x, y + 2x, y + 3x, y + 4x\}$  belongs to precisely  $\lambda_2 = 71$  blocks containing y. Hence

$$\lambda_1 \cdot 4 + \lambda_2 \cdot 20 = r(k-1),$$

that is, 20 + 4 = v - 1, and  $70 \cdot 4 + 71 \cdot 20 = 425 \cdot 4$ .

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# Colombeau Algebras and convolutions generated by self-adjoint operators

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#### Abstract

The role of convolution of functions in the construction of Colombeau algebras of generalized functions is analyzed, with particular referring to the commutative relation with the derivation operator. The possibility to consider the A-convolution, with A an unbounded self-adjoint operator in Hilbert space, is discussed.

 $Key\ words:$  Colombeau algebras, convolution, unbounded self-adjoint operator. MSC: 46F30, 47A05.

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# 1 Introduction

As known, multiplication of distributions is defined only in particular circumstances. However in several applications (as, for example, partial differential equations and physics), a correct definition of multiplication of distributions is of crucial

importance. In this sense the literature include several situations of "impossibility" results" (you can see in [14, 8] for a review). One of them is due to L. Schwartz, who consider the question if it is possible to define an associative algebra that it contains distributions, such that the derivation operator extends the usual derivation of distributions  $\mathcal{D}'(\Omega)$ , and such that the product becomes the usual multiplication between continuous functions. In other words, in some circumstances recurring in partial differential equation theory, it is natural to ask yourself if there exists an associative algebra  $\mathcal{A}$  of "generalized functions" such that: 1) it contains the identity and  $\mathcal{D}'(\Omega)$ is linearly embedded; 2) there exists a derivation operator  $\hat{\partial}$  (i.e. an operator with Leibnitz property) such that 3) restricted to  $\mathcal{D}'(\Omega)$  become the usual (distributional) derivative, 4) the product in  $\mathcal{A}$  becomes the usual pointwise product between continuous functions. The incompatibility of the coexistence at the same time of these conditions has been proved by L. Schwartz on 1954. Subsequently, several approach to define an algebra of generalized functions according with the "impossibility result" are considered. For a detailed review, you can se [14, 8, 26] and references therein. In this paper is considered the approach due to J.F. Colombeau, who, in [3, 2], defines an associative, differential algebra that contains distributions and such that the properties 1)-3) are maintained, but the condition 4) is modified by the 4b), where it is the product on the space  $C^{\infty}(\Omega)$  of infinite differentiable functions that coincides with the usual product of functions. Such algebras are called Colombeau algebras, usually denoted by  $\mathcal{G}$ . As stated in [14], the properties 1),2), 3), 4b) are "optimal, that is, it is not possible to do better in the setting of associative differential algebras". In defining the Colombeau algebra, a fundamental role is played by the convolution, that linearly embeds the space of the continuous functions and of the distributions in  $\mathcal{G}$ . Starting from an idea in [16], in this paper is studied the possibility to consider the Aconvolution, where A is an unbounded self-adjoint operator in Hilbert space and that become the convolutions of functions for a particular choice of A. The A-convolution was defined and their properties are studied by C. Trapani and the author in [26], [16], [27], [23], [24], [28]. The paper is organized as follows. In section 2, the definition and the construction of Colombeau algebras is reviewed, in Section 3 is described the general construction scheme, putting in evidence the interplay between commutativity of diagrams w.r. to the derivation and the embedding  $\iota$  of distributions in  $\mathcal{G}$ . In Section 3, is reviewed the definition and the properties of the A-convolution and finally is considered its extension to a general scheme of construction of Colombeau.

In this paper, for simplicity, we assume that the domain of the independent variables is  $\Omega = \mathbb{R}^n$  and the following notations are adopted: a Schwartz distribution and test functions are denoted, respectively, by Greek capital letters:  $\Psi, \Phi \ldots \in \mathcal{D}'(\mathbb{R}^n)$  and lowercase Greek letters:  $\psi, \phi \ldots \in \mathcal{D}(\mathbb{R}^n)$ ; the set of positive integer numbers is denoted by  $\mathbb{N}$ , while  $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$ ;  $\bar{k} := (k_1, k_2, \ldots, k_n)$  is a multi-index, and  $|\bar{k}| := k_1 + k_2 + \ldots + k_n$ , for  $x \in \mathbb{R}^n, x^k := x_1^{k_1} x_2^{k_2} \cdots x_n^{k_n}$ .

# 2 Colombeau algebras

The idea is to define an algebra of generalized functions as opportune classes of equivalence of linear maps  $\mathcal{D}(\mathbb{R}^n) \to C^{\infty}(\mathbb{R}^n)$ . Let consider the subsets  $\mathcal{A}_q$  of  $\mathcal{D}(\mathbb{R}^n)$  so defined:  $\mathcal{A}_0 := \{\phi \in \mathcal{D}(\mathbb{R}^n) : \int_{\mathbb{R}^n} \phi(x) dx = 1\}$ , and for  $q \in \mathbb{N}$ ,  $\mathcal{A}_q := \{\phi \in \mathcal{A}_0 : \int_{\mathbb{R}^n} x^k \phi(x) dx = 0, \quad 1 \leq |k| \leq q\}$ . We define  $\phi_{\epsilon} \in \mathcal{D}$  for  $\epsilon \in \mathbb{R}^+$  by  $\phi_{\epsilon}(x) = \frac{1}{\epsilon^n} \phi(\frac{x}{\epsilon})$ . One has that  $\phi_{\epsilon}(x) \in \mathcal{A}_q$  for all  $\epsilon > 0$  if, and only if  $\phi \in \mathcal{A}_q$ . Let us consider the space:

 $\mathcal{E}(\mathbb{R}^n) := C^{\infty}(\mathbb{R}^n)^{\mathcal{A}_0} = \{ R : \mathcal{A}_0 \times \mathbb{R}^n \to \mathbb{C}, \ R(\phi, x) \text{ is smooth in the second variable} \}.$ 

This means that for all  $\phi \in \mathcal{A}_0$ , the map  $R^{\phi} : x \mapsto R(\phi, x)$  is a function in  $C^{\infty}(\mathbb{R}^n)$ . In [14] the maps  $\phi \to R^{\phi}$  are denoted by  $u : \mathcal{A}_0 \to C^{\infty}(\mathbb{R}^n)$ , but here, until otherwise specified, is adopted the notations of [2, 8]. The space  $\mathcal{E}(\mathbb{R}^n)$  is a differential algebra, w.r. to the product of functions and the usual derivative on  $R(\phi, x)$ . However the set  $\mathcal{E}(\mathbb{R}^n)$  is "too large" to define a quotient w.r. to a nontrivial ideal. So, it is usual to define a subalgebra  $\mathcal{E}_M(\mathbb{R}^n)$  of  $\mathcal{E}(\mathbb{R}^n)$ . If  $K \subset \mathbb{R}^n$  denote a compact set, then  $\mathcal{E}_M(\mathbb{R}^n)$  is a subset of  $\mathcal{E}(\mathbb{R}^n)$  such that:

$$R \in \mathcal{E}(\mathbb{R}^n) : \forall K \subset \mathbb{R}^n, \ \forall \alpha \in \mathbb{N}_0^n, \exists m \in \mathbb{N} : \ \forall \phi \in \mathcal{A}_m(\mathbb{R}^n)$$
  
$$\exists c > 0, \ \eta > 0 : \sup_{x \in K} |\partial^{\alpha} R(\phi_{\epsilon}, x)| \le c\epsilon^{-m}, 0 < \epsilon < \eta.$$
  
(2.1)

The space  $\mathcal{E}_M(\mathbb{R}^n)$  is a differential subalgebra of  $\mathcal{E}(\mathbb{R}^n)$  and its elements are called *moderates.* Further, let us define the following ideal of  $\mathcal{E}_M(\mathbb{R}^n)$ :  $\forall K \subset \mathbb{R}^n, \ \forall \alpha \in \mathbb{N}_0^n, \ \exists m \in \mathbb{N} : \ \forall \phi \in \mathcal{A}_q(\mathbb{R}^n), \ q \geq m$ , it holds:

$$\exists c > 0, \ \exists \eta > 0: \ \sup_{x \in K} |\partial^{\alpha} R(\phi_{\epsilon}, x)| \le c \epsilon^{q-m}, \ 0 < \epsilon < \eta.$$

$$(2.2)$$

Then  $\mathcal{N}(\mathbb{R}^n)$  is a subalgebra  $\mathcal{E}(\mathbb{R}^n)$  closed by per differentiation, but is not ideal of  $\mathcal{E}(\mathbb{R}^n)$  (see [3, 2, 14]). However, it results that  $\mathcal{E}_M(\mathbb{R}^n)$  is a subalgebra in  $\mathcal{E}(\mathbb{R}^n)$  and  $\mathcal{N}(\mathbb{R}^n)$  is an ideal of  $\mathcal{E}_M(\mathbb{R}^n)$ . Finally, the algebra of generalized functions of Colombeau is defined as:

$$\mathcal{G}(\mathbb{R}^n) = \mathcal{E}_M(\mathbb{R}^n) / \mathcal{N}(\mathbb{R}^n).$$

It follows that  $\mathcal{G}(\mathbb{R}^n)$  is an associative, commutative algebra.

Remark 2.1. The choice of the space  $\mathcal{E}(\mathbb{R}^n)$  is not unique in literature. For example, another definition is  $\mathcal{E}(\mathbb{R}^n) := C^{\infty}(\mathbb{R}^n)^I$ , with I = (0, 1]. In this case, it is defined a "variant", otherwise said a "Colombeau-type" algebra of generalized functions (wellknown as *special* Colombeau algebra, see [8]). The possibility to unify the variants of Colombeau algebras is discussed in [6].

Remark 2.2. The definitions (2.1) and (2.2) respectively of  $\mathcal{E}_M$  and  $\mathcal{N}$  are based on the behavior of  $R(\phi_{\epsilon}, x)$  with respect  $\epsilon > 0$  for  $\phi \in A_q$ . However, the definitions of  $\mathcal{E}_M$  and  $\mathcal{N}$  are not univocal in literature. Here are considered that are defined in [14]. But, for

example, in [8] asymptotic conditions for  $\epsilon \to 0$  using Landau big-O are considered. For an approach for a definition of Colombeau algebras without asymptotic estimates see [13].

Remark 2.3. As remarked in [18], the algebra  $\mathcal{G}$  is not a completion w.r. to a vectors space topology on  $C^{\infty}(\mathbb{R}^n)$  and  $R(\phi_{\epsilon}, x), \epsilon > 0, \phi \in \mathcal{A}_q$  have not to be intended as a "Cauchy net". In this sense, an order structure have to be defined. See [6] for a discussion in this direction.

We have the following inclusions:

$$\partial^p \mathcal{N}(\mathbb{R}^n) \subset \mathcal{N}(\mathbb{R}^n), \quad \partial^p \mathcal{E}_M(\mathbb{R}^n) \subset \mathcal{E}_M(\mathbb{R}^n), \quad \forall p \in \mathbb{N}.$$

Then we can define the partial derivative operator  $\widehat{\partial} : \mathcal{G} \to \mathcal{G}$  such that  $\widehat{\partial}^p(R + \mathcal{N}) = \partial^p R + \mathcal{N}$ . Let us show the following embedding relations:

$$C^{\infty}(\mathbb{R}^n) \subset \ldots \subset C^0(\mathbb{R}^n) \subset \mathcal{D}'(\mathbb{R}^n) \subset \mathcal{G}(\mathbb{R}^n).$$

The relation of " $\subset$ " inclusion of sets is here intended as injective, linear embedding. To embed  $C^{\infty}(\mathbb{R}^n)$  in  $\mathcal{G}(\mathbb{R}^n)$ , we consider the following map  $\sigma : C^{\infty}(\mathbb{R}^n) \to \mathcal{E}_M(\mathbb{R}^n)$  so defined:

$$C^{\infty} \ni f \mapsto R + \mathcal{N}, \quad R = R(\phi, x) := f(x), \quad \phi \in \mathcal{A}_0.$$
 (2.3)

To prove that the map is well defined, we prove that:

$$f \mapsto R \in \mathcal{E}_M(\mathbb{R}^n)$$

considering that:

$$\partial^p R(\phi_{\epsilon}, x) = \partial^p f(x), p \in \mathbb{N}^n, \phi \in \mathcal{A}_0, \epsilon > 0, x \in \mathbb{R}^n$$

the condition (2.1) is satisfied. Furthermore, the mapping (2.3) is injective: in fact from (2.2) we have that  $f \in C^{\infty}(\mathbb{R}^n), R \in \mathcal{N}(\mathbb{R}^n)$  imply f = 0. It follows that the map  $\sigma : C^{\infty} \to \mathcal{G}$  defined by (2.3) is an algebra homomorphism. The embedding  $\sigma$  is called *standard copy* in [14]. The operator  $\partial^p$  on  $\mathcal{G}(\mathbb{R}^n)$  restricted on  $C^{\infty}(\mathbb{R}^n)$ coincide with the usual partial derivative of functions. We have proved the following:

**Theorem 2.4.** The embedding defined in  $\sigma : C^{\infty}(\mathbb{R}^n) \to \mathcal{G}(\mathbb{R}^n)$  is an embedding differential algebra and the function  $1 \in C^{\infty}(\mathbb{R}^n)$  is the unit in  $\mathcal{G}(\mathbb{R}^n)$  (i.e.  $\sigma(1) = 1$ ).

It is noteworthy that the embedding of  $C^{\infty}(\mathbb{R}^n)$  in  $\mathcal{G}(\mathbb{R}^n)$  with the standard copy  $\sigma$  implies the fact that  $C^{\infty}(\mathbb{R}^n)$  is embedded in Colombeau algebra with the usual product of functions, compatibly with Schwartz result, as mentioned in the introduction. The next step is to define the embedding  $C^0(\mathbb{R}^n) \subset \mathcal{G}(\mathbb{R}^n)$ . Clearly, in this case, the standard copy don't work. For simplicity, let us consider in the case n = 1, and let us define the following map:  $\iota : C^0(\mathbb{R}) \to \mathcal{G}(\mathbb{R})$  by:

$$C^0 \ni f \mapsto R_f + \mathcal{N} \in \mathcal{G}, \quad R_f \equiv R_f(\phi, x) =: (f * \phi)(x) := \int_{\mathbb{R}} f(x - y)\phi(y)dy.$$

In order to prove that the map  $\iota$  is well defined, we have to show that  $R_f \in \mathcal{E}_M$ . As known, from convolution properties one has  $R_f \in \mathcal{E}$ . Then, we have:

$$\partial^p R_f(\phi_\epsilon, x) = \frac{(-1)^p}{\epsilon^{1+p}} \int f(y) \phi\Big(\frac{x-y}{\epsilon}\Big) dy$$

and the condition (2.1) is satisfied. The map  $\iota$  is injective, in fact:  $f \in C^0(\mathbb{R}), R_f \in \mathcal{N}(\mathbb{R})$  imply f = 0. Then  $\iota : C^0(\mathbb{R}) \to \mathcal{G}(\mathbb{R})$  is a linear embedding of vectors spaces. The map  $\iota$  can be extended to define the following embedding:

$$\mathcal{D}'(\mathbb{R})\subset \mathcal{G}(\mathbb{R})$$

by:

 $\mathcal{D}'(\mathbb{R}) \ni \Phi \mapsto R_{\Phi} + \mathcal{N} \in \mathcal{G}(\mathbb{R}), \quad R_{\Phi} \equiv R_{\Phi}(\phi, x) := (\Phi * \phi)(x) = \Phi_y(\phi(x-y)) = \Phi(\tau_x \check{\phi}).$ 

Since  $(\Phi * \phi)(x) \in C^{\infty}(\mathbb{R})$ , this imply obviously that  $(\Phi * \phi)(x) \in \mathcal{E}(\mathbb{R})$ . Furthermore:

$$\partial^p R_{\Phi}(\phi_{\epsilon}, x) = \Phi_y(\partial^p \phi_{\epsilon}(x-y)), p \in \mathbb{N}, \phi \in \mathcal{A}_0, \epsilon > 0$$

then condition (2.1) is satisfied and the map  $\iota : \mathcal{D}'(\mathbb{R}) \to \mathcal{E}_M(\mathbb{R})$  given by  $\iota : \Phi \mapsto R_{\Phi}$ , is well defined. At this point, one could to note that the embedding  $\sigma : C^{\infty}(\mathbb{R}) \to \mathcal{E}_M(\mathbb{R})$  is different from  $\iota : C^{\infty}(\mathbb{R}) \to \mathcal{E}_M(\mathbb{R})$ , since  $f(x) \neq \int_{-\infty}^{\infty} f(x-y)\phi(y)dy$ . However it holds the following:

**Proposition 2.5.** If  $f \in C^{\infty}(\mathbb{R})$ , then  $\iota(f) - \sigma(f) \in \mathcal{N}(\mathbb{R})$ .

We sketch the proof to put in evidence the role of the sets  $\mathcal{A}_q(\mathbb{R})$  and of the convolution of functions.

*Proof.* The argument is based on the use of the Taylor formula (with Lagrange rest): there exists  $\xi$  between x and  $x - \epsilon y$  such that:

$$g(x) := (f * \phi_{\epsilon} - f)(x) = \int_{-\infty}^{+\infty} (f(x - \epsilon y) - f(x))\phi(y)dy =$$
$$= \sum_{j=1}^{q} f^{(j)}(x) \int_{-\infty}^{+\infty} \frac{(-\epsilon y)^{j}}{j!}\phi(y)dy + \int_{-\infty}^{+\infty} \frac{(-\epsilon y)^{q+1}}{(q+1)!} f^{(q+1)}(\xi)\phi(y)dy$$

The terms in the sum vanish if  $\phi \in \mathcal{A}_q$ . Furthermore, if  $x \in K$  (compact), the second term is estimated by  $C\epsilon^{q+1}$ . A similar result can be obtained considering  $\partial^p g(x) := (\partial^p f * \phi_\epsilon - \partial^p f)(x)$ . Then, it holds condition (2.2), so we have that  $g \in \mathcal{N}(\mathbb{R})$ .

#### 3 A general construction scheme

Let us resume here a general scheme of construction of Colombeau algebras (see [7, 8] for more details).

- (a) To define a space  $\mathcal{E}$  (called *basic space*) such that  $\mathcal{E}$  is an associative algebra with unit; a *linear embedding of vector spaces*:  $\iota : \mathcal{D}'(\mathbb{R}^n) \to \mathcal{E}$ ; an *algebra* homomorphism embedding:  $\sigma : C^{\infty}(\mathbb{R}^n) \to \mathcal{E}$  such that  $\sigma(1) = e$ ;
- (b) to define a derivation  $\widehat{\partial} : \mathcal{E} \to \mathcal{E}$  that extend  $\partial$ , i.e. such that the following diagrams are commutative:

- (c) to define the subspaces  $\mathcal{E}_M$  and  $\mathcal{N}$  of  $\mathcal{E}$  respectively of *moderate elements* and *null elements* such that  $\mathcal{E}_M$  is a subalgebra of  $\mathcal{E}$  and  $\mathcal{N}$  an ideal of  $\mathcal{E}_M$ ;
- (d) to prove the following:

 $(d_1)$ 

$$\iota(\mathcal{D}'(\mathbb{R}^n)) \subset \mathcal{E}_M, \quad \sigma(C^{\infty}(\mathbb{R}^n)) \subset \mathcal{E}_M;$$

 $(d_2)$ 

$$(\iota - \sigma)(C^{\infty}(\mathbb{R}^n)) \subset \mathcal{N}, \quad \iota(\mathcal{D}'(\mathbb{R}^n)) \cap \mathcal{N} = \{0\};$$

(e) to prove that:

$$\widehat{\partial}(\mathcal{E}_M) \subset \mathcal{E}_M, \quad \widehat{\partial}\mathcal{N} \subset \mathcal{N};$$

(f) finally, we have to define the Colombeau algebra as:

$$\mathcal{G} = \mathcal{E}_M / \mathcal{N}.$$

As already said in Remarks 2.1 and 2.2, in literature there are some variants of definition of Colombeau algebras (see for example [14], [8]), that maintain the general scheme of construction already described. However all the approaches have in common the central rôle of convolution to define the embedding  $\iota$ . There are strong motivations for using convolution for this purpose: for a detailed discussion see [8, 18, 19]. One of them is based on well known theorems on distribution theory that put derivation and convolution in commutation relation (see, for example, [20],[9]). To be more precisely,

if  $\iota$  is defined by the convolution, the diagram (3.2) is commutative. Conversely, let us suppose that (3.2) was commutative, i.e. if:

$$\widehat{\partial}(\iota(\Phi)) = \iota(\partial(\Phi), \quad \forall \Phi \in \mathcal{D}'(\mathbb{R}^n), \tag{3.3}$$

then  $\iota$  is a convolution. Let us dwell on the last statement. Let us suppose that the application  $\iota$  is defined considering a bilinear map  $k : \mathcal{D}(\mathbb{R}^n) \times \mathcal{D}'(\mathbb{R}^n) \to C^{\infty}(\mathbb{R}^n)$  separately continuous. The linear embedding of  $\mathcal{D}'(\mathbb{R}^n)$  in  $\mathcal{E}, \iota : \mathcal{D}'(\mathbb{R}^n) \to \mathcal{E}, \iota(\Phi) = u_{\Phi}$ , is defined by:  $u_{\Phi}(\phi) := k(\phi, \Phi)$ , so  $u_{\Phi} : \mathcal{D}(\mathbb{R}^n) \to C^{\infty}(\mathbb{R}^n)$ . On the other hand, let us consider the map  $L_{\phi} : \mathcal{D}'(\mathbb{R}^n) \to C^{\infty}(\mathbb{R}^n)$  defined by  $L_{\phi}(\Phi) := k(\phi, \Phi)$ : one has that for all  $\phi, L_{\phi}$  is linear and continuous. From the condition (3.3),  $\partial(u_{\Phi}(\phi)) = u_{\partial\Phi}(\phi)$ , one has  $\partial(L_{\phi}(\Phi)) = L_{\phi}(\partial\Phi)$ , then  $[\partial, L_{\phi}](\Phi) = 0$  for all  $\Phi \in \mathcal{D}'(\mathbb{R}^n)$ . The continuity of  $L_{\phi} : \mathcal{D}'(\mathbb{R}^n) \to C^{\infty}(\mathbb{R}^n)$  imply the continuity of  $L_{\phi} : \mathcal{D}'(\mathbb{R}^n) \to \mathcal{D}'(\mathbb{R}^n)$ , and from [9, Corollary pag. 399], there exists a distribution with compact support  $\Xi_{\phi}$  such that:  $L_{\phi}(\Phi) = \Xi_{\phi} * \Phi$ . From the condition  $\Xi_{\phi} * \Phi \in C^{\infty}(\mathbb{R}^n)$  for all  $\Phi \in \mathcal{D}'(\mathbb{R}^n)$ , we can put in particular  $\Phi = \delta$ , so  $\Xi_{\phi} \in C^{\infty}(\mathbb{R}^n)$  with compact support, i.e.  $\Xi_{\phi} \in \mathcal{D}(\mathbb{R}^n)$ . The bilinearity of k implies  $\Xi_{\phi} = \lambda\phi$ , so necessarily it follows that:  $k(\phi, \Phi) = \phi * \Phi$ .

Then, if the diagram (3.2) is commutative, it follows that the embedding  $\iota$  is defined by the convolution. However, if we assume the commutativity of the following diagram:

the condition (3.3) can be replaced by:

$$\widehat{\partial}(\iota(\Phi)) - \iota(\partial(\Phi)) = \mathcal{N}, \quad \forall \Phi \in \mathcal{D}'(\mathbb{R}^n).$$
(3.5)

From this point of view, it is not very clear if the use of ordinary convolution to define embedding of  $\mathcal{D}'(\mathbb{R}^n)$  in  $\mathcal{G}$  is necessary. In this sense, it can be put a question: it can be reasonable to consider a generalization of convolution, maintaining the previous general construction scheme already considered?

#### 4 A-convolution

In [24][28] a generalization of convolution is defined, considering an unbounded self-adjoint operator A on the domain  $\mathcal{D}(A)$  in the Hilbert space  $\mathcal{H}$ . Let U(t) be the strongly continuous one parameter unitary groups which has A as infinitesimal generator (see [17]). Then one has:

$$\mathcal{D}(A) = \left\{ f \in \mathcal{H} : \lim_{t \to 0} \frac{U(t) - \mathbf{1}}{t} f \text{ exists in } \mathcal{H} \right\}, \quad U(t)f = e^{itA}f, \quad \forall f \in \mathcal{H}.$$

As usual, the set of  $C^{\infty}$ -vectors of A is defined by:

$$\mathcal{D}^{\infty}(A) = \bigcap_{n=1}^{\infty} \mathcal{D}(A^n)$$

This set, also denoted  $C^{\infty}(A)$ , endowed with the topology  $t_A$  generated by the set of seminorms  $f \mapsto ||A^n f||$ ,  $n \in \mathbb{N}$ , is a Frechèt and reflexive domain [21, Section 2.2]. Its conjugate dual, with respect to the scalar product of  $\mathcal{H}$ , is denoted by  $\mathcal{D}_{-\infty}(A)$  and endowed with the strong dual topology  $t'_A$ .

As known, the operator A leaves  $\mathcal{D}^{\infty}(A)$  invariant, and  $A : \mathcal{D}^{\infty}(A) \to \mathcal{D}^{\infty}(A)$ is continuous in  $t_A$  topology: so, being symmetric,  $A \upharpoonright_{\mathcal{D}^{\infty}(A)}$  has a unique extension  $\widehat{A} : \mathcal{D}_{-\infty}(A) \to \mathcal{D}_{-\infty}(A)$  which is continuous in the strong dual topology of  $\mathcal{D}_{-\infty}(A)$ . The same results are true for the positive integer powers of A. Furthermore  $e^{itA} : \mathcal{D}^{\infty}(A) \to \mathcal{D}^{\infty}(A)$  is continuous, so U(t) admits a continuous extension  $\widehat{U}(t)$  to  $\mathcal{D}_{-\infty}(A)$  given by:

$$\langle \phi, \widehat{U}(t)F \rangle = \langle U(-t)\phi, F \rangle, \quad F \in \mathcal{D}_{-\infty}(A), \quad \phi \in \mathcal{D}^{\infty}(A).$$

**Definition 4.1.** Let  $\phi \in \mathcal{D}(\mathbb{R})$  and  $f \in \mathcal{H}$ ; in [26, 24, 28] is defined the <u>A</u>-convolution of  $\phi$  and f as the vector  $\phi^A f \in \mathcal{H}$  given by:

$$\phi^{^{A}}_{*}f := \int_{\mathbb{R}} \phi(t) U(t) f dt.$$

It is well-known from Stone's theorem (see [10, Th.5.6.36]) that  $\phi^A f = \tilde{\phi}(A)f$ , where  $\tilde{\phi}$  denote the Fourier transform of  $\phi$ . In [26, 24, 28] it is shown the following Proposition: for all  $\phi \in \mathcal{D}(\mathbb{R})$ , the map  $T_{\phi} : \mathcal{H} \to \mathcal{H}$  defined by:

$$T_{\phi}f := \phi^{A}_{*}f = \int_{\mathbb{R}} \phi(t)U(t)fdt$$

is linear and bounded. Furthermore, one has  $T_{\phi}f \in \mathcal{D}^{\infty}(A)$ ,  $\forall f \in \mathcal{H}$ , and  $T_{\phi}$  is a continuous operator from  $\mathcal{H}$  to  $\mathcal{D}^{\infty}(A)$ . It follows that the corresponding bilinear map  $k: \mathcal{D}(\mathbb{R}) \times \mathcal{H} \to \mathcal{H}$ , defined by  $K(\phi, f) := T_{\phi}f$  is separately continuous, in fact, if  $|\phi|_0 = \sup_{\mathbb{R}} |\phi(t)|$ , one has:  $||k(\phi, f)|| \leq |\phi|_0||f||$ . From [24] one has  $||A^n T_{\phi}f|| \leq ||f|| \int_{\mathbb{R}} |\phi^{(n)}(t)| dt$  so it follows that  $k: \mathcal{D}(\mathbb{R}) \times \mathcal{H} \to \mathcal{D}^{\infty}(A)$  is separately continuous too, and that there exists an extension  $\mathcal{D}(\mathbb{R}) \times \mathcal{D}_{-\infty}(A) \to \mathcal{D}^{\infty}(A)$  given by:

$$\widehat{T}_{\phi}F = \phi_{*}^{A}F = \int_{\mathbb{R}} \phi(t)\widehat{U}(t)Fdt$$

For example, when  $A = -i\frac{d}{dx}$ , then U(t) is the translation operator, in this case the A-convolution is the convolution of functions. If A = x, the A-convolution is the multiplication by  $\tilde{\phi}$ .

#### 5 A-convolution and the general construction scheme

To extend the previous results between a locally convex space  $\mathcal{D}$  and its dual  $\mathcal{D}'$ , we proceed in the following way. Let  $\mathcal{D}$  be a dense subspace of Hilbert space  $\mathcal{H}$ . Let us endow  $\mathcal{D}$  with a locally convex topology t, stronger than the one induced on  $\mathcal{D}$  by the Hilbert norm and let  $\mathcal{D}'[t']$  be its topological conjugate dual endowed with the strong dual topology t' defined by the set of seminorms

$$F \mapsto \|F\|_{\mathcal{M}} := \sup_{\phi \in \mathcal{M}} |\langle F, \phi \rangle|$$
(5.1)

where  $\mathcal{M}$  runs in the family of bounded subsets of  $\mathcal{D}[t]$ . In this way, if  $\hookrightarrow$  denote a continuous linear injection, we get the familiar triplet:

$$\mathcal{D} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{D}'$$

called a rigged Hilbert space. Well-known examples of rigged Hilbert spaces are given by  $\mathcal{D}(\Omega) \hookrightarrow L^2(\Omega) \hookrightarrow \mathcal{D}'(\Omega)$  and  $\mathcal{S}(\mathbb{R}^n) \hookrightarrow L^2(\mathbb{R}^n) \hookrightarrow \mathcal{S}'(\mathbb{R}^n)$ , where  $\mathcal{S}(\mathbb{R}^n)$  is the Schwartz space of infinitely differentiable functions rapidly decreasing. Such spaces have often been considered from mathematical point of view: see for example [5] in distributions theory, and see [11, 12, 21, 25] where are considered space of linear maps acting on them; and see [4] for their applications to quantum physics. Let us consider a subspace  $\mathcal{D} \subset \mathcal{D}^{\infty}(A)$  with locally convex topology t finer than the topology induced from  $\mathcal{D}^{\infty}(A)$ . If  $\mathcal{D}'$  is the dual space of  $\mathcal{D}$ , we have the following chain of embedding:

$$\mathcal{D} \hookrightarrow \mathcal{D}^{\infty}(A) \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{D}_{-\infty}(A) \hookrightarrow \mathcal{D}'.$$

We suppose that  $A : \mathcal{D} \to \mathcal{D}$  continuously. In this way, A has a unique continuous extension to  $\widehat{A} : \mathcal{D}' \to \mathcal{D}'$  in the strong dual topology of  $\mathcal{D}'$ . It follows that we can extend U(t) to  $\mathcal{D}'$ , and so the A-convolution map can be extended to  $\mathcal{D}'$ :

$$\widehat{T}_{\phi}: \mathcal{D}' \to X$$

where  $X = Img \hat{T}_{\phi}$ . Obviously,  $\mathcal{D}^{\infty}(A) \subset X$ . The convolution map is represented by:

$$\widehat{T}_{\phi}F = \phi^{A}_{*}F = \int_{\mathbb{R}} \phi(t)\widehat{U}(t)Fdt, \quad F \in \mathcal{D}'.$$

Let us consider the following bilinear map:

$$K_A(\phi, F) : \mathcal{D}(\mathbb{R}) \times \mathcal{D}' \longrightarrow X$$

defined by:

$$(\phi, F) \mapsto K_A(\phi, F) := \phi^A F.$$

Let us sketch a possible guideline to construct a Colombeau-like algebra with A-convolution.

To follow the general scheme of construction of the previous section, we suppose that X is a topological algebra [29], with topology generated by a family of seminorms  $\{p_{\alpha}\}_{\alpha \in I}$ . The *basic space* is defined by  $\mathcal{E}_A := X^{\mathcal{D}(\mathbb{R})}$ , i.e.:

$$\mathcal{E}_A := \{ all \, the \, maps \, u : \mathcal{D}(\mathbb{R}) \to X \}.$$

We define the following embedding of  $\mathcal{D}'$  in  $\mathcal{E}_A$  by:

$$\iota_A: F \mapsto K_A(\cdot, F),$$

and the "standard copy"  $\sigma_A : X \to \mathcal{E}_A$  by:

$$\sigma_A: f \mapsto u(\phi) = f \quad \forall \phi \in \mathcal{D}(\mathbb{R}).$$

Let us define the "parameter sets":  $\mathcal{A}_0 := \{\phi \in \mathcal{D}(\mathbb{R}) : \int \phi(t) dt = 1\}$  and

$$\mathcal{A}_q = \Big\{ \phi \in \mathcal{A}_0 : \quad \int_{\mathbb{R}} t^k \phi(t) A^k f dt = 0 \quad \forall f \in \mathcal{D}, \, \forall k : \, 1 \le k \le n \Big\}.$$

The space of A-moderate elements is defined by:

$$\mathcal{E}_{A\mathcal{M}} \coloneqq \left\{ u \in \mathcal{E}_A : \forall \alpha \in I, \exists m \in \mathbb{N} : \forall \phi \in \mathcal{A}_m \; \exists c > 0, \, \eta > 0 : p_\alpha[u(\phi_\epsilon)] \le c\epsilon^{-m}, \, 0 < \epsilon < \eta \right\}$$

and A-null elements are defined by:

$$\mathcal{N}_A := \Big\{ u \in \mathcal{E}_A : \forall \alpha \in I, \exists N \in \mathbb{N} : \forall \phi \in \mathcal{A}_m, m \ge N, \exists c > 0, \eta > 0 : p_\alpha[u(\phi_\epsilon)] \le c\epsilon^{m-N}, 0 < \epsilon < \eta \Big\}.$$

To go further, we have to control if the general scheme to construction "works", considering X,  $\mathcal{E}_{A\mathcal{M}}$ ,  $\mathcal{N}_A$  at the place of  $C^{\infty}(\mathbb{R})$ ,  $\mathcal{E}_{\mathcal{M}}$ ,  $\mathcal{N}$ . In this sense, some additional hypothesis can occur: for example, we can suppose that X and  $\mathcal{D}$  are differential algebras. If it is defined a derivation  $\partial : \mathcal{D} \to \mathcal{D}$ , we can define a derivation in its conjugate dual  $\mathcal{D}'$  by  $\langle f | \partial^n F \rangle := (-1)^n \langle \partial^n f | F \rangle$ , and consequently a derivation  $\widehat{\partial}$  on  $\mathcal{E}_A$  such that the following commutation relation is well defined:

$$\widehat{\partial}(\iota_A(F)) = \iota_A(\partial F) + [\widehat{\partial}, \iota_A]F$$

equivalently:

$$\partial(\phi^{A}_{*}F) = \phi^{A}_{*}\partial F + \int_{\mathbb{R}} \phi(t)[\partial,\widehat{U}(t)]Fdt \quad \forall \phi \in \mathcal{D}(\mathbb{R})$$

With the choice  $A = -i\frac{d}{dx}$ ,  $\mathcal{D}(A) = W^{1,2}(\mathbb{R})$  and  $X = C^{\infty}(\mathbb{R})$ , one has  $[\partial, \widehat{U}(t)] = 0$ , and we obtain the usual Colombeau algebra.

### 6 Conclusion

The considerations of the previous sections provide some hints to consider, in a future paper, an unbounded self-adjoint operator satisfying the previous commutation relation, and to define a "Colombeau-like" algebra with the linear embedding of vector spaces defined by A-convolution.

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# From the Classical Boltzmann Equation to the Generalized Kinetic models of Biological Systems

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#### Abstract

This paper deal with the classical Boltzmann Equation generalized to model cell populations in complex biological system. In particular, the populations refer to the cells of the immune system and to those of an aggressive host (cancer cells) in a human being. We will focus with the study of a spatially homogeneous continuous model, and derivation of the macroscopic model. The paper starts from a simple description of the classical Boltzmann equation and goes to the mathematical approach proposed to model the large systems of interacting entities focusing the competition between immune system and cancer cells.

Key words: classical Boltzmann equation, kinetic theory, active particles MSC: 70Fxx, 76P05, 37N25

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### 1 Introduction

Ludwig Eduard Boltzmann, (1844-1906), was an Austrian physicist famous in the development of statistical mechanics, where he explains and predicts that the properties of atoms and molecules "microscopic properties" determine the macroscopic properties of matter such as viscosity and diffusion coefficient. Boltzmann's most important scientific contributions were in kinetic theory including the Maxwell-Boltzmann distribution for molecular speeds in a gas. The classical Boltzmann equation, define the evolution of a statistical distribution function over the physical internal state of interacting individuals or objects belonging to a large population. The distribution function means the probability of finding particles within a certain range of velocities at a certain range of locations at a given time, which that mean, it gives a mathematical description of the state and how to change it. The Boltzmann equation is the fundamental model of rarefied gas dynamics, which has been successfully applied to the analysis of several molecular fluid dynamic problems [2]. Moreover, the term Boltzmann equation is often used to refer to any kinetic equation that describes the change of a macroscopic quantity in a thermodynamic system, such as energy and momentum, when a fluid is in transport, and other properties characteristic to fluids such as viscosity. The classic example is a fluid with temperature gradients in space causing heat to flow from hotter regions to colder ones, by the random transport of particles. Non equilibrium gases can be, for example, surrounding a body in flight in the atmosphere or flowing in a pipe [11]. In physics, specifically non-equilibrium statistical mechanics, the Boltzmann equation or Boltzmann transport equation (BTE) describes the statistical behaviour of a thermodynamic system not in thermodynamic equilibrium. It was devised by Ludwig Boltzmann in 1872. As we know, the Boltzmann equation define the evolution equation for the one particle distribution function of a mono-atomic perfect gas, where this distribution function represents the number of particles that occupy the corresponding element of the phase space at the given time in insulated system [3]. In the recent years, the generalization of the Boltzmann equation has been widely discussed in the scientific literature. These generalizations have been based on the term "generalized Boltzmann equation", which usually refers to any new modification of a publication. As mentioned in paper [1], recent research activities have shown that the statistical methods in applied sciences can take advantage of mathematical methods of the phenomenological kinetic theory of gases. This was done by developing the classical Boltzmann equation.

A simple model of population dynamics with kinetic type interactions was proposed by Jager and Segel to describe the evolution of social dynamics of certain insects (bumble-bees) whose interactions modify the physical state and end up into a splitting of the populations of dominant and dominated individuals.

Here we will deals with suitable generalization of methods of classical kinetic theory, in complex biological systems, such as the propagation of an infection, or in the anomalous proliferation of tumor cells. In these systems, the early stage is mainly stochastic while at large times, by some law of large numbers, the predominant effects are deterministic. So the mathematical tools offer a conceptual framework to modeling the complex biological systems, and allow to model the dynamics of large systems of interacting particles. These interactions are rules non only by laws of classical mechanics, but also by biological functions.

The mathematical approach is based on the Kinetic Theory of Active Particles (KTAP) developed to describe the dynamics of large systems of interacting objects [4], [5], [8]. This approach to living systems was initiated by the pioneer paper [6] and developed and applied by various authors. According to KTAP, the overall system is divided into different populations (functional subsystems) each of them consisting of entities, called active particles, which collectively express the same function, called activity, which is related to the intrinsic biological function of particles. The evolution of each functional subsystem is described by a distribution function and the time evolution of the subsystem is governed by interactions.

In this paper, the contents are organized in six additional sections. In section 2, we first briefly recall the mean lines of classical Boltzmann theory. In section 3, we outline the KTAP. In section 4, as an example, we present the general mathematical structure of KTAP. In section 5 we present a spatially homogeneous continuous model as the particular cases of competition between immune system and cancer cells (continuous model). In section 6 we deal with a simplified situation to derivation equations for macroscopic averaged quantities.

#### 2 Classical Boltzmann Equation

The kinetic theory of the gas is a theory devoted to study the evolutionary behaviors of gases in the one-particle phase space of position and velocity. To statistically describe the state of the gas, we consider a mono-atomic (one species) gas with N molecules enclosed in a space domain  $\Omega \subseteq \mathbb{R}^3$ . Each molecule can be specified at a given time as a point in a six dimensional space spanned by its position coordinate  $\mathbf{x} = (x_1, x_2, x_3)$  and velocity component  $\mathbf{v} = (v_1, v_2, v_3)$ . According to the laws of classical mechanics:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \tag{1}$$

$$\frac{d\mathbf{v}}{dt} = \mathbf{F} \tag{2}$$

where the strength  $\mathbf{F}$  refers to the mass *m* acting on each particle.

In the kinetic theory, the state of the gas is described by a distribution function  $f = f(t, \mathbf{x}, \mathbf{v}) : \mathbb{R}^+ \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^+$  which stands for the mass density of gas particles having position  $\mathbf{x} \in \mathbb{R}^3$  and velocity  $\mathbf{v} \in \mathbb{R}^3$  at time  $t \in \mathbb{R}$ . By definition, f is a non-negative function such that for any region D of the one-particle phase space  $\mathbb{R}^3 \times \mathbb{R}^3$ , the average number of particles contained in a volume element  $d^3\mathbf{x}$  about  $\mathbf{x}$  within the range  $\mathbf{x} + d\mathbf{x}$  and a velocity space element  $d^3\mathbf{v}$  about  $\mathbf{v}$  within the range  $\mathbf{v} + d\mathbf{v}$ , is given by  $n = f(t, \mathbf{x}, \mathbf{v})d^3\mathbf{x}d^3\mathbf{v}$ . The total number of particles is:

$$N(t) = \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t; \mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v}$$
(3)

If f is a known distribution function, then we can compute the following macroscopic quantities such as mass density  $(\rho)$ , mass velocity  $\mathbf{U} = (U_1, U_2, U_3)$ , and mass translational energy  $(\varepsilon)$ , as follows:

$$\rho(t, \mathbf{x}) = mn(\mathbf{x}, t) = m \int_{\mathbb{R}^3} f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}$$
(4)

$$\mathbf{U}(t,\mathbf{x}) = \frac{m}{n(\mathbf{x},t)} \int_{\mathbb{R}^3} \mathbf{v} f(t,\mathbf{x},\mathbf{v}) d\mathbf{v}$$
(5)

$$\varepsilon(t, \mathbf{x}) = \frac{1}{3(k \setminus m)n(\mathbf{x}, t)} \int_{\mathbb{R}^3} [\mathbf{v} - U]^2 f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}$$
(6)

where m is the mass of a single particle, and k is the Boltzmann constant. In general, Boltzmann transport equation 'BTE' is an integro-differential equation of the distribution function f in terms of position, velocity, and time. It takes in account the change in this function that is caused by collisions between the particles and the external force. The general equation can then be written in the following form:

$$\frac{df}{dt} = C[f] \tag{7}$$

where the term C[f] is given by the following:

$$C[f] = \left(\frac{\partial f}{\partial t}\right)_{force} + \left(\frac{\partial f}{\partial t}\right)_{diff} + \left(\frac{\partial f}{\partial t}\right)_{coll} \tag{8}$$

where the "force" term corresponds to the forces exerted on the particles by an external influence (not by the particles themselves), the "diff" term represents the diffusion of particles, and "coll" is the collision term - accounting for the forces acting between particles in collisions.

The equation is called Valsov equation (collisionless Boltzmann equation) if:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f = 0 \tag{9}$$

In the case of collisions between particles, the term  $\left(\frac{\partial f}{\partial t}\right)_{coll}$  is added on the right hand side of the Eq. (9), then the Eq. (9) will be modified as follows:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f = \left(\frac{\partial f}{\partial t}\right)_{coll} \tag{10}$$

# 3 Statistical Representation of Biological Systems by Using the Kinetic Theory of Active Particles

In this generalized model, we consider a biological system constituted by a large number of interacting particles (called active particles), distributed in space, whose microscopic state includes not only geometrical and mechanical variables (typically position and velocity), but also biological functions, called activities, which are related to the intrinsic biological functions of particles. According to KTAP, the overall system is divided into a number of subsystems each of them composed by particles that collectively express the same biological function (functional subsystems). The evolution of each functional subsystem is described by a distribution function over the microscopic state of the particles, and the time evolution of the subsystem is governed by interaction, which changes both the microscopic state (conservative interaction) and the number of particles (non-conservative interaction). Essentially, complex biological closed systems are composed of a large number of interacting individuals, in the absence of any effective external action. The mathematical kinetic theory methods describes the system by identifying the microscopic state of the entities interacting within a large system, and the distribution function over this state.

In this generalized model, we will deal with the competition between immune cells and tumor cells.

**Remark 3.1.** The biological microscopic state of the active particles is a scalar variable  $u \in D_u$ , ( $D_u$  is the domain of existence of the variable u), which defines the physical state of active particles. The same variable is used for all particles, yet this variable attains different values for each particle.

#### 3.1 Mathematical Representation

A large system of object, or individuals, is constituted by some differential populations of interacting entities called **active particles**.

**Definition 3.1.** The physical variable denoting the state of each active particle is called the **microscopic state**, and is denoted by  $\mathbf{w}$ , which is formally written as follows:

$$\mathbf{w} = (\mathbf{x}, \mathbf{v}, u) \in D_{\mathbf{x}} \times D_{\mathbf{v}} \times D_{u},$$

where  $\mathbf{x} \in D_{\mathbf{x}}$  is the geometrical microscopic variable (position),  $\mathbf{v} \in D_{\mathbf{v}}$  is the microscopic mechanical variable (velocity), and  $u \in D_u$  characterizes the **biological microscopic internal state**, of each subject. Moreover,  $D_{\mathbf{x}}$ ,  $D_{\mathbf{v}}$ , and  $D_u$  refer to the domains of existence of these variables, while the space  $D_{\mathbf{w}} = D_{\mathbf{x}} \times D_{\mathbf{v}} \times D_u$  of microscopic states is called the **state space**.

Definition 3.2. The dependent variable

$$f_i = f_i(t, \mathbf{x}, \mathbf{v}, u) = f_i(t, \mathbf{w}) : [0, T] \times D_{\mathbf{x}} \times D_{\mathbf{v}} \times D_u \to \mathbb{R}^+$$

for i = 1, 2, ..., M, defines the distribution at the time t, of individuals of the *i*-th functional subsystem, over the microscopic state  $\mathbf{w}$ . Each quantity  $f_i(t, \mathbf{w})d\mathbf{w}$  denotes the number of particles, whose state at time t, is in the elementary volume of the space of the microscopic states  $[\mathbf{w}, \mathbf{w} + d\mathbf{w}]$ , defined as  $[\mathbf{w}, \mathbf{w} + d\mathbf{w}] = [\mathbf{x}, \mathbf{x} + d\mathbf{x}] \times [\mathbf{v}, \mathbf{v} + d\mathbf{v}] \times [u, u + du]$ .

#### 3.2 Modeling Microscopic Interactions

The KTAP is a new mathematical approach that develops methods of mathematical kinetic theory to deal with active particles (cells, for example) rather than with classical particles. Thus, according to the modeling of microscopic interactions, particles are classified into three types [4]:

• Test particles of  $i^{th}$  functional subsystem with microscopic state, at time t, delivered by the variable  $\mathbf{w} = (\mathbf{x}, \mathbf{v}, u)$ , whose distribution function is

$$f_i = f_i(t, \mathbf{x}, \mathbf{v}, u) = f_i(t, \mathbf{w}).$$

The test particle is assumed to be representative of the whole system.

• Field particles of the  $k^{th}$  functional subsystem with microscopic state, at time t, defined by the variable  $\mathbf{w}^* = (\mathbf{x}^*, \mathbf{v}^*, u^*)$ , whose distribution function is

$$f_k = f_k(t, \mathbf{x}^*, \mathbf{v}^*, u^*) = f_k(t, \mathbf{w}^*).$$

• Candidate particles, of the  $h^{th}$  functional subsystem, with microscopic state, at time t, defined by the variable  $\mathbf{w}_* = (\mathbf{x}_*, \mathbf{v}_*, u_*)$ , whose distribution function is

$$f_h = f_h(t, \mathbf{x}_*, \mathbf{v}_*, u_*) = f_h(t, \mathbf{w}_*).$$

The above definitions depend upon modeling of microscopic interactions based on binary interactions involving test or (candidate) particles and field particles, where the field particles enters into the action domain of the test particles. In this modeling, there are two type of microscopic interactions for derivation the mathematical framework [5] [8]:

**Definition 3.3.** The short-range binary interactions refer to the mutual actions between test and field cells, when the test cell enters into the action domain  $\Sigma \subset D_{\mathbf{x}}$ of the field cell;  $\Sigma$  is relatively small with respect to  $D_x$  and only binary encounters are assumed to be relevant.
**Definition 3.4. Long range mean field interactions** refer to the action over the test active particles applied by all field active particles which are in the long range action domain  $D_{\mathbf{x}} \subseteq \mathbb{R}^3$  of the field particle. The action is still of the type of binary encounters.

For both types of interactions, we consider the following classifications:

- **Conservative interactions** which modify the state, mechanical and/or activity, of the interacting active particles, but not their number.
- Non-Conservative (Proliferative or Destructive) interactions which generate birth or death of active particles respectively due to pair interactions.

**Assumption 3.1.** Microscopic state of individuals is going to change after the interaction between individuals. Any interactions depends on the microscopic state of interacting individuals, and can generate changes in population of different species too. They do not preserve the total number of individuals of each population, because proliferation or destruction of individuals are both possible.

## 4 General Mathematical Structure

Let us consider a large system of interacting active particles subdivided into M functional subsystems labeled by the subscript i. The evolution equation of the distribution function of the *i*-th population can be written similarly as the case of the classical Boltzmann equation in Eq. (10), as follows:

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}}\right) f_i(t, \mathbf{x}, \mathbf{v}, u) = J_i[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u), \qquad \forall i = 1, 2, ..., M,$$
(11)

where  $\nabla_{\mathbf{x}}$  is the gradient operator, and where

 $J_{i}[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u) = (C_{i} + P_{i} + M_{i} - D_{i} - L_{i})[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u), \qquad \forall i = 1, 2, ..., M.$ (12)

- $J_i[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u)$  models the flow, at time  $t \in [t_0, T)$ , of particles that fall into the state  $\mathbf{w}$  of the functional subsystem i;
- $C_i[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u)$  is the net flux, at time  $t \in [t_0, T]$ , into the state  $\mathbf{w} \in D_{\mathbf{w}}$  of the functional subsystem *i*, due to conservative interactions. These only modify the micro-state, but not the number of particles, and include the flux rate  $C_i^+$  and  $C_i^-$  of particles which enter or leave the elementary volume  $d\mathbf{w}$  of the state space, therefore:

$$C_i[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u) = C_i^+[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u) - C_i^-[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u).$$
(13)

•  $P_i[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u)$  is the inflow, at time  $t \in [t_0, T]$ , into the state  $\mathbf{w} \in D_{\mathbf{w}}$  of the functional subsystem *i*, due to proliferative events that occur within the same functional subsystem, and generate the birth or gain of particles due to pair interactions;

- $M_i[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u)$ , refers to the inflow, at time  $t \in [t_0, T]$ , into the state  $\mathbf{w} \in D_{\mathbf{w}}$  of the functional subsystem *i*, due to mutation events, where daughter particles occur in a subsystem different from that of the mother cell;
- $D_i[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u)$  is the outflow, at time  $t \in [t_0, T]$ , into the state  $\mathbf{w} \in D_{\mathbf{w}}$  of the functional subsystem *i*, due to destructive events that generate the death or the loss of particles due to pair interactions;
- $L_i[\mathbf{f}](t, \mathbf{x}, \mathbf{v}, u)$ , refers to the natural activity loss or cell death (apoptosis).

The modelling of interactions at the micro-scale is based on the knowledge of the following quantities:

- Interaction rates (Encounter rates),  $\eta_{hk}[\mathbf{f}](\mathbf{w}_*, \mathbf{w}^*)$  and  $\mu_{hk}[\mathbf{f}](\mathbf{w}_*, \mathbf{w}^*)$ ; these are parameters which model the frequency of the interactions between a candidate *h*-particle with state  $\mathbf{w}_*$  and a field *k*-particle with state  $\mathbf{w}^*$ . So the encounter rate depends both on the states and on the type of populations of the interacting pairs. In general, different rates  $\eta$  and  $\mu$  are used corresponding to conservative and proliferative/mutation/destructive interactions, respectively;
- **Transition probability density**  $\mathcal{B}_{hk}^{i}[\mathbf{f}](\mathbf{w}_{*} \to \mathbf{w}; \mathbf{w}^{*})$ , which denotes the probability density that a candidate *h*-particle ends up into the state of the test particle of the *i*<sup>th</sup> functional subsystem after an interaction (with rate  $\eta_{hk}$ ) with a field *k*-particle, while test *i*-particles interact with field particles and lose their state;
- Proliferative term events P<sup>i</sup><sub>hk</sub>[f](w<sub>\*</sub> → w; w<sup>\*</sup>), which models the proliferative events for a candidate h-particle into the *i*-th functional subsystem after interaction (with rate μ<sub>hk</sub>) with a field k-particle;
- Mutation term events  $\mathcal{M}_{hk}^{i}[\mathbf{f}](\mathbf{w}_{*} \to \mathbf{w}; \mathbf{w}^{*})$ , which models the mutation events for a candidate *h*-particle into the functional subsystem  $i \neq h$  after interaction (with rate  $\mu_{hk}$ ) with a field *k*-particle;
- **Destructive term events**  $\mathcal{D}_{ik}[\mathbf{f}](\mathbf{w};\mathbf{w}^*)$ , which models the rate of destruction for a candidate *i*-particle in its own functional subsystem after an interaction (with rate  $\mu_{ik}$ ) with a field *k*-particle.
- **Relaxation and apoptosis events**  $\mathcal{L}_i[\mathbf{f}](\mathbf{w})$ , which models the natural loss of activity and death (apoptosis) of the cells, due to their damage or age.

**Remark 4.1.** In the above expressions **f** denotes the set of all distribution functions:  $\mathbf{f} = \{f_i\}, \quad i = 1, \dots M.$ 

**Remark 4.2.** The encounter rate depends both on the states and on the type of populations of the interacting pairs.

**Remark 4.3.** An important concept that is useful in the definition of the encounter rate, is the introduction of a distance  $d_{hk}$  between the cells of the h-th and the k-th functional subsystems, and in the assumption that the encounter rate depends on the distance between the interacting particles [7]:

$$\eta_{hk}[\mathbf{f}] = \eta_{hk}^0(d_{hk}[\mathbf{f}]). \tag{14}$$

In some situations one expects that the encounter rate decays with the distance between the activity state of the interacting particles  $d_{hk}(u_*, u^*) = |u_* - u^*|$ . In other cases  $d_{hk}$  may depend on distribution function  $f_h(t)$  and  $f_k(t)$ . A simple possibility is to consider the distance induced by the norm  $L^1$  where  $||f_i(t)|| = \int_{D_u} |f_i(t, u)| du$ , and

$$d_{hk}[\mathbf{f}](t) = \|f_h(t) - f_k(t)\|.$$
(15)

In the equation (13)  $(C_i = C_i^+ + C_i^-)$ ,  $C_i^+$  refers to the gain term, which is the number of test particles of the  $i^{th}$  population appearing in the state **w**, after interactions between candidate particles of the same population with microscopic state **w**<sub>\*</sub>, and field particles of the  $i^{th}$  population with microscopic state **w**<sup>\*</sup>. The term  $C_i^+$  can be written as follows:

$$C_{i}^{+}[f](\mathbf{x}, \mathbf{v}, u) = \sum_{h,k=1}^{M} \int_{(\Omega \times D_{u}^{2} \times D_{v}^{2})[\mathbf{f}]} \eta_{hk}[\mathbf{f}](\mathbf{x}, \mathbf{x}^{*}, \mathbf{v}_{*}, \mathbf{v}^{*}, u_{*}, u^{*})$$

$$\cdot \mathcal{B}_{hk}^{i}[\mathbf{f}](\mathbf{v}_{*} \to \mathbf{v}, u_{*} \to u; \mathbf{v}_{*}, \mathbf{v}^{*}, u_{*}, u^{*})$$

$$\cdot f_{h}(t, \mathbf{x}, \mathbf{v}_{*}, u_{*})f_{k}(t, \mathbf{x}^{*}, \mathbf{v}^{*}, u^{*})d\mathbf{x}^{*}d\mathbf{v}_{*}d\mathbf{v}^{*}du_{*}du^{*}.$$
(16)

The term  $C_i^-$  refers to the lose term, which is the number of test particles which leave the state  $\mathbf{w}_*$ , per unit of time and volume, after having interacted with field particles with state  $\mathbf{w}^*$ , the lose term is defined as:

$$C_{i}^{-}[\mathbf{f}](\mathbf{x}, \mathbf{v}, u) = f_{i}(t, \mathbf{x}, \mathbf{v}, u) \sum_{k=1}^{M} \int_{(\Omega \times D_{u} \times D_{v})[f]} \eta_{ik}[\mathbf{f}](\mathbf{x}, \mathbf{x}^{*}, \mathbf{v}, \mathbf{v}^{*}, u, u^{*})$$
  
 
$$\cdot f_{k}(t, \mathbf{x}^{*}, \mathbf{v}^{*}, u^{*}) d\mathbf{x}^{*} d\mathbf{v}^{*} du^{*}, \qquad (17)$$

**Remark 4.4.** The function  $\mathcal{B}_{hk}^i$  has the structure of a probability density function with respect to the variable  $\mathbf{w}$ :

$$\int_{D_{\mathbf{w}}} \mathcal{B}_{hk}^{i}(\mathbf{w}_{*}, \mathbf{w}^{*}; \mathbf{w}) \mathbf{dw} = \mathbf{1}$$
(18)

The terms  $P_i$ ,  $M_i$ ,  $D_i$  and  $L_i$ , corresponding to proliferation, mutation, destruction, and relaxation are defined respectively as:

$$P_{i}[\mathbf{f}](\mathbf{x}, \mathbf{v}, u) = \sum_{h,k=1}^{M} \int_{(\Omega \times D_{u}^{2} \times D_{v}^{2})[\mathbf{f}]} \mu_{hk}[\mathbf{f}](\mathbf{x}, \mathbf{x}^{*}, \mathbf{v}_{*}, \mathbf{v}^{*}, u_{*}, u^{*}) \mathcal{P}_{hk}^{i}[f](u_{*} \to u; u^{*})$$

$$\cdot f_{h}(t, \mathbf{x}, \mathbf{v}_{*}, u_{*}) f_{k}(t, \mathbf{x}^{*}, \mathbf{v}^{*}, u^{*}) d\mathbf{x}^{*} d\mathbf{v}_{*} d\mathbf{v}^{*} du_{*} du^{*}$$
(19)

$$M_{i}[\mathbf{f}](\mathbf{x}, \mathbf{v}, u) = \sum_{h,k=1}^{M} \int_{(\Omega \times D_{u}^{2} \times D_{\mathbf{v}}^{2})[\mathbf{f}]} \mu_{hk}[\mathbf{f}](\mathbf{x}, \mathbf{x}^{*}, \mathbf{v}_{*}, \mathbf{v}^{*}, u_{*}, u^{*}) \mathcal{M}_{hk}^{i}[f](u_{*} \to u; u^{*})$$

$$f_h(t, \mathbf{x}, \mathbf{v}_*, u_*) f_k(t, \mathbf{x}^*, \mathbf{v}^*, u^*) d\mathbf{x}^* d\mathbf{v}_* d\mathbf{v}^* du_* du^*, \quad i \neq h$$
(20)

$$D_{i}[\mathbf{f}](\mathbf{x}, \mathbf{v}, u) = f_{i}(\mathbf{x}, \mathbf{v}, u) \sum_{k=1}^{M} \int_{(\Omega \times D_{u} \times D_{v})[\mathbf{f}]} \mu_{ik}[\mathbf{f}](\mathbf{x}, \mathbf{x}^{*}, \mathbf{v}, \mathbf{v}^{*}, u, u^{*}) \mathcal{D}_{ik}[\mathbf{f}](u, u^{*})$$
  

$$\cdot f_{k}(t, \mathbf{x}^{*}, \mathbf{v}^{*}, u^{*}) d\mathbf{x}^{*} d\mathbf{v}^{*} du^{*}$$
(21)

$$L_i[\mathbf{f}](\mathbf{x}, \mathbf{v}, u) = \lambda_i \left[ f_i(t, \mathbf{x}, \mathbf{v}, u) - f_i(t_0, \mathbf{x}_0, \mathbf{v}_0, u_0) \right]$$
(22)

The general system of evolution equations is obtained substituting the formal expressions (16), (17), (19), (20), (21) and (22) into the equation (11).

## 5 Spatially Homogeneous Continuous Case

Now we will consider a simplified model related to the previous mathematical framework, this model suitable for describing the evolution and competition between cells of the immune system and cancer cells. This simplification corresponds to the spatially homogeneous continuous case, in which the space and velocity variables are not significant or they are constant in time, and the activity variable  $u \in (0, \infty)$ . The description of the framework of the model follows the same line of followed in [10] and [13], where discrete values of the activity were considered, but with a continue activity, as made in [12]. In this Section, we will recall the results of [12], for the sake of completeness.

The first step of the modeling approach is the identification of the functional subsystems. The first four subsystems contain epithelial (subsystem 1) and cancer cells (subsystems 2,3,4), the other four functional subsystems contain cells of the innate immune system (subsystem 5) and cells of the adaptive immune system (subsystems 6,7,8).

The tumor cells are distinguished according to their progressive hallmarks, while the immune cells are characterized by the capability to recognize specific hallmarks. Accordingly, the eight functional subsystems are as follows:

- i = 1 Normal epithelial cells. It is supposed that the organism is a source of epithelial cells, so their quantity can be regarded as constant in time;
- i = 2 Cancer cells of the first hallmark that have the ability to thrive in a chronically inflamed micro-environment;
- i = 3 Cancer cells of the second hallmark, that have the ability to evade the immune recognition;

- i = 4 Cancer cells of the third hallmark that have acquired the ability to suppress the immune reaction;
- i = 5 Cells of the innate immune system which have the ability to acquire, by a learning process, the capacity of contrasting the development of cancer cells of the first hallmark (labeled by i = 2);
- i = 6 Cells of the adaptive immune system which have the ability to contrast the development of cancer cells labeled by i = 2;
- i = 7 Cells of the adaptive immune system which have the ability of contrasting the development of cancer cells labeled by i = 2 and i = 3;
- i = 8 Cells of the adaptive immune system which have the ability of contrasting the development of cancer cells labeled by i = 2, i = 3 and i = 4.

The overall state of each functional subsystem is described by the one-cell generalized distribution function:

$$f_i = f_i(t, u) : [t_0, T] \times D_u \to \mathbb{R}^+, \text{ for } i \in \{1, 2, \dots, 8\},$$
 (23)

so that  $f_i(t, u)du$  denotes the number of cells whose state, at time t, is in the interval [u, u + du]. In the KTAP, the interactions involve three types of particles: test, field and candidate. As we have said in Section 3, the interaction rule is as follows: candidate particles can acquire, in probability, the state of the test particles, after an interaction with field particles, while test particles lose their state after interactions.

The domain  $D_u$  of the microscopic state is assumed to coincide with interval  $[u^{(0)}, +\infty)$ , where  $u^{(0)} > 0$  is the lowest value of the biological function of each active particle. Then we will assume  $f_i(t, u) = 0$ , for  $u < u^{(0)}$ .

The time evolution of the distribution function  $f_i$ , is obtained by a suitable balance of particles in the elementary interval [u, u + du] of the microscopic state as follows:

$$\frac{\partial f_i}{\partial t}(t,u) = J_i[\mathbf{f}](t,u) \quad i \in \{1, 2, \dots, 8\}$$
(24)

with  $\mathbf{f} = (f_1, f_2, \dots, f_8)$  the vector of the densities, and where

$$J_{i}[\mathbf{f}](t,u) = C_{i}[\mathbf{f}](t,u) + M_{i}[\mathbf{f}](t,u) + P_{i}[\mathbf{f}](t,u) - D_{i}[\mathbf{f}](t,u) - L_{i}[\mathbf{f}](t,u).$$
(25)

The operators  $C_i$ ,  $M_i$ ,  $P_i$ ,  $D_i$  and  $L_i$ , acting over the whole set of distribution functions, have been introduced in Section 4. In spatially homogeneous continuous case, they are modeled as follows:

$$C_{i}[\mathbf{f}](t,u) = \sum_{k=1}^{n} \int_{D_{u} \times D_{u}} \eta_{ik}[\mathbf{f}] \mathcal{B}_{ik}[\mathbf{f}] f_{i}(t,u_{*}) f_{k}(t,u^{*}) du_{*} du^{*}$$
  
-  $f_{i}(t,u) \sum_{k=1}^{n} \int_{D_{u}} \eta_{ik}[\mathbf{f}] f_{k}(t,u^{*}) du^{*},$  (26)

$$P_{i}[\mathbf{f}](t,u) = \sum_{k=1}^{n} \int_{D_{u} \times D_{u}} \eta_{ik}[\mathbf{f}] \mathcal{P}_{ik}[\mathbf{f}] f_{i}(t,u_{*}) f_{k}(t,u^{*}) du_{*} du^{*}$$
(27)

$$M_{i}[\mathbf{f}](t,u) = \sum_{h,k=1}^{n} \int_{D_{u} \times D_{u}} \eta_{hk}[\mathbf{f}] \,\mathcal{M}_{hk(h\neq i)}[\mathbf{f}] \,f_{h}(t,u_{*}) \,f_{k}(t,u^{*}) \,du_{*} \,du^{*}$$
(28)

$$D_{i}[\mathbf{f}](t,u) = f_{i}(t,u) \sum_{k=1}^{n} \int_{D_{u}} \eta_{ik}[\mathbf{f}] \mathcal{D}_{ik}[\mathbf{f}] f_{k}(t,u^{*}) du^{*}$$
(29)

$$L_{i}[\mathbf{f}](t,u) = \lambda_{i}[\mathbf{f}][f_{i}(t,u) - f_{i}(t_{0},u_{0})]$$
(30)

**Remark 5.1.** In this model, we suppose that the encounter rate  $\eta_{ik} = \eta_{ik}[\mathbf{f}](u_*, u^*)$  is the same for all events (conservative/proliferative/mutation/destructive interactions).

### 5.1 Encounter Rate

In the modeling of encounter rate, which is obviously a symmetric function, this modeling is achieved in a fashion that increasing values of the distance  $d_{hk}$  between the *h*-th and the *k*-th functional subsystems correspond to decreasing values of the encounter rate  $\eta_{hk}$ , which is defined as follows:

$$\eta_{hk}[\mathbf{f}] = \eta_{hk}^{(0)} d_{hk}[\mathbf{f}], \qquad (31)$$

with  $\eta_{hk}^{(0)}$  suitable constants (that in the following will be denoted with  $\eta_{hk}$ , for sake of simplicity), and where [10]:

$$d_{hk}[\mathbf{f}] = \begin{cases} \exp\left(-\tau \frac{\|f_h - f_k\|}{\|f_h\| + \|f_k\|}\right) & \|f_h\|, \|f_k\| \neq 0, \tau > 0, \\ 0 & \|f_h\| = \|f_k\| = 0, \end{cases}$$
(32)

and  $\tau$  is a positive real constant.

• The encounter between epithelial and tumor cells (h = 1, 2, 3, 4) with epithelial cells (k = 1) is assumed proportional to a constant

$$\eta_{h1}[\mathbf{f}] = \eta_{h1} \, d_{h1}[\mathbf{f}],\tag{33}$$

with  $0 < \eta_{11} \le \eta_{21} \le \eta_{31} \le \eta_{41}$ .

• For the encounters between immune and cancer cells, only those corresponding to couples (h, k) = (5, 2), (6, 2), (7, 2), (7, 3), (7, 4), (8, 2), (8, 3), (8, 4) are considered. Therefore, we assume

$$\eta_{hk}[\mathbf{f}] = \eta_{hk} \, d_{hk}[\mathbf{f}],\tag{34}$$

with  $0 < \eta_{5k} \le \eta_{6k} \le \eta_{7k} \le \eta_{8k}$ .

Thus one gets the following matrix expression for the encounter rate [12]:

|               | $(\eta_{11}d_{11})$ | $\eta_{21} d_{21}$ | $\eta_{31} d_{31}$ | $\eta_{41}d_{41}$  | 0                 | 0                  | 0                  | 0                  | ١    |
|---------------|---------------------|--------------------|--------------------|--------------------|-------------------|--------------------|--------------------|--------------------|------|
| $\eta_{hk} =$ | $\eta_{21} d_{21}$  | 0                  | 0                  | 0                  | $\eta_{52}d_{52}$ | $\eta_{62} d_{62}$ | $\eta_{72} d_{72}$ | $\eta_{82} d_{82}$ |      |
|               | $\eta_{31}d_{31}$   | 0                  | 0                  | 0                  | 0                 | $\eta_{63} d_{63}$ | $\eta_{73} d_{73}$ | $\eta_{83} d_{83}$ |      |
|               | $\eta_{41} d_{41}$  | 0                  | 0                  | 0                  | 0                 | 0                  | $\eta_{74} d_{74}$ | $\eta_{84} d_{84}$ |      |
|               | 0                   | $\eta_{52}d_{52}$  | 0                  | 0                  | 0                 | 0                  | 0                  | 0                  |      |
|               | 0                   | $\eta_{62}d_{62}$  | $\eta_{63}d_{63}$  | 0                  | 0                 | 0                  | 0                  | 0                  |      |
|               | 0                   | $\eta_{72} d_{72}$ | $\eta_{73} d_{73}$ | $\eta_{74} d_{74}$ | 0                 | 0                  | 0                  | 0                  |      |
|               | 0                   | $\eta_{82} d_{82}$ | $\eta_{83} d_{83}$ | $\eta_{84} d_{84}$ | 0                 | 0                  | 0                  | 0 /                | /    |
|               |                     |                    |                    |                    |                   |                    |                    | ,                  | (35) |

with  $d_{hk} = d_{hk}[\mathbf{f}]$  expressed by (32), and  $\eta_{hk} = \eta_{kh}$ 

### 5.2 Transition Probability Density

 $\mathcal{B}_{ik}$  represents the probability density that a candidate particle, with state  $u_*$ , of the *i*-th functional subsystem ends up into the state *u* of the test particle of the same functional subsystem after the interaction with the field particle, with state  $u^*$ , of the *k*-th functional subsystem.  $\mathcal{B}_{ik}$  satisfies, for all  $i, k \in \{1, 2, ..., n\}$ , the following condition:

$$\int_{D_u} \mathcal{B}_{ik}[\mathbf{f}](u_* \to u | u_*, u^*) \, du = 1, \quad \forall \, u_*, u^* \in D_u.$$

$$(36)$$

The function  $\mathcal{B}_{ik}(u_*, u^*, u)$  has different expressions for the subsystems i = 1, 2, 3, 4 corresponding to epithelial and cancer cells, and the subsystems k = 5, 6, 7, 8 corresponding to immune system cells. Specifically we assume [12]:

$$\mathcal{B}_{ik} = \begin{pmatrix} \mathcal{B}_{11} & \mathcal{B}_{12} & \mathcal{B}_{13} & \mathcal{B}_{14} & 0 & 0 & 0 & 0 \\ \mathcal{B}_{21} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathcal{B}_{31} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathcal{B}_{41} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathcal{B}_{52} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathcal{B}_{62} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathcal{B}_{73} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathcal{B}_{84} & 0 & 0 & 0 & 0 \end{pmatrix}$$
(37)

We will assume that transition probability density does not depend on the activity  $u^*$  of the cell (field) that interacts with the candidate particle:

$$\mathcal{B}_{ik} = \mathcal{B}_{ik}(u_*, u). \tag{38}$$

Consider first the interaction that involve the interactions between epithelial and cancer cells (k = 1, 2, 3, 4) and epithelial cells (i = 1). Epithelial cells are assumed to feed progression of cancer cells without changing their activity. Thus, we assume:

$$\mathcal{B}_{1k}(u_*, u) = \delta(u_* - u)$$
 for  $k = 1, 2, 3, 4$  (39)

Consider now the interactions that involve functional subsystem k = 1 and i = 2, 3, 4. The progression in the activity of cancer cells (i = 2, 3, 4) is due to the interaction with epithelial cells (k = 1). In this case, we will assume that the probability of transition depends on the interacting populations and decrease with the activity state of the cancer cells. So we will assume

$$\mathcal{B}_{i1} = \alpha_i [1 - (u_* + a_i)] \,\delta(u - (u_* + a_i)) + [1 - \alpha_i (1 - (u_* + a_i)] \,\delta(u - u_*) \tag{40}$$

For the interaction that involve the innate immune system (functional subsystem i = 5) and the cancer cells, we assume that the innate immune system has the ability to recognize the cancer cell of the first hallmark,(functional subsystem k = 2) without changing their activity. Thus, we assume:

$$\mathcal{B}_{52}(u_*, u) = \delta(u_* - u) \tag{41}$$

For what concerns the cells of the adaptive immune system, these cells acquire progressively the ability to identify the tumor cells. Thus for the pairs (i, k) = (6, 2), (7, 2), (7, 3), (8, 4) we will assume

$$\mathcal{B}_{ik} = \alpha_i [1 - (u_* + a_i)] \,\delta(u - (u_* + a_i)) + [1 - \alpha_i (1 - (u_* + a_i))] \,\delta(u - u_*) \tag{42}$$

The conservative events are expressed by the quantity (26). Substituting (39) - (42) in it, we get

• we get for i = 1:

$$C_1[\mathbf{f}](t,u) = 0, (43)$$

• for i = 2, 3, 4:

$$C_{i}[\mathbf{f}](t,u) = \eta_{i1}d_{i1}n_{1}\alpha_{i}(1-u)\left[f_{i}(t,u-a_{i}) - (1-(u+a_{i}))f_{i}(t,u)\right], \quad (44)$$

• we get also for i = 5

$$C_5[\mathbf{f}](t,u) = 0, \tag{45}$$

• and for i = 6, 7, 8:

$$C_{i}[\mathbf{f}](t,u) = \eta_{i(i-4)}d_{i(i-4)}n_{i-4}\alpha_{i}(1-u)\left[f_{i}(t,u-a_{i}) - (1-(u+a_{i}))f_{i}(t,u)\right].$$
(46)

### 5.3 Modeling Proliferative Events

 $P_i[\mathbf{f}](t, u)$  is the gain, at time  $t \in [0, T]$ , into the state  $u \in [u^{(0)}, +\infty)$  of the functional subsystem *i*, due to proliferative events. We model these events, in which generation of a daughter cell occurs in the same functional subsystem of the mother cell, choosing for the rate  $\mathcal{P}_{hk}[\mathbf{f}](u_*, u^*, u)$  the following matrix expression [12]:

The proliferative events dynamics in the *h*-th functional subsystems is assumed to follow the following rules: A candidate particle (mother cell) of functional subsystem h with state  $u_*$  by interacting with a cell (field) from subsystem k, with state  $u^*$ , proliferate a daughter cell of the same functional subsystem, with the same activity  $u = u_*$ . More precisely:

• The proliferative events in the cancer subsystems h = 2, 3, 4, owing to their interaction with epithelial cells, increase with the hallmarks of cancer cells due to the increasing proliferation program, which is an acquired capability of tumor cells. So we assume:

$$\mathcal{P}_{h1} = \beta_h u_* \delta(u_* - u), \tag{48}$$

with  $0 < \beta_2 \le \beta_3 \le \beta_4$ .

• The proliferative events in the immune subsystems h = 6, 7, 8 are due to the interactions with the cancer cells. Following [9], we assume, for each pair (h, k) = (6, 2), (7, 2), (7, 3), (8, 2), (8, 3), (8, 4):

$$\mathcal{P}_{hk} = \beta_h \delta(u_* - u), \qquad \beta_h > 0. \tag{49}$$

with  $0 < \beta_6 \leq \beta_7 \leq \beta_8$ .

BmP,

These proliferative events are expressed by the equation (27). Substituting (48) and (49) in it, we get

$$P_2[\mathbf{f}](t,u) = \eta_{21} d_{21} \beta_2 n_1 u f_2(t,u)$$
(50)

$$P_3[\mathbf{f}](t,u) = \eta_{31} d_{31} \beta_3 n_1 u f_3(t,u)$$
(51)

$$P_4[\mathbf{f}](t,u) = \eta_{41} d_{41} \beta_4 n_1 u f_4(t,u)$$
(52)

$$P_6[\mathbf{f}](t,u) = \eta_{62} d_{62} \beta_6 n_2 f_6(t,u)$$
(53)

$$P_{7}[\mathbf{f}](t,u) = \eta_{72} d_{72} \beta_{7} n_{2} f_{7}(t,u) + \eta_{73} d_{73} \beta_{7} n_{3} f_{7}(t,u)$$
(54)

 $P_8[\mathbf{f}](t,u) = \eta_{82} d_{82} \beta_8 n_2 f_8(t,u) + \eta_{83} d_{83} \beta_8 n_3 f_8(t,u) + \eta_{84} d_{84} \beta_8 n_4 f_8(t,u) (55)$ 

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### 5.4 Modeling Mutations

 $M_i[\mathbf{f}](t, u)$  is the gain, at time  $t \in [t_0, T]$ , into the state  $u \in [u^{(0)}, +\infty)$  of the functional subsystem *i*, due to mutation events, where generation of a daughter cell occurs in a subsystem different from that of the mother cell. We model mutation events choosing for the rate  $\mathcal{M}_{ik}[\mathbf{f}](u_*, u^*, u)$  the following matrix expression [12]:

The mutation events dynamics in the *i*-th functional subsystems is assumed to follow the following rules: A candidate particle (mother cell) of functional subsystem h with state  $u_*$ , by interacting with a cell (field) from subsystem k, with state  $u^*$ , proliferate a daughter cell belonging to the following functional subsystem i = h + 1 with the lowest activity values  $u = u^{(0)}$ .

Following [9], we will make the assumptions:

• The mutation events in the cancer subsystems i = 2, 3, 4 are related to the encounters of particles of the functional subsystems h = 1, 2, 3 respectively with the cells of the first functional subsystem, indeed the epithelial cells k = 1 are those that furnish to the mother cell the nutrient to create a mutated daughter. So we assume, for i = 2, 3, 4:

$$M_{i}[\mathbf{f}](t,u) = \int_{D_{u} \times D_{u}} \eta_{(i-1)1} d_{(i-1)1}[\mathbf{f}] \,\mathcal{M}_{(i-1)1} \,f_{i-1}(t,u_{*}) \,f_{1}(t,u^{*}) \,du_{*} \,du^{*}$$
(57)

where

$$\mathcal{M}_{(i-1)1} = \varepsilon_{(i-1)1} u_* \delta(u - u^{(0)}), \tag{58}$$

with  $0 < \varepsilon_{11} \le \varepsilon_{21} \le \varepsilon_{31}$ .

Substituting (58) in (57), we get for i = 2, 3, 4:

$$M_2 = \eta_{11} d_{11} \varepsilon_{11} n_1 A_1 \delta(u - u^{(0)})$$
(59)

$$M_3 = \eta_{21} d_{21} \varepsilon_{21} n_1 A_2 \delta(u - u^{(0)})$$
(60)

$$M_4 = \eta_{31} d_{31} \varepsilon_{31} n_1 A_3 \delta(u - u^{(0)})$$
(61)

• The mutation events in the immune subsystems i = 6, 7, 8 are related to the increasing capability of the immune cells to recognize a specific cancer hallmark.

Therefore, mutations in the immune system cells are due to encounters of particles of the functional subsystems h = 5, 6, 7 with the cells of the subsystems k = 2, 3, 4 respectively. We assume, for i = 6, 7, 8:

$$M_{i}[\mathbf{f}](t,u) = \int_{D_{u} \times D_{u}} \eta_{(i-1)(i-4)} d_{(i-1)(i-4)} \mathcal{M}_{(i-1)(i-4)} f_{i-1}(t,u_{*}) f_{i-4}(t,u^{*}) du_{*} du^{*}$$
(62)

where

$$\mathcal{M}_{(i-1)(i-4)} = \varepsilon_{(i-1)(i-4)} u_* \delta(u - u^{(0)}), \qquad \varepsilon_{(i-1)(i-4)} > 0.$$
(63)

with  $0 < \varepsilon_{52} \le \varepsilon_{63} \le \varepsilon_{74}$ .

Substituting (63) in (62), we get, for i = 6, 7, 8

$$M_6 = \eta_{52} d_{52} \varepsilon_{52} n_2 A_5 \,\delta(u - u^{(0)}) \tag{64}$$

$$M_7 = \eta_{63} d_{63} \varepsilon_{63} n_3 A_6 \delta(u - u^{(0)})$$
(65)

$$M_8 = \eta_{74} d_{74} \varepsilon_{74} n_4 A_7 \,\delta(u - u^{(0)}) \tag{66}$$

**Remark 5.2.** The quantities  $n_1, \dots, n_4$  and  $A_1, \dots, A_8$ , refer to the size of the *i*-th population and the activation, respectively, which we will address in the section 6.

### 5.5 Modeling Destructive Events

 $D_i[\mathbf{f}](t, u)$  is the loss, at time  $t \in [t_0, T]$ , in the state  $u \in [u^{(0)}, +\infty)$  of the functional subsystem *i*, due to destructive events. The dynamics of the destructive interactions follow the following rules. A candidate cell from functional subsystem *i* with state  $u_*$ , interacting with a field cell of the *k*-th functional subsystem with activity  $u^*$ , can undergo a destructive action which occurs within the same state of the candidate particle, only cancer cell can be destructed, owing to the interactions with the immune cells that are able to identify them. We assume that the ability of the immune cells is proportional to their activity  $u^*$ .

For the rate  $\mathcal{D}_{ik}[\mathbf{f}](u, u^*)$  we obtain the following matrix [12]:

Where, for each pair (h, k) = (2, 6), (2, 7), (2, 8), (3, 7), (3, 8), (4, 8), the destructive rate  $\mathcal{D}_{ik}[\mathbf{f}](u, u^*) = \gamma_k u^*$ , with  $0 < \gamma_6 \leq \gamma_7 \leq \gamma_8$ . Consequently, by using the general

expression (67), we obtain:

$$D_{2}[\mathbf{f}](t,u) = f_{2}(t,u) (\eta_{26}d_{26}\gamma_{6}A_{6} + \eta_{27}d_{27}\gamma_{7}A_{7} + \eta_{28}d_{28}\gamma_{8}A_{8})$$

$$D_{3}[\mathbf{f}](t,u) = f_{3}(t,u) (\eta_{37}d_{37}\gamma_{7}A_{7} + \eta_{38}d_{38}\gamma_{8}A_{8})$$

$$D_{4}[\mathbf{f}](t,u) = f_{4}(t,u) \eta_{48}d_{48}\gamma_{8}A_{8}$$
(69)

### 5.6 Modeling the Relaxation Term

The immune cells in the absence of tumor cells tend to return to their healthy initial state. Then we will assume  $\lambda_i = 0$  for i = 2, 3, 4, and for i = 6, 7, 8 [12]:

$$L_{i}[\mathbf{f}](t,u) = \lambda_{i}[f_{i}(t,u) - f_{i}(t_{0},u_{0})]$$
(70)

with  $0 < \lambda_6 \leq \lambda_7 \leq \lambda_8$ .

## 6 Macroscopic model

The mathematical model analyzed in the preceding section allow us to describe several interesting phenomena related to several aspects of the immune-cancer competition. In what follows, we shall derive macroscopic equations macroscopic equations for averaged quantities, from the underlying microscopic description.

If the distribution functions  $f_i$  are known, then macroscopic variables can be computed, under suitable integrability properties, as moments weighted by the above distribution function [5], [8].

For our purpose, we consider the following macroscopic variables of each cellular population:

• Number density: The size of the *i*-th population at time *t*, given by

$$n_i[\mathbf{f}](t) = \int_{D_u} f_i(t, u) \, du \quad \text{for} \quad i \in \{1, 2, \dots, 8\},\tag{71}$$

where  $D_u = [u_0, +\infty)$ .

• Activation density: The activation at time t of the *i*-th population, defined as:

$$A_{i}[\mathbf{f}](t) = \int_{D_{u}} u f_{i}(t, u) \, du \quad \text{for} \quad i \in \{1, 2, \dots, 8\},$$
(72)

• Quadratic activation density:

$$E_i[\mathbf{f}](t) = \int_{D_u} u^2 f_i(t, u) \, du \quad \text{for} \quad i \in \{1, 2, \dots, 8\},\tag{73}$$

• Cubic activation density:

$$Q_i[\mathbf{f}](t) = \int_{D_u} u^3 f_i(t, u) \, du \quad \text{for} \quad i \in \{1, 2, \dots, 8\}.$$
(74)

Because our aim is to determine macroscopic equations by using a multiscale analysis, we will make here some simplifying assumptions for the coefficients introduced in this section. This model obtained is sufficiently appealing for a qualitative understanding of some biological features influencing the immune-cancer competition.

• In the simplest case we assume that  $\eta_{hk}[\mathbf{f}]$  depends only on h and k and not on the functional expression of  $f_h$  and  $f_k$ .

Different choice can be made for  $\eta_{hk}^{(0)}$ . Here, the encounter between tumor (h = 2, 3, 4) and epithelial cells (h = 1) is assumed proportional to h, as progressive hallmarks corresponds to increasing activations to search nutrients for increasing proliferation:

$$\eta_{h1}^{(0)} = \eta_0 h, \qquad \eta_0 > 0 \tag{75}$$

The encounter rate between immune and cancer cells is assumed constant, for each pair (h, k) = (5, 2), (6, 2), (6, 3), (7, 2), (7, 3), (7, 4), (8, 2), (8, 3), (8, 4). Therefore, we assume:

$$\eta_{hk}^{(0)} = \eta_0 \sigma, \qquad \sigma > 0 \tag{76}$$

in agreement with the representation of the system, one gets the following matrix expression for the encounter rate:

$$\eta_{hk} = \begin{pmatrix} 1 & 2 & 3 & 4 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & \sigma & \sigma & \sigma & \sigma \\ 3 & 0 & 0 & 0 & 0 & \sigma & \sigma & \sigma \\ 4 & 0 & 0 & 0 & 0 & 0 & \sigma & \sigma \\ 0 & \sigma & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma & \sigma & \sigma & 0 & 0 & 0 & 0 \\ 0 & \sigma & \sigma & \sigma & 0 & 0 & 0 & 0 \end{pmatrix}$$
(77)

The dimensionless parameter  $\eta_0$  corresponds to interaction between epithelial cells, and can be included in the time scale.

- For the coefficients appearing in the transitions events, as modeled in Section 5.2, we assume  $\alpha_i = \alpha$  and  $a_i = a = u^{(0)}$ .
- We consider now the proliferation events introduced in Section 5.3. We assume that in the cancer subsystems h = 2, 3, 4, owing to the interactions with epithelial cells k = 1, the proliferation rate is  $\beta_h = h\beta$ , and the proliferation rate in the immune subsystems h = 5, 6, 7, 8, owing to their interactions with cancer

cells k = 2, 3, 4 is  $\beta_h = \beta'$ . Thus, we get the following matrix expression for the rate  $\mathcal{P}_{hk}$ :

where  $U = u_* - u$ .

• In the modeling of the mutation events introduced in Section 5.4 we will assume that the mutation rate in cancer subsystems h = 2, 3, 4 related with the encounters of cells of the functional subsystems h = 1, 2, 3 respectively with the cells of first functional subsystem, is  $\varepsilon_{(h-1)1} = \varepsilon$ .

On the other hand, the mutation rate in immune subsystems h = 6, 7, 8 related with the encounters of particles of the functional subsystems h = 5, 6, 7 respectively with the cancer cells of functional subsystems k = 2, 3, 4, is  $\varepsilon_{(h-1)k} = \varepsilon'$ . Thus, we get the following matrix expression for the rate  $\mathcal{M}_{hk}$ :

where  $U_0 = u - u^{(0)}$ .

• In the modeling of destruction events we will assume that the destruction rate  $\gamma_i = \gamma$  for i = 6, 7, 8. We get:

BPP: N. Mohammed :From the Classical Boltzmann Equation to the Generalized Kinetic models of Biological Systems(pp. 95 - 118) • The relaxation of the immune system defined in Section 5.6 is assumed as follows:  $\lambda_i = \lambda$  for i = 6, 7, 8.

In the following, for sake of mathematical simplicity, we will assume that the cubic activation Q is constant in time.

By substituting the above assumptions in evolution equations (24), and in the expressions of  $C_i$ ,  $P_i$ ,  $M_i$ ,  $D_i$  and  $L_i$  found in previous section, we obtain  $\frac{\partial f_1}{\partial t}(t, u) = 0$ ,  $\frac{\partial f_5}{\partial t}(t, u) = 0$  and the following system of integro-differential equations:

$$\begin{cases} \frac{\partial f_2}{\partial t}(t,u) = 2\alpha n_1(1-u) \left[ f_2(t,u-u^{(0)}) - (1-(u+u^{(0)}))f_2(t,u) \right] \\ +4\beta n_1 u f_2(t,u) + \varepsilon n_1 A_1 \delta(u-u^{(0)}) - f_2(t,u) (\sigma \gamma A_6 + \sigma \gamma A_7 + \sigma \gamma A_8) \\ \frac{\partial f_3}{\partial t}(t,u) = 3\alpha n_1(1-u) \left[ f_3(t,u-u^{(0)}) - (1-(u+u^{(0)}))f_3(t,u) \right] \\ +9\beta n_1 u f_3(t,u) + 2\varepsilon n_1 A_2 \delta(u-u^{(0)}) - f_3(t,u) (\sigma \gamma A_7 + \sigma \gamma A_8) \\ \frac{\partial f_4}{\partial t}(t,u) = 4\alpha n_1(1-u) \left[ f_4(t,u-u^{(0)}) - (1-(u+u^{(0)}))f_4(t,u) \right] \\ +16\beta n_1 u f_4(t,u) + 3\varepsilon n_1 A_3 \delta(u-u^{(0)}) - \sigma \gamma A_8 f_4(t,u) \\ \frac{\partial f_6}{\partial t}(t,u) = \sigma \alpha n_2(1-u) \left[ f_6(t,u-u^{(0)}) - (1-(u+u^{(0)}))f_6(t,u) \right] \\ +\sigma n_2 \beta' f_6(t,u) + \sigma \varepsilon' n_2 A_5 \delta(u-u^{(0)}) - \lambda \left[ f_6(t,u) - f_6(t_0,u_0) \right] \\ \frac{\partial f_7}{\partial t}(t,u) = \sigma \alpha n_3(1-u) \left[ f_7(t,u-u^{(0)}) - (1-(u+u^{(0)}))f_7(t,u) \right] \\ + (\sigma n_2 + \sigma n_3)\beta' f_7(t,u) + \sigma \varepsilon' n_3 A_6 \delta(u-u^{(0)}) - \lambda \left[ f_7(t,u) - f_7(t_0,u_0) \right] \\ \frac{\partial f_8}{\partial t}(t,u) = \sigma \alpha n_4(1-u) \left[ f_8(t,u-u^{(0)}) - (1-(u+u^{(0)}))f_8(t,u) \right] \\ + (\sigma n_2 + \sigma n_3 + \sigma n_4)\beta' f_8(t,u) + \sigma \varepsilon' n_4 A_7 \delta(u-u^{(0)}) \\ -\lambda \left[ f_8(t,u) - f_8(t_0,u_0) \right] \end{cases}$$
(81)

The system in (81) is a complicated system of six integro-differential equations in the unknown functions  $f_2$ ,  $f_3$ ,  $f_4$ ,  $f_6$ ,  $f_7$ ,  $f_8$ .

A different approach is to work in a macroscopic framework, that gives us also important information as the evolution of the disease (cancer-immune system competition). By differentiating each of the both sides of the equations (71), (72), (73), with respect to t, and use the equations in the system (81). We can get a macroscopic model allowing to examine the number density n, the activation density A and the energy density E of each cellular population, as the following:

$$\frac{dn_2}{dt} = 2a\alpha n_1 n_2 + 4\beta n_1 A_2 + \varepsilon n_1 A_1 - n_2 \sigma \gamma (A_6 + A_7 + A_8)$$
(82)

$$\frac{dA_2}{dt} = 2a\alpha n_1 A_2 + 4\beta n_1 E_2 + \varepsilon n_1 A_1 u^{(0)} - A_2 \sigma \gamma (A_6 + A_7 + A_8)$$
(83)

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$$\frac{dE_2}{dt} = 2a\alpha n_1 E_2 + 4\beta n_1 Q_2 + \varepsilon n_1 A_1 [u^{(0)}]^2 - E_2 \sigma \gamma (A_6 + A_7 + A_8)$$
(84)

For i = 3 we get:

$$\frac{dn_3}{dt} = 3a\alpha n_1 n_3 + 9\beta n_1 A_3 + 2\varepsilon n_1 A_2 - n_3 \sigma \gamma (A_7 + A_8)$$
(85)

$$\frac{dA_3}{dt} = 3a\alpha n_1 A_3 + 9\beta n_1 E_3 + 2\varepsilon n_1 A_2 u^{(0)} - A_3 \sigma \gamma (A_7 + A_8)$$
(86)

$$\frac{dE_3}{dt} = 3a\alpha n_1 E_3 + 9\beta n_1 Q_3 + 2\varepsilon n_1 A_2 [u^{(0)}]^2 - E_3 \sigma \gamma (A_7 + A_8)$$
(87)

For i = 4 we get:

$$\frac{dn_4}{dt} = 4a\alpha n_1 n_4 + 16\beta n_1 A_4 + 3\varepsilon n_1 A_3 - \sigma\gamma n_4 A_8 \tag{88}$$

$$\frac{dA_4}{dt} = 4a\alpha n_1 A_4 + 16\beta n_1 E_4 + 3\varepsilon n_1 A_3 u^{(0)} - \sigma \gamma A_4 A_8 \tag{89}$$

$$\frac{dE_4}{dt} = 4a\alpha n_1 E_4 + 16\beta n_1 Q_4 + 3\varepsilon n_1 A_3 (u^{(0)})^2 - \sigma \gamma E_4 A_8 \tag{90}$$

For i = 6 we get:

$$\frac{dn_6}{dt} = \sigma a \alpha n_2 n_6 + \sigma \beta' n_2 n_6 + \sigma \varepsilon' n_2 A_5 - \lambda n_6 \tag{91}$$

$$\frac{dA_6}{dt} = \sigma a \alpha n_2 A_6 + \sigma \beta' n_2 A_6 + \sigma \varepsilon' n_2 A_5 u^{(0)} - \lambda A_6 \tag{92}$$

$$\frac{dE_6}{dt} = \sigma a \alpha n_2 E_6 + \sigma \beta' n_2 E_6 + \sigma \varepsilon' n_2 A_5 (u^{(0)})^2 - \lambda E_6 \tag{93}$$

For i = 7 we get:

$$\frac{dn_7}{dt} = \sigma a \alpha n_3 n_7 + \sigma \beta' n_7 (n_2 + n_3) + \sigma \varepsilon' n_3 A_6 - \lambda n_7 \tag{94}$$

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$$\frac{dA_7}{dt} = \sigma a\alpha n_3 A_7 + \sigma \beta' A_7 (n_2 + n_3) + \sigma \varepsilon' n_3 A_6 u^{(0)} - \lambda A_7$$
(95)

$$\frac{dE_7}{dt} = \sigma a \alpha n_3 E_7 + \sigma \beta' E_7 (n_2 + n_3) + \sigma \varepsilon' n_3 A_6 (u^{(0)})^2 - \lambda E_7$$
(96)

For i = 8 we get:

$$\frac{dn_8}{dt} = \sigma a \alpha n_4 n_8 + \sigma \beta' n_8 (n_2 + n_3 + n_4) + \sigma \varepsilon' n_4 A_7 - \lambda n_8 \tag{97}$$

$$\frac{dA_8}{dt} = \sigma a \alpha n_4 A_8 + \sigma \beta' A_8 (n_2 + n_3 + n_4) + \sigma \varepsilon' n_4 A_7 u^{(0)} - \lambda A_8 \tag{98}$$

$$\frac{dE_8}{dt} = \sigma a \alpha n_4 E_8 + \sigma \beta' E_8 (n_2 + n_3 + n_4) + \sigma \varepsilon' n_4 A_7 (u^{(0)})^2 - \lambda E_8 \tag{99}$$

**Remark 6.1.** Note that, we have assumed null initial conditions in the system 81, that is:  $f_i(t_0, u_0) = 0$  for i = 6, 7, 8.

## 7 Conclusions

In this work, we deal with a generalization of the classical Boltzmann Equation to model complex biological systems. The distribution function in the Boltzmann equation, may represent the number of particles that occupy the corresponding element of the phase space at the given time. On the other hand, in the generalized biological model, where the overall system is divided into a number of subsystems, the distribution function represents the number of active particles within the microscopic state that at a certain time are found in an elementary volume with a certain value of the activation of the active particles themselves. All this in the absence of any effective external action.

We have also presented, as a particular case, a spatially homogeneous model with continue activity  $u \in (0, \infty)$ . This continuous model is appropriate to examine macroscopic averaged quantities, as the number density n, the activation density A and the quadratic activation density E of each cellular population. Macroscopic equations for these averaged quantities are written, that are useful for giving some information about the state of healthy given individuals.

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# Non equilibrium phase–field descriptions of phase transitions in superconductors and superfluids

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### Abstract

In this review paper an overview is given on some phase–field models of phase transitions in the theory of superfluidity and superconductivity. The Gross-Pitaevskii equation, that describes a weakly non-ideal Bose gas at zero temperature, is reviewed and its conditions of applicability to superfluids and superconductors are discussed. The Ginzburg-Landau equation for superconductors and the Ginzburg-Pitaevskii equation for superfluids are recalled. Recent models describing dynamical aspects of phase–transition in superconductors and superfluids as well as the influence of external fluxes are presented. Further applications of the models are suggested to phase transitions in the presence of quantized vortices, or in superfluid <sup>3</sup>He, or in superfluid cosmological models.

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## 1 Introduction

The study of critical phenomena in non-equilibrium systems is an intense field of research, both from an experimental and a theoretical point of view. Studies have been made in non equilibrium systems also at very low temperature [2], [35], [66]. Two systems which have been extensively studied both experimentally and theoretically are the superconductor transition in metals carrying an electric current [74], [75] and the superfluid transition of liquid <sup>4</sup>He [74], [81], [84] in the presence of a heat flux. Having a dynamical description for the transitions is very important from the practical point of view, in view of the relevant applications of superconductors carrying high electric currents and superfluids conveying high heat fluxes. In both situations, an excessive value of the currents may induce vortices that increase the electrical or the thermal resistance, thus reducing the efficiency of the sought effect. The situation may become much more dangerous, however, if the fluxes induce a phase transition from the superconducting (or the superfluid) state to the normal state, with a fast increase of the respective resistances. This may produce severe accidents, because of a fast heating of the corresponding systems. Thus, accurate analyses of the effects of fluxes on the phase transitions, as well as their dynamical aspects, are needed, because of the behaviour of the systems close to the transition point exhibits peculiar features.

In order to develop a common framework to these phase transitions, incorporating dynamical aspects and the influence of external fluxes, in this small review paper an overview is given on some recent phase–field models in the theory of superfluidity and superconductivity. The Gross-Pitaevskii equation, that describes a weakly nonideal Bose gas at zero temperature, is reviewed in Section 2 and its conditions of applicability to superfluids and superconductors are discussed.

After a brief recall of the Landau theory of second-order phase transitions, in Section 3 the Ginzburg-Landau equation for superconductors and the Ginzburg-Pitaevskii equation for superfluids are written. Section 4 is devoted to present the phase-field theory of phase transitions. Two recent points of view are considered. The use of a balance equation for the order structure proposed by Fabrizio in [20] with applications to superconductor is presented in Subsection 4.1; a model able to describe the behavior of liquid <sup>4</sup>He, both in the normal and in the superfluid phase, recently proposed [22], [23], [61] is presented in Subsection 4.2. In the concluding Section 5 some interesting problems in other kinds of systems to which the phase-field theory can be applied are presented, as for instance, comparisons between the role of magnetic fields on superconductors and rotations in superfluids, regarding the formation of quantized electric current vortices or velocity vortices; phase transitions in cosmological models with fast expansion, as modelized by a superfluid vacuum; and phase transition to superfluidty in helium 3.

## 2 Gross-Pitaevskii equation

A simple theory to describe superfluids is the Gross-Pitaevskii theory, describing a weakly non-ideal Bose gas (with repulsion between the particles) at zero temperature. Indeed, in dilute gases of bosons cooled below a critical temperature the phenomenon of Bose-Einstein condensation occurs, i.e. a large fraction of bosons occupy the lowest quantum state, and macroscopic quantum phenomena become apparent. The Gross-Pitaevskii theory assumes that the behaviour of a weakly-interacting Bose gas at zero temperature is described by a single condensate wave function  $\psi(\mathbf{x}, t)$ , that is a complex function  $\psi = |\psi|e^{i\phi}$  [11].

This collective wave function must satisfy a nonlinear Schrödinger equation, also called the Gross-Pitaevskii equation. Assuming that  $\psi$  varies very slowly at distances of the interatomic scales, such Schrödinger equation takes the form [50]:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi - \mu\psi + V_0|\psi|^2\psi, \qquad (2.1)$$

where m is the mass of bosons,  $\hbar$  the reduced Planck constant,  $\mu$  the chemical potential and  $V_0$  the potential of the (repulsive) short-range interatomic forces. For an ideal gas it is  $\mu = 0$ . In a weakly interacting gas  $\mu = nV_0$  where n is the particle density. In this case, the Schrödinger equation (2.1) becomes

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi - V_0\left(n\psi - |\psi|^2\psi\right). \tag{2.2}$$

The r.h.s. is the energy (kinetic plus potential) of the condensate state. This equation was obtained by [32] and [68] in 1961 and it is much used in the analysis of Bose–Einstein condensates.

It is usual to interpret the square modulus of the wave function as the density number of particles in the condensed state, also in non–uniform and time dependent situations, i.e.  $\psi\psi^* = |\psi|^2 = n$ . So,  $mn = \rho$  is the density of the superfluid. Note that the density of the condensate atoms  $\rho_s = mn$  coincides with  $\rho$  for a weakly interacting gas at low temperature, where almost all atoms are the condensate.

According to (2.1), the rate of change of  $\psi\psi^*$  is given by

$$\frac{\partial}{\partial t}\psi\psi^* = -i\frac{\hbar}{2}\nabla\cdot\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right].$$
(2.3)

If we introduce the particle flow  $\mathbf{J}$ , by using the quantum-mechanical expression of the momentum per unit volume

$$\mathbf{J} = -i\frac{\hbar}{2} \left[\psi^* \nabla \psi - \psi \nabla \psi^*\right] = \hbar n \nabla \phi \tag{2.4}$$

equation (2.3) becomes

$$\frac{\partial}{\partial t}\psi\psi^* = -\nabla\cdot\mathbf{J}.\tag{2.5}$$

So, we are lead to define the particle velocity in a weakly interacting Bose gas as

$$\mathbf{v} = \frac{\mathbf{J}}{\rho} = \frac{\hbar}{m} \nabla \phi. \tag{2.6}$$

This relation outlines the relevant role of the phase  $\phi$  in connection to the velocity. The corresponding equation of motion is [50], [74]:

$$m\frac{\partial \mathbf{v}}{\partial t} = -\nabla \left(\mu + \frac{1}{2}m\mathbf{v}^2\right). \tag{2.7}$$

As shown in [50], to construct a kinetic model of superfluids by using the Gross-Pitaevskii equation the characteristic length of spatial variations (coherence length) of the wave function, given by

$$\xi = \frac{\hbar}{\sqrt{2mV_0 n}} \tag{2.8}$$

must be  $\xi \gg d$ , being d the interatomic distance. Therefore, the weakly-interacting Bose gas describes only approximatively superfluids. Nevertheless, some useful results can be obtained; indeed particular solutions of equation (2.1) describe straight vortices and long wavelength phonons [50]. For the purpose of this paper, the role of vortices deserves a special attention.

**Vortex solution**. A time independent solution of equation (2.2), in cylindrical coordinates  $(r, \theta, z)$ , is [50]:

$$\psi = \sqrt{n} f(r/\xi) e^{ik\theta}, \qquad (2.9)$$

with k an integer; it describes a straight vortex line with velocity circulation given by:

$$\oint \mathbf{v} \cdot d\gamma = \frac{\hbar}{m} \oint \nabla \phi \cdot d\gamma = \frac{2\pi\hbar k}{m} = k\kappa$$
(2.10)

where

$$\kappa = \frac{2\pi\hbar}{m} \tag{2.11}$$

is the quantum of circulation. We deduce therefore that in a weakly interacting Bose gas, the velocity circulation is quantized. This is relevant both for superfluids as for as for superconductors, where velocity of charges is related to electrical currents.

The Gross-Pitaevskii equation describes, in an approximate way, a superfluid, below the transition temperature, but it is not able to describe the transition from normal to superfluid state. Semimicroscopic models to describe phase transitions in superconductor and superfluids can be obtained by using Landau theory of second– order phase transitions.

## 3 Landau theory of second–order phase transitions

Landau theory of second-order phase transitions [29] is a mathematical physical theory formulated to describe all transformations which involve a broken symmetry and a continuous change in the free energy.

The basic ideas of this theory are that a phase transition can be characterized by one or more order parameters and that the free energy can be expanded as a power series in these order parameters. An order parameter, for a given system, is a quantity which is zero in the disordered phase and non-zero in the ordered phase.

For instance, consider a material that suffers a phase transition depending on the temperature T, and in which broken symmetry can be described by a single real order parameter  $\varphi$ . Denoting with  $F = F(T, \varphi, \mathbf{x})$  the free energy density of this system, the Landau theory assumes that to find the stable state at a given temperature, the total free energy  $\mathcal{F}$ 

$$\mathcal{F} = \int F(T, \varphi, \mathbf{x}) d^3 \mathbf{x}, \qquad (3.1)$$

must be minimized with respect to the order parameter. This implies:

$$\frac{\delta \mathcal{F}}{\delta \varphi} = 0. \tag{3.2}$$

Landau assumed that the functional  $\mathcal{F}$  can be split in the following way

$$\mathcal{F}(T,\varphi) = \mathcal{F}_0(T) + \mathcal{F}_L(T,\varphi) \tag{3.3}$$

where  $\mathcal{F}_0$  is a function of temperature, and  $\mathcal{F}_L(T,\varphi)$  contains all the information about dependence on the order parameter. The Landau functional  $\mathcal{F}_L$  is assumed to obey all possible symmetries associated with the order parameter  $\varphi$ . The most important part of the model consists in the construction of the Landau functional  $\mathcal{F}_L$ .

The first assumption is that, since the order parameter is small near the phase transition, the free energy density  $F(T, \varphi)$  can be approximated by the first few terms of a Taylor expansion in the order parameter:

$$\mathcal{F}(T,\varphi) = \int \left( F_0(T) + \alpha_0(T)\varphi + \alpha_1(T)\varphi^2 + \alpha_2(T)\varphi^3 + \alpha_3(T)\varphi^4 + \dots \right) d^3\mathbf{x} \quad (3.4)$$

In equation (3.4) the coefficients have been taken as functions of T, since the equilibrium values of  $\mathcal{F}$  and  $\varphi$  are functions of T. A further assumption is that all the coefficients can be expanded in powers of  $T - T_c$ , where  $T_c$  is the critical value of the temperature. These two simple assumptions are not valid for any system, but here we will made this simplified hypothesis.

We further consider the simple case in which the local free energy F at the point  $\mathbf{x}$  depends only on the value of the order parameter  $\varphi$  at  $\mathbf{x}$ . We will assume also that

the temperature dependence appears only in the lowest order term in the expansion of  $F(T, \varphi)$ , and that the following symmetry is present:

$$F(T,\varphi) = F(T,-\varphi). \tag{3.5}$$

In this case, the power series has only even powers of  $\varphi$  and one obtains for F:

$$F(T,\varphi) = F_0 + \frac{1}{2}A(T - T_c)\varphi^2 + \frac{1}{4}B\varphi^4$$
(3.6)

with A and B positive constants.

Since the equilibrium phase corresponds to a minimum of F, according to (3.2), at the phase transition it must be

$$\frac{\partial F}{\partial \varphi} = A(T - T_c)\varphi + B\varphi^3 = 0.$$
(3.7)

The solutions of this equation are  $\varphi = 0$  and

$$\varphi = \pm \sqrt{\frac{A}{B}(T_c - T)}.$$
(3.8)



**Figure 1:** Plots of  $\mathcal{F}$  with respect to  $|\varphi|$  at various temperatures.

The plot of the free energy at various temperature is shown in the figure. For  $T > T_c$  the free energy has only a minimum in the point  $\varphi = 0$ . Therefore, for  $T > T_c$  the stable solution is  $\varphi = 0$ , and the system is in the disordered state. For  $T < T_c$  the minimum  $\varphi = 0$  becomes unstable and the system goes in one of the two solutions (3.8) that are stable, and which correspond to a broken symmetry with respect to the order parameter  $\varphi$ .

### 3.1 Ginzburg–Landau theory of superconductivity

Superconductivity is a phenomenon observed in several metals and ceramic materials, which when cooled below a critical temperature, their electrical resistance suddenly drops to zero. Experiments made with *persistent currents* in superconducting rings have shown that electric currents flow without measurable decrease for years.

The *critical temperature* is a characteristic of the superconductor in consideration and depends on the current density and the magnetic field as shown in the Figure 2.



Figure 2: Phase diagram for a given supercontucors.

Another property of superconducting materials is the *Meissner effect*. It was observed that, as a magnet is brought near a superconductor, the magnet encounters a repulsive force. It can be said that the superconductor completely expels the magnetic field and behaves as a perfect diamagnet.

Depending on the response to magnetic fields, there are two main types of superconductor. Type-I superconductors expel magnetic flux from the material and are in the Meissner state, but when the applied magnetic field is higher than a (single) critical value  $H_c$ , superconductivity is lost. In type-2 superconductors there are two critical values  $H_{c1}$  and  $H_{c2}$  of the magnetic fields. For applied field intensity less that  $H_{c1}$  superconductor exhibits the usual Meissner effect; for an applied field higher that  $H_{c2}$  superconductivity is destroyed. In between  $H_{c1}$  and  $H_{c2}$  the superconductor allows partial penetration of the magnetic field; this state is called a mixed-state vortex lattice. In type-II superconductors magnetic flux can penetrate in the form of Abrikosov vortices [1]. If in a type-II superconductor one applies a magnetic field H larger than the lower critical field  $H_{c1}$  (but smaller than the upper critical field  $H_{c2}$ ), an Abrikosov vortex lattice will form. Each vortex carries a quantum of the flux of magnetic field, given by

$$\Phi_1 = h/2e, \tag{3.9}$$

with e electronic charge. This quantized flux is analogous to the quantized velocity circulation of vortices in superfluids, given in (2.11). The supercurrent circulates around the normal (i.e. non-superconducting) core of the vortex. Abrikosov vortices tend to arrange themselves in a flux-line (usually) triangular lattice, which however can be perturbed by material inhomogeneities (defects/dislocations) that pin the flux lines [55], [74], [75].

Ginzburg-Landau theory for superconducting transition. Ginzburg-Landau theory [29] is a phenomenological model describing the phase transition which occurs in a metal or alloy superconductor, under the critical temperature  $T_c$ . This transition is associated with a jump of the specific heat and no latent heat (second-order transition). The order parameter in the superconductor transition is a complex-valued parameter  $\psi$ , whose microscopic meaning is the wave function of the condensate.

By analogy with the Gross-Pitaevskii equation, the physical meaning of  $\psi$  is specified by saying that  $|\psi|^2$  is the number density  $n_s$  of superconducting electrons, while the phase  $\phi$  of the wave function is linked to the electron supercurrent:

$$|\psi|^2 = n_s, \qquad \frac{\hbar}{m} \nabla \phi = \mathbf{v}_s.$$
 (3.10)

Hence  $\psi = 0$  means that the material is in the normal state,  $T > T_c$ , while  $|\psi| = 1$  corresponds to a perfect superconductor (T = 0).

Ginzburg and Landau [29] assumed that the (Helmholtz) free energy density F of the superconductor, in the absence of magnetic fields, can be expanded in powers of  $|\psi|^2$  and  $|\nabla \psi|^2$ :

$$F(\mathbf{x}) = F_n + \alpha |\psi(\mathbf{x})|^2 + \frac{1}{2}\beta |\psi(\mathbf{x})|^4 + \frac{\hbar^2}{2m} |\nabla\psi(\mathbf{x})|^2.$$
(3.11)

where  $F_n$  is the free energy density of the electrons in the normal state, and m the electron mass. In this relation, higher–order terms in  $|\psi|^2$  are neglected and therefore the model is valid for small values of  $|\psi|$ .

Decomposing the wave function  $\psi$  in its modulus f and its phase  $\phi$ , equation (3.11) can be written:

$$F(\mathbf{x}) = F_n + \alpha f^2 + \frac{1}{2}\beta f^4 + \frac{\hbar^2}{2m} \left( |\nabla f|^2 + f^2 |\nabla \phi|^2 \right).$$
(3.12)

Recalling equation (3.10), we see that the last term in (3.12) can be interpreted as a kinetic term. In fact it is:

$$\frac{\hbar^2}{2m} f^2 |\nabla \phi|^2 = \frac{1}{2} \rho v_s^2.$$
(3.13)

In order to found the equilibrium states of the phase transition, following Landau theory of second-order phase transitions, this quantity must be minimized with respect to  $\psi$ . Note that in the GL theory of superconductor transition the quantity that must be minimized does not contain only the internal energy density, but also the kinetic energy of the electron flux with respect to the lattice.

In the presence of a magnetic field, Ginzburg and Landau [29] recognized that the quantity to be minimized is the Gibbs free energy

$$\mathcal{G}(T, H_0) = \mathcal{F} - \mathbf{H}_0 \cdot \mathbf{M} = \mathcal{U} - T\mathcal{S} - \mathbf{H}_0 \cdot \mathbf{M}, \qquad (3.14)$$

where  $\mathcal{U}$  is the total energy,  $\mathcal{S}$  the total entropy,  $\mathbf{H}_0$  the applied magnetic field and  $\mathbf{M}$  the magnetization vector. So, they modified the free energy expansion (3.12) including in it terms dependent on the applied magnetic field  $\mathbf{H}_0$ , obtaining

$$F(\mathbf{x}) = F_n + \alpha |\psi(\mathbf{x})|^2 + \frac{1}{2}\beta |\psi(\mathbf{x})|^4 + \frac{1}{2m} \left| \left( -i\hbar\nabla - 2q\mathbf{A} \right)\psi \right|^2 - \mathbf{H}_0 \cdot \mathbf{B} + \frac{1}{2}\mu_0 H_0^2, \quad (3.15)$$

where q is the effective electric charge, and **A** is the vector potential associated to the magnetic induction **B** by the equation

$$\nabla \times \mathbf{A} = \mathbf{B}.\tag{3.16}$$

The dependence of the free energy on the vector potential **A** must satisfy gaugeinvariance requirements. Here the gauge is  $\nabla \cdot \mathbf{A} = 0$ .

To obtain the equilibrium states in the phase transition the total Gibbs free energy

$$\mathcal{G} = \int G(\mathbf{x}) d^3 \mathbf{x} \tag{3.17}$$

must be minimized with respect to the order parameter  $\psi$  and to the vector potential  ${\bf A}.$ 

The corresponding Euler-Lagrange equations for the unknowns  $\psi$  and  ${\bf A}$  are:

$$\frac{\delta \mathcal{G}}{\delta \psi^*} = \frac{\partial G}{\partial \psi^*} - \sum_j \frac{\partial}{\partial x_j} \frac{\partial G}{\partial (\nabla_j \psi^*)} = 0, \qquad (3.18)$$

$$\frac{\delta \mathcal{G}}{\delta \psi} = \frac{\partial G}{\partial \psi} - \sum_{j} \frac{\partial}{\partial x_{j}} \frac{\partial G}{\partial (\nabla_{j} \psi)} = 0, \qquad (3.19)$$

$$\frac{\delta \mathcal{G}}{\delta A_k} = \frac{\partial G}{\partial A_k} - \sum_j \frac{\partial}{\partial x_j} \frac{\partial G}{\partial (\nabla_j A_k)} = 0$$
(3.20)

where  $\nabla_j$  is the component of the gradient in the *j* direction and  $A_k$  is the component of **A** in the *k* direction. Equations (3.18) and (3.19) lead to the same equation. After some manipulation, and with the restriction that use the gauge  $\nabla \cdot \mathbf{A} = 0$ , equation (3.18) leads to:

$$\frac{1}{2m} \left( -i\hbar\nabla - 2q\mathbf{A} \right)^2 \psi + \alpha\psi + \beta|\psi|^2 \psi = 0.$$
(3.21)

Equation (3.19) leads to the corresponding complex conjugated expression.

Following Landau theory, one assumes that the coefficients  $\alpha$  and  $\beta$  can be expanded in powers of  $T - T_c$ ; in particular we assume  $\beta = B > 0$  constant and

$$\alpha = A(T - T_c),$$
 (A > 0). (3.22)

The GL equation for superconductor transition is then

$$A(T - T_c)|\psi| + \beta|\psi|^3 - \frac{\hbar^2}{m_4} \left(\nabla^2 |\psi| - |\psi| |\nabla\phi|^2\right) = 0.$$
(3.23)

Finally, from equation (3.20), using Maxwell's equations, we obtain the standard expression for a quantum-mechanical current [20]:

$$\mathbf{J}_{\mathbf{e}} = -i\frac{\hbar q}{m} \left[\psi^* \nabla \psi - \psi \nabla \psi^*\right] - 4\frac{q^2}{m} |\psi|^2 \mathbf{A}$$
(3.24)

Introducing module f and phase  $\phi$  of the wave function, this equation is written:

$$\mathbf{J}_{\mathbf{e}} = \frac{\hbar q}{m} f^2 \nabla \phi - 4 \frac{q^2}{m} |f|^2 \mathbf{A} = \Lambda^{-1} \left( \frac{\hbar}{q} \nabla \phi - \mathbf{A} \right) = \frac{n_s q^2}{m} \left( \frac{\hbar}{q} \nabla \phi - \mathbf{A} \right)$$
(3.25)

Putting

$$\Lambda = \frac{m}{n_s q^2} \tag{3.26}$$

one recovers London equation for superconductors:

$$\nabla \times (\Lambda \mathbf{J}_{\mathbf{e}}) = -\mathbf{B}.\tag{3.27}$$

### 3.2 Ginzburg-Pitaevskii equation for superfluid transition

Between the cryogenic fluids, helium (isotope <sup>4</sup>He) exhibits one of the most interesting behavior [48], [52], [54], [56], [76]. Unlike all other substances, the solid state cannot exist at any temperature, unless an external pressure higher than 2.5 MPa is applied. Further, there are two liquid phases: liquid He I and liquid He II. He I is a normal heat conducting fluid. As the normal liquid He I is cooled below a critical temperature, it transforms in a new state, known as He II. The line separating the two physical states is termed  $\lambda$ -line, from the peculiar shape of its specific heat, as shown in Figure 3;  $T_{\lambda}$  is the transition temperature at vapor pressure. He II has exceptional physical features. Most notable are the transport properties, with a vanishing small viscosity and a thermal conductivity many orders larger than that of liquid He I.

The transition of <sup>4</sup>He to superfluidity is related to the phenomenon of Bose– Einstein condensation. It is a complex quantum fluid of strongly interacting particles and corresponds to a flowing ground state in which quasiparticles move. This ground state is described by the complex macroscopic wave function  $\psi = |\psi| \exp(i\phi)$ , with  $\phi$ the phase of the wave function.



Figure 3: Phase diagram of <sup>4</sup>He.

The Landau theory of second-order phase transitions [29], [74] was applied to liquid <sup>4</sup>He, near the  $\lambda$ -point by Ginzburg and Pitaevskii [30]. As for the superconductor transition, the complex wave function  $\psi(\mathbf{x})$  is the order parameter used for the transition. It is assumed that:

$$\rho_s = m_4 |\psi|^2, \qquad \mathbf{v}_s = \frac{\hbar}{m_4} \nabla \phi \tag{3.28}$$

so that the dimensions of  $\psi$  are  $length^{-3/2}$ .

Ginzburg and Pitaevskii consider the fluid at rest in an inertial frame and assume that the free-energy density G can be expanded in powers of  $|\psi|^2$  and  $|\nabla \psi|^2$ , as in (3.11):

$$G(\mathbf{x}) = G_I + \frac{1}{2}\alpha|\psi(\mathbf{x})|^2 + \frac{1}{4}\beta|\psi(\mathbf{x})|^4 + \frac{1}{2}\frac{\hbar^2}{m_4}|\nabla\psi(\mathbf{x})|^2, \qquad (3.29)$$

where  $G_I$  is the free-energy density of He I.

To find the stable state at a given temperature and pressure, the total free energy

$$\mathcal{G}(T,\psi,\mathbf{x}) = \int G(\mathbf{x}) d^3 \mathbf{x}$$
(3.30)

must be minimized with respect to the wave function  $\psi$ .

For minimization with respect to  $\psi^*$  the corresponding Euler-Lagrange equation is

$$\frac{\delta G}{\delta \psi^*} = \frac{\partial G}{\partial \psi^*} - \sum_j \frac{\partial}{\partial x_j} \frac{\partial G}{\partial (\nabla_j \psi^*)} = 0, \qquad (3.31)$$

where  $\nabla_j \psi^*$  is the component of the gradient in the *j* direction. One obtains the following equation

$$\frac{1}{2}\alpha\psi + \frac{1}{2}\beta|\psi|^2\psi - \frac{\hbar^2}{2m_4}\nabla^2\psi = 0.$$
(3.32)

If we had minimized with respect to  $\psi$  rather than to  $\psi^*$  we would simply have the complex conjugate equation. In terms of modulus and phase of the wave function, this equation is written:

$$\alpha |\psi| + \beta |\psi|^3 - \frac{\hbar^2}{m_4} \left( \nabla^2 |\psi| - |\psi| \, |\nabla\phi|^2 \right) = 0.$$
(3.33)

Following Landau theory, one assumes that the coefficients  $\alpha$  and  $\beta$  can be expanded in powers of  $(T - T_{\lambda})$ ; in particular we assume, as in (3.22),  $\beta = B > 0$  constant and

$$\alpha = A(T - T_{\lambda}), \qquad (A > 0). \tag{3.34}$$

The GP equation for superfluid helium is then the analogous of (3.23), namely

$$A(T - T_{\lambda})|\psi| + \beta|\psi|^{3} - \frac{\hbar^{2}}{m_{4}} \left(\nabla^{2}|\psi| - |\psi| |\nabla\phi|^{2}\right) = 0.$$
(3.35)

The free energy assumes the form

$$G(\mathbf{x}) = G_1 + \frac{1}{2}A(T - T_\lambda)|\psi|^2 + \frac{1}{4}\beta|\psi|^4 + \frac{1}{2}\frac{\hbar^2}{m_4}\left[(\nabla|\psi|)^2 + |\psi|^2|\nabla\phi|^2\right].$$
 (3.36)

The contributions to the energy density and to the entropy density due to the order parameter  $|\psi|$  are

$$E^{(f)} = -\frac{1}{2}AT_{\lambda}|\psi|^{2} + \frac{1}{4}\beta|\psi|^{4} + \frac{1}{2}\frac{\hbar^{2}}{m_{4}}|\nabla\psi|^{2}$$
(3.37)

$$S^{(f)} = \frac{1}{2}AT|\psi|^2 \tag{3.38}$$

In particular, if we suppose that the phase  $\phi$  of the wave function is homogeneous, the GP equation simplifies as:

$$A(T - T_{\lambda})|\psi| + \beta|\psi|^3 - \frac{\hbar^2}{m_4}\nabla^2|\psi| = 0.$$
(3.39)

while the free-energy (3.36) becomes:

$$G(\mathbf{x}) = G_1 + \frac{1}{2}A(T - T_\lambda)|\psi|^2 + \frac{1}{4}\beta|\psi|^4 + \frac{1}{2}\frac{\hbar^2}{m_4}(\nabla|\psi|)^2.$$
 (3.40)

Neglecting also inhomogeneities in the modulus of the wave function, we get simply:

$$A(T - T_{\lambda})|\psi| + \beta|\psi|^{3} = 0.$$
(3.41)

$$G = G_1 + \frac{1}{2}A(T - T_\lambda)|\psi|^2 + \frac{1}{4}\beta|\psi|^4$$
(3.42)

## 4 Phase-field models of phase transitions

A phase-field model is a mathematical physical model describing the dynamics of microstructure in complex materials [14], [26], [28], [73]. The method introduces a phase-field variable as an auxiliary field (the phase field) that takes the role of an order parameter. The formalism allows a mesoscopic (coarse-grained) description of the material undergoing a phase transformation, where particles can be thought small enough to resolve micro-scale variations in microstructure. This approach allows also to determine the interface dynamics in a given phase transition problem by integrating a set of partial differential equations for the whole system. It was initially applied to solidification dynamics [10], [27] but also to other systems, as for example vesicle dynamics in biological systems [9], or fracture propagation [47], or ultrafast crystallization [49].

Some formulations of the phase field model are based on a free energy functional depending on an order parameter (variational formulations). Other formulations start by writing directly the phase field equations, without referring to any thermodynamical functional (non-variational formulations).

In the following subsections, two recent formulations of the phase—field model are presented for superconductor and superfluid phase transition.

### 4.1 Phase-field model of superconductor transition

A new phase field model for second order phase transitions was proposed by Fabrizio in [20]. In it the evolution equation for the order parameter was written through a balance equation of the microforces which are assumed to occur during the phase transition (see [25], [26]).

He considered that in any phase transition the states of the two phases are endowed with different structures or symmetries. Noting that for many materials the structure order below a critical temperature is greater than above, He propose a view of the phase equation as a balance law for the action associated to the structure order.

In this framework, consider a body  $\mathcal{B}$  and let the mass density  $\rho$  be constant. For any sub-body  $S \subseteq \mathcal{B}$  the balance of the structure order is represented as

$$\int_{S} \rho Y d^{3} \mathbf{x} = \int_{\partial S} \mathbf{\Pi} \cdot \mathbf{n} dS + \int_{S} \rho \sigma d^{3} \mathbf{x},$$

where  $\rho Y$  is the order structure density,  $\mathbf{\Pi}$  is the order structure flux,  $\mathbf{n}$  is the outward normal to  $\partial S$  and  $\rho \sigma$  is the order supply.

The divergence theorem, the arbitrariness of S and the smoothness of  $Y,\, \Pi$  and  $\sigma$  allow us to write

$$\rho Y = \nabla \cdot \mathbf{\Pi} + \rho \sigma. \tag{4.1}$$

Denoting with f the order parameter, from this equation one can obtain the following balance equation on the power of the structure order:

$$\rho Y f_t = \nabla \cdot (\mathbf{\Pi} f_t) - \mathbf{\Pi} \cdot \nabla f_t + \rho \sigma f_t.$$
(4.2)

For any sub-body S, from (4.2), we have:

$$\int_{S} (\rho Y f_t + \mathbf{\Pi} \cdot \nabla f_t) d^3 \mathbf{x} = \int_{\partial S} \mathbf{\Pi} f_t \cdot \mathbf{n} dS + \int_{S} \rho \sigma f_t d^3 \mathbf{x}.$$
(4.3)

in this equation the left-hand side is the internal power of the structure order, the first term in the right-hand side is the power flux of the order and the last term denotes the external power supply.

In order to study the phase transition, Fabrizio supposed that the terms introduced in equation (4.1) assume the following form [20]

$$\rho Y = \gamma \partial_t f + u_0 F'(f) + u G'(f), \qquad \mathbf{\Pi} = \nu \nabla f, \qquad (4.4)$$

where  $\gamma$  and  $\nu$  are two positive constants while F'(f) and G'(f) are the derivatives of two suitable functions F(f) and G(f), such that F(f) enters as a potential in the free energy and u - G(f) is the entropy function. Therefore, the evolution equation of the order parameter assumes the expression

$$\gamma \partial_t f + u_0 F'(f) + u G'(f) = \nu \nabla^2 f.$$
(4.5)

In this framework, u is the parameter that controls the transition.

Equation (4.5) was specified to describe superconductor transition, by choosing [20]

$$u = \frac{T}{T_c}, \qquad u_0 = 1 \tag{4.6}$$

$$F(f) = -AT_c \frac{f^2}{2} + \beta \frac{f^4}{4}, \qquad G(f) = \frac{1}{2}ATf^2$$
(4.7)

Namely, when the coefficient  $u_0$  of F' is less of the coefficient u of G', we are in the disordered phase. Vice versa, if  $u_0 > u$  we are in ordered phase.

Further applications of this method of superconductivity can be found in [6], [7].

### 4.2 A thermodynamic description of superfluid transition

A phase field model of transition of superfluidity of liquid helium that use the structure order balance equation introduced in previous Subsection was made in [21] and in [22].

Here we will use a different approach, formulated in papers [3], [23], [61]. This approach uses the methods of extended thermodynamics [40], [41], [53], [63] and permits to describe with a unique system both normal liquid helium I and superfluid liquid helium II. Further this model allows to describe the influence of the pressure and of the heat flux on the superfluid transition, a subject which has received much attention in recent years [8], [18], [31], [33], [65].

The model was obtained performing a suitable modification of the non standard one-fluid model of liquid He II [57], [58], [59], [60], [62]. This model selects as fundamental fields the density  $\rho$ , the velocity  $\mathbf{v}$ , the absolute temperature T and the

heat flux  $\mathbf{q}$ . The evolution equations for these fields were determined starting from the balance equations of density, velocity and energy and a Maxwell-Cattaneo-type equation for the heat flux [13].

To describe also normal liquid He I and phase-transition from normal liquid He I to superfluid liquid He II, in [23] a new variable was added, which can be interpreted as the order parameter that controls the transition. This scalar phase field f has dimension of density and is linked to the modulus of the wave function  $\psi(\mathbf{x}, t)$  by the relation

$$f^{2}(\mathbf{x},t) = \rho m_{4} |\psi(\mathbf{x},t)|^{2} = \rho \rho_{s}.$$
 (4.8)

The construction of the theory starts from a general set of evolution equations, adding to the balance equations of mass, momentum and energy two additional balance equations for the order parameter f and for the vector field  $\mathbf{q}$ . Then the constitutive relations are particularized in order to describe the material in consideration. The following set of equations was obtained [61]:

$$\begin{cases} \dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0, \\ \rho \dot{\mathbf{v}} + \nabla p = 0, \\ \rho \dot{\epsilon} + \nabla \cdot \mathbf{q} + p \nabla \cdot \mathbf{v} = 0, \\ \dot{f} + f \nabla \cdot \mathbf{v} + \nabla \cdot (\nu \nabla f) = Q^{f}, \\ \dot{\mathbf{q}} + \mathbf{q} \cdot \nabla \mathbf{v} + \beta \nabla T = \mathbf{Q}^{\mathbf{q}}, \end{cases}$$
(4.9)

where p is the pressure and  $\epsilon$  the internal specific energy, and  $\nu$  and  $\beta$  are suitable coupling coefficients.

In order to determine the expressions of the production terms  $Q^f$  and  $\mathbf{Q}^{\mathbf{q}}$  of the two fields f and  $\mathbf{q}$ , we will suppose that the free-energy density G has the simple expression

$$G = G_1 + G^f = G_1 + \frac{1}{2}\tilde{a}f^2 + \frac{1}{4}\tilde{b}f^4, \qquad (4.10)$$

where  $G_1$  is the free-energy density of He I, and coefficients  $\tilde{a}$  and  $\tilde{b}$  are general functions of the field variables

$$\tilde{a} = \tilde{a}(\rho, T, q^2), \qquad \tilde{b} = \tilde{b}(\rho, T, q^2).$$
(4.11)

Now, we will assume that the production term in the equation of the order parameter is proportional to  $\partial G/\partial f$ 

$$Q^{f} = -K \frac{\partial G}{\partial f} = -K \left[ \tilde{a}(\rho, T, q^{2})f + \tilde{b}(\rho, T, q^{2})f^{3} \right], \qquad (4.12)$$

where K is a positive constant. We obtain the following evolution equation for the phase field f

$$\dot{f} + f\nabla \cdot \mathbf{v} + \nabla \cdot (\nu\nabla f) = Q^f = -K \left[ \tilde{a}(\rho, T, q^2) f + \tilde{b}(\rho, T, q^2) f^3 \right].$$
(4.13)

Now we will determine some constrains for coefficients  $\tilde{a}$  and  $\tilde{b}$ . The first observation is that the stationary solution of equation (4.13), neglecting spatial inhomogeneities of the field variables, are

$$f = 0,$$
  $f^2 = -\frac{\tilde{a}(\rho, T, q^2)}{\tilde{b}(\rho, T, q^2)}.$  (4.14)

The first of them describes the normal phase, and therefore this solution must be stable for T greater than a critical temperature  $T_c$ , instead, the second stationary solution describes the superfluid phase, and must be stable for  $T < T_c$ .

As usual in the thermodynamics of liquid helium, in the following, we will assume the pressure p as independent variable instead of the density  $\rho$ . Further, we will suppose that  $\tilde{a}$  depends on p,  $q^2$  and on the critical temperature  $T_c$ , while  $\tilde{b}$  is independent by the temperature, then we assume

$$\tilde{a} = \mathcal{A}(p, q^2)(T - T_c) \quad \text{and} \quad \tilde{b} = \mathcal{B}(p, q^2).$$
(4.15)

Experiments show that the critical temperature  $T_c$  depends on the pressure and on the heat current, so we have:

$$T_c = T_c(p, q^2).$$
 (4.16)

Therefore, in the space of the thermodynamic variables  $(p, T, q^2)$  we will have a surface of  $\lambda$ -points, of equation  $T = T_c(p, q^2)$ . The equation of this surface can be obtained by using experimental data. First, we will observe that in the absence of heat flux the equation (4.16) must reduce to

$$T_c(p,0) = T_\lambda (1-ap),$$
 (4.17)

where a is the slope of the line of critical points, the so-called  $\lambda$ -line. A glance to Figure 3 shows that coefficient a is positive. If we suppose q not too high, equation (4.16) can be approximated by:

$$T_c = T_c(p, q^2) \simeq T_\lambda \left[1 - ap - bq^2\right], \qquad (4.18)$$

where b can be determined from experimental data. Noting that the presence of the heat flux can create vortices, so destroying superfluidity, we deduce that also coefficient b is a positive coefficient. Equation (4.18) represents a plane of critical points in the space of the variables  $p, q^2$  and T, that we will call  $\lambda$ -plane.

Recalling the microscopic meaning of the order parameter,  $f^2 = \rho \rho_s$ , we can determine the link between coefficients  $\mathcal{A}$  and  $\mathcal{B}$ . In fact, with the assumptions (4.15)

for  $\tilde{a}$  and  $\tilde{b}$ , if we neglect spatial inhomogeneities of the field variables, the non zero stationary solution of equation (4.13) is

$$f^{2} = \frac{\mathcal{A}(p,q^{2})}{\mathcal{B}(p,q^{2})} \left( T_{c}(p,q^{2}) - T \right).$$
(4.19)

Since  $\rho_s/\rho \to 1$ , when  $T \to 0$ , then f must be equal to  $\rho$  when  $T \to 0$ . So we infer that

$$\mathcal{B} = \frac{\mathcal{A}T_c}{\rho^2}.\tag{4.20}$$

Finally, we obtain the following equation:

$$\dot{f} + f\nabla \cdot \mathbf{v} + \nabla \cdot (\nu\nabla f) = -Kf\mathcal{A}(p,q^2) \left[ \left( T - T_c(p,q^2) \right) + \frac{1}{\rho^2} T_c(p,q^2) f^2 \right].$$
(4.21)

Using relations (4.15) and (4.20), the free energy G becomes

$$G(\mathbf{x},t) = G_1 + \frac{1}{2}\mathcal{A}(T - T_c)f^2 + \frac{1}{4\rho^2}\mathcal{A}T_c f^4.$$
(4.22)

This choice of G allows us to obtain the expressions for the entropy density  $S^f$  and the energy density  $E^f$  that depend on the order parameter

$$S^{f} = -\frac{\partial G}{\partial T} = -\frac{1}{2}\mathcal{A}f^{2}, \qquad E^{f} = G^{f} + TS^{f} = \mathcal{A}T_{c}\left(\frac{1}{4\rho^{2}}f^{4} - \frac{1}{2}f^{2}\right). \quad (4.23)$$

For the production terms  $\mathbf{Q}^{\mathbf{q}}$  in the equation for the heat flux, we will choose the expression

$$\mathbf{Q}^{\mathbf{q}} = -\frac{1}{\tau_q(\rho, f)} \mathbf{q},\tag{4.24}$$

with  $\tau_q(\rho, f)$  a scalar coefficient of the dimension of time, that can be interpreted as relaxation time. This coefficient depends on the order parameter f, and it results zero above the  $\lambda$ -line, while it becomes extremely high below the  $\lambda$ -line. As a tentative expression, in the following we will choose

$$\tau_q(\rho, f) = \tau_0 \frac{f^2}{\rho^2 - f^2},\tag{4.25}$$

where  $\tau_0$  is a constant having the dimension of time. Further, we will choose [61]:

$$\beta = \frac{\rho^2}{f^2} \zeta. \tag{4.26}$$

Note that coefficient  $\zeta$  is a nonnegative coefficient. Indeed when f = 0 it results  $\zeta = 0$ , while, in the superfluid state, when  $f = \rho$ , it determines the second sound velocity, that is given by  $V_2 = \zeta/(\rho c_V)$ ,  $c_V$  being the constant volume specific heat [58].

In this way the evolution equation for the heat flux is

$$\dot{\mathbf{q}} + \mathbf{q} \cdot \nabla \mathbf{v} + \frac{\rho^2 \zeta}{f^2} \nabla T = -\frac{\rho^2 - f^2}{\tau_0 f^2} \mathbf{q}$$
(4.27)

When  $f = \rho$  we get the equation:

$$\dot{\mathbf{q}} + \mathbf{q} \cdot \nabla \mathbf{v} + \zeta \nabla T = 0, \tag{4.28}$$

that is identical with the evolution equation for the heat flux found in [57].

We will briefly comment the Maxwell-Cattaneo equation (4.27) that allows us to explore the influence of the heat flux on the phase transition. Writing this equation as

$$\mathbf{q} = -\frac{\tau_0 \rho^2 \zeta}{\rho^2 - f^2} \nabla T - \frac{\tau_0 f^2}{\rho^2 - f^2} \left( \dot{\mathbf{q}} + \mathbf{q} \cdot \nabla \mathbf{v} \right)$$
(4.29)

we see that the thermal conductivity  $\chi$  near the phase transition is:

$$\chi = \frac{\tau_0 \rho^2 \zeta}{\rho^2 - f^2}; \tag{4.30}$$

as one sees  $\chi$  becomes extremely high below the  $\lambda$ -line, when the helium is in the superfluid phase (in fact  $k \to \infty$  when  $f \to \rho$ ), while when f = 0 one get  $\chi = \tau_0 \zeta$ , i.e. the heat conductivity of He I.

## 5 Concluding remarks

In this paper, phase-field models to describe phase transition in superconductors and superfluids have been revised, both in the stationary (Section 3) and in the non stationary case (Section 4). The phase field models to describe time-dependent phase transitions, which have been applied here to superconductors and superfluids, can be also applied to describe other aspects of phase transitions.

We will focus on three situations: 1) Comparison of the influence of quantized vortices in superconductor phase transition and in superfluid phase transition; 2) phase transition in cosmological models, and in particular with models using a supe-fluid vaccuum; 3) superfluid phase transitions in <sup>3</sup>He. Of course, another interesting situation would be to generalize this analysis to rotating Bose-Einstein condensates.

Comparison of the influence of quantized vortices in superconductor phase transition and in superfluid phase transition. We have provided this short review of phase-field models of superconductor and superfluid phase transitions in order to foster the comparison of them. This comparison is well known in equilibrium situations, but our interest is to extend it to nonequilibrium regimes. In particular, two aspects should be considered. On the one side, a comparison of the role of quantized vortices on the phase transition (electric current vortices with quantized magnetic flux in superconductors, and mass current vortices with quantized velocity circulation in superfluids).
These vortices could be respectively produced by a magnetic external field [1] (in superconductors) and by an imposed global rotation [19], [44], [55] (in superfluids), or by means of an electric current (in superconductors) and a heat flow [77](in superfluids). Indeed, we have mentioned the different responses of superconductors of type I and II with respect to the penetration of a magnetic field, and the Meissner effect. One could consider, analogously, the superfluid phase transition in helium superfluid in a rotating container. For the usual helium I phase, the fluid behaves as a normal viscous fluid, and it exhibits a global rotation. Instead, when the system becomes superfluid, the global rotation (the global angular momentum of the fluid) becomes an ensemble of localized rotations in the form of vortex lines with quantized velocity circulation, with the quantum of circulation given by (2.11) and with vortex lines distributed in a regular way. Thus, the dynamics from the global to the local form is of much interest [34], [85].

The second aspect is to consider the influence of an electric current or a heat flow on the respective phase transitions. This topic is of especial practical interest, because superconductors are used to carry high intensity electric currents, and superfluids helium is used in cryogenic situations to remove heat. In both cases, a too high value of the current destroys the superconductivity or the superfluidity, with dangerous consequences for the control and the evolution of the corresponding system.

Phase transitions in cosmology. Symmetry-breaking phase transitions are assumed to play an important role in cosmology. For instance, it has been speculated that, in the hot early universe, the quantum vacuum (i.e. the various quantum fields that fill space) possessed a large number of symmetries. As the universe expanded and cooled, the vacuum underwent a series of symmetry-breaking phase transitions. For example, the electroweak transition broke the SU(2)xU(1) symmetry of the electroweak field into the U(1) symmetry of the present-day electromagnetic field.

Since the several symmetry-breaking phase transition proposed in cosmology are difficult to consider from a direct experimental perspective, there are several proposals to consider them by means of analogies with superfluids [12], [64], [79], [80], [82]. Several models incorporating superfluidity are considered for several ingredients of the cosmological models: dark matter [36], [37], [45], [83], dark energy [17], [37], [38], quantum vacuum [39], [46], [70], [71], [72], [86], and Higgs field [15]. For instance, the action of the Higgs field, giving mass to elementary particles, could be analogous to a superfluid [70], [71], [72]. Particles moving at constant speed in the superfluid do not experience any resistance, but those accelerating throught it exhibit a resistance to change their velocity, i.e. the analogous of an inertial mass appears related to the several particles, according to their coupling to the Higgs field. Models proposing superfluid features for dark matter [5] are able to match the successes of the L cold dark matter model at cosmological scales with the added feature of yielding the modified Newtonian dynamics at the galactic scale. Instead, the connection between dark energy and superfluidity has been carried out through quantum turbilence [38]. A relatively simple model of the relation between quantum turbulence and dark energy

has been carried out in [42], [43], where the properties of the quantized vortex loops in superluids have been compared to those of cosmic string loops. This rich interface between superfluid models and cosmology is still lacking apossibly relevant feature, namely, the role of the cosmic expansion as a possible source of quantized vortices. In this sense, having a phase-field model as those described in this could be of special interest in the early inflationary eras of the universe, or in the decoupling eras.

Phase transition in superfluid  ${}^{3}He$ . Helium 3 boils at 3.191 K. The first observations of a superfluid transition in liquid  ${}^{3}He$  were made by Osheroff, Richardson and Lee [67]. They observed two phase transitions: the first, called the A-transition. occurs at 2.65 mK and is a higher-order phase transition. The lower-temperature B, occurring at 1.8 mK, is a first-order phase transition, with an associated latent heat.

The phase diagram of  ${}^{3}$ He at low temperatures is shown in the following figure. There are two superfluid phases, A and B, which both show very unusual properties. For increasing magnetic fields, a widening phase A1 develops.



Figure 4: Phase diagram of <sup>3</sup>He plotted against temperature, pressure, and magnetic field H.

The superfluid transition temperature of <sup>3</sup>He depends on the magnetic field, a unique feature for pure liquid. At H = 0 there are two phases, A and B. For increasing magnetic fields, a widening phase A1 develops, which forms between the A-phase and the normal liquid.

The diagram indicates the existence of three phases in addition to the normal fermi liquid occurring above  $T_c$ . The intersection point between the A, B and normal Fermi liquid is called the *polycritical point*. It is suggested that the three phases occur in <sup>3</sup>He because it is a magnetic superfluid. In <sup>3</sup>He three orientations are possible for the nuclear spin, two with parallel and one with anti-parallel alignment.

One of the most interesting aspects of  ${}^{3}$ He in the superfluid regime are those associated to its anomalous behavior in the energy transport mechanisms. Among these are temperature waves (second sound), viscosity that depends on the mechanism used for measurement, the existence of vortex lines in the bulk fluid, and extremely high thermal conductivity.

In superfluid <sup>4</sup>He, these properties are explained in terms of the two-fluid hydrodynamics or of the one-fluid model deduced by extended thermodynamics. Also the similar properties of superfluid <sup>3</sup>He can be explained by using the usual two-fluid model or equivalently by using the one fluid model with internal variable. There is a fundamental difference between <sup>3</sup>He and <sup>4</sup>He in that <sup>3</sup>He atoms have spin  $\frac{1}{2}$  whereas <sup>4</sup>He atoms have spin 0. Since the Bose-Einstein transition can take place only in bosonic systems (namely, with spin integer), the only form for <sup>3</sup>He to become a superfluid is to couple two <sup>3</sup>He in a way analogous to Cooper electron pairs in metals for superconductivity. Therefore, the existence of several transitions and several superfluid phases is to be expected: in one of them, the pair of <sup>3</sup>He atoms will have spin 0, and in another one it will have spin 1. Spin 1 situations are characterized by an angular momentum and a magnetic momentum: it is not surprising that in this case a magnetic field may have an effect on the corresponding superfluid phase transition. The phenomenology of <sup>3</sup>He is therefore much richer than that of <sup>4</sup>He, but since it takes place at much lower temperaturas it has less practical interest than that of <sup>4</sup>He.

The vortex lines in <sup>3</sup>He quantum turbulence will be more complicated than in <sup>4</sup>He. In the latter one, a vortex line may be described by a simple line, characterized at each point by its unit tangent; instead, in <sup>3</sup>He the vortex line will have at each point two characteristic vectors: the unit tangent and the magnetic moment. This will give to the dynamics of the vortex lines a wider diversity of possibilities [4], [16], [24], [51], [69]. From the point of view of cosmological applications this wider diversity is of interest, as it allows to describe scalar bosons (like Higgs boson) and vectorial bosons (as photons and gluons) [78].

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