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Decomposability of Mixed States into Pure States and Related Properties

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The nonunique decomposability of mixtures into pure states, the occurrence of dispersion for pure states, the existence of coherent superpositions of pure states, and the non-Boolean structure of the associated logic are typical quantum features. Connections among these properties are examined in the general framework of the so-called convex description.

1. INTRODUCTION

Moving from the standard formulation of classical mechanics to the standard Hilbert-space formulation of quantum mechanics, we are faced with a number of concomitant features: the pure states take dispersion, different pure states no longer need to be orthogonal and there arise coherent superpositions of them, the convex decomposition of nonpure states into pure ones becomes nonunique and the convex set of states is no longer a simplex, there arise mutual incompatibility among observables, and the ordered structure of the two-valued observables that form the quantum logic loses the distributivity.

The studies on the foundations of classical and quantum mechanics, the quantum measurement issue (see, e.g. Busch *et al.*, 1991), the recently developing theory of mesoscopic systems, the phase-space representations of quantum theories (see, e.g., Bugajski, 1993), the problem of nonlinear extensions of quantum theories (Bugajski, 1991), and many other issues of theoretical physics have pushed the characterization of classicality and of quantum behavior into more general frameworks within which one can ask

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which features should be basic for any *classical* or *quantum* theory, and how these features are intertwined.

So, questions arise like (Beltrametti and Cassinelli, 1981*a*):

(i) To what extent does the nonunique decomposition of mixed states have to accompany the birth of coherent superpositions and of nonorthogonal pure states?

(ii) To what extent does a theory in which the mixed states have or have not a unique decomposition into pure states imply that the pure states are or are not dispersion-free?

(iii) Under which hypotheses is the nondistributivity of the ordered structure $\mathscr{L}$ of the two-valued observables forming the quantum logic equivalent to the nonsimplex nature of the set $S(\mathscr{L})$ of probability measures on $\mathscr{L}$?

The nonunique decomposition of nonpure states translates the fact that quantum mixtures do not have a memory of the pure states of which they are made, i.e., there are infinitely many different families of pure states which can generate, by suitable convex combinations, one and the same physical state. The existence of coherent superpositions of pure states is intrinsic to the linearity of the theory. The presence of dispersion for pure states is a typical expression of the nondeterministic nature of the theory. The lack of distributivity of $\mathscr{L}$ accompanies the fact that such a structure is no longer an algebraic model of classical logic. Thus by the questions above we ask, loosely speaking, to what extent the memory the mixtures have of the pure states of which they are made is related to linearity, to determinism, or to the kind of logic mirrored by $\mathscr{L}$.

An answer to these questions is the purpose of this paper. Of course, the characterization of classical and quantum theories has to be viewed within some sufficiently general frame, able to encompass a number of physical theories, including those commonly considered as classical, nonclassical, and of an intermediate type.

An adequate framework is offered by the so-called convex description [see, for a review, Lahti and Bugajski (1985) and Busch *et al.* (1989)], which gives a major role to the shape of the convex set of states of the physical system under consideration. Classical theories there appear as associated to sets of states which are a type of simplex, whereas a similarly simple intrinsic characterization of the set of states of a quantum theory appears less definite. In the next section we sketch some basic elements of the convex description, and in Section 3 the notion of unique decomposability of mixed states is given. The questions (i) and (ii) above are then discussed in Sections 4 and 5 respectively.

The traditional *logical* approach (see, e.g., Beltrametti and Cassinelli, 1981*b*), which gives a major role to the ordered structure of the two-valued observables that form the quantum logic (associating Boolean structures to classical theories and orthomodular nondistributive structures to quantum theories), can be to some extent translated into the convex description by the linearization procedure of Rüttimann (1993): we come to this in Section 6, where the question (iii) is examined.

Let us mention that the convex description admits a Hilbert-space realization called "generalized quantum mechanics" (Busch *et al.*, 1989), and encompasses, besides the standard quantum mechanics, all C^*- and W^*-algebraic theories, including the commutative (hence *classical*) ones.

2. CONVEX DESCRIPTION

Let S_0 be a convex set whose elements we interpret as states of the physical system. Let ∂S_0 denote the set of extreme points of S_0, i.e., the set of pure states contained in S_0.

An affine mapping from S_0 into the convex set $M_1^+(\mathbb{R})$ of all probability measures on the family $\mathscr{B}(\mathbb{R})$ of Borel subsets of $\mathbb{R}$ is naturally interpreted as an observable. Write $O(S_0)$ for the set of all affine mapping from S_0 into $M_1^+(\mathbb{R})$, i.e., all possible observables related to S_0 with values in $\mathbb{R}$. For $B\in O(S_0)$ and $\alpha\in S_0$, $B(\alpha)$ is thus a probability measure on $\mathscr{B}(\mathbb{R})$; if we evaluate $B(\alpha)$ at $X\in\mathscr{B}(\mathbb{R})$, we get a number $[B(\alpha)](X)$, contained in the unit interval $[0, 1]$ of $\mathbb{R}$, to be interpreted as the probability that the observable B takes a value in X given that the physical system is in the state α. When we look at the number $[B(\alpha)](X)$ as defining a function from S_0 into $[0, 1]$, we write for this function $E_{B,X}$, i.e., $E_{B,X}(\alpha) = [B(\alpha)](X)$. The functions of the form $E_{B,X}$ obviously belong to the family $A^b(S_0)$ of all real affine bounded functions on S_0.

We assume that S_0 is the base of a base normed space, which implies that $A^b(S_0)$ is an order-unit Banach space with respect to the pointwise ordering. The functions of the form $E_{B,X}$ belong to the order interval $[0, e]_0$ of $A^b(S_0)$, where 0 is the constant zero function [the origin of $A^b(S_0)$] and e the constant unity function [the order unit of $A^b(S_0)$]. Actually we have more: every element of the order interval $[0, e]_0$ is of the form $E_{B,X}$ for some $B\in O(S_0)$ and $X\in\mathscr{B}(\mathbb{R})$. Indeed, if $u\in[0, e]_0$ we take the observable B_u defined by the property that $B_u(\alpha)$ is the probability measure on $\mathscr{B}(\mathbb{R})$ concentrated at the real numbers 1 and 0 where it assumes the values $u(\alpha)$ and $1-u(\alpha)$, respectively.

The elements of the order interval $[0, e]_0$ of $A^b(S_0)$, hence the functions of the form $E_{B,X}$, are called effects. For any observable $B\in O(S_0)$ the function $E_B:\mathscr{B}(\mathbb{R})\to[0, e]_0$ defined by $E_B(X) = E_{B,X}$ is an effect-valued measure on $\mathscr{B}(\mathbb{R})$ which we call the semispectral resolution of B. Conversely, any effect-valued measure on $\mathscr{B}(\mathbb{R})$ defines an observable.

The set $[0, e]_0$ is convex, and its extreme elements are called decision effects or sharp effects. If u is a sharp effect, then its norm is 1, and $e - u$ is also sharp. An observable is called sharp if the range of its semispectral resolution is contained in the set $\partial[0, e]_0$ of sharp effects. In standard quantum mechanics sharp observables correspond to projection-valued measures.

The weak topology defined on S_0 by $[0, e]_0$, i.e., the weakest topology that makes continuous all elements of $[0, e]_0$, will be called the physical topology.

3. UNIQUE DECOMPOSABILITY

We can now approach the notion of unique decomposability of a mixed state into pure states: intuitively it means that any (mixed) state can be represented in a unique way as a convex sum, or integral, of pure states. Thus, if $\alpha \in S_0$ has the unique decomposability property, then there must exist one and only one measure μ_α (possibly discrete) on ∂S_0 such that

$$u(\alpha) = \int_{\partial S_0} u(\beta)\, d\mu_\alpha(\beta) \qquad \text{for any} \quad u \in [0, e]_0$$

But to guarantee a precise meaning to this notion, we should be sure that the set of pure states is sufficiently rich and meets some regularity properties. To overcome this problem, let us first notice that the elements of S_0 can be viewed as real bounded functions on $A^b(S_0)$ [if $f \in A^b(S_0)$, just define $\alpha(f) := f(\alpha)$], hence as elements of the base normed Banach space $A^b(S_0)^*$, the dual of $A^b(S_0)$. More specifically, S_0 is embedded into the base S of $A^b(S_0)^*$. The physical topology of S_0 coincides with the one induced on S_0 by the weak* topology of $A^b(S_0)^*$, and we shall thus call physical the weak* topology restricted to S. With respect to this topology, S is compact and S_0 is dense in S. Going from S_0 to S, we just add states which, loosely speaking, can be approached by the elements of S_0.

Since S is compact, the notion of unique decomposability for its elements becomes precise without any further assumption. Denoting by ∂S the set of extreme points of S (of course $\partial S_0 \subseteq \partial S$), we can then state that $\alpha \in S$ is uniquely decomposable into pure states if there exists one and only one probability (Radon) measure μ_α on the weak* closure $\overline{\partial S}$ of ∂S (notice that ∂S does not need to be measurable, while $\overline{\partial S}$ does) such that

$$u(\alpha) = \int_{\overline{\partial S}} u(\beta)\, d\mu_\alpha(\beta) \qquad \text{for any} \quad u \in [0, e]_0$$

If every $\alpha \in S$ is uniquely decomposable, we shall say that S is classical. In such a case a number of consequences follow (Alfsen, 1971, pp. 103, 104): (1) S is a Bauer simplex, (2) ∂S is closed, i.e., $\overline{\partial S} = \partial S$, (3) S is homeomorphic and affinely isomorphic to the convex set $M_1^+(\partial S)$ of all probability measures on ∂S (equipped with the vague topology), and (4) $A^b(S_0)$ and $A^b(S_0)^*$ are vector lattices.

Notice that every element of $A^b(S_0)$ has a unique continuous extension on S, hence $A^b(S_0)$ is embedded into the order-unit Banach space $A^b(S)$ of all real bounded affine functions on S, and consists of the (weak*) continuous elements of $A^b(S)$. To emphasize this fact, $A^b(S_0)$ will also be denoted by $A(S)$, the set of all real, affine, (weak*) continuous functions on S. Writing $[0, e]$ for the order interval of $A^b(S)$, we have that $[0, e]_0$ is a (weak*) dense subset of $[0, e]$ and consists of its continuous elements.

4. CLASSICAL STATES AND COHERENT SUPERPOSITIONS

The existence of coherent superpositions of quantum pure states expresses, in standard quantum mechanics, the linearity of the underlying Hilbert space. In the present, more general approach a pure state $\alpha \in \partial S$ will be said to be a coherent superposition of two other pure states α_1, α_2 ($\neq \alpha$) whenever α belongs to the smallest norm-exposed face of S containing both α_1 and α_2, i.e., whenever $u(\alpha_1) = u(\alpha_2)$ implies $u(\alpha) = u(\alpha_1)$ for any effect $u \in [0, e]$ (Lahti and Bugajski, 1985).

If S is classical, then any of its extreme points is a split face of S (Alfsen, 1971, p. 144), and we define the projective unit $u_\alpha \in [0, e]$ associated to α by $u_\alpha(\beta) := \lambda$, with $\beta = \lambda\alpha + (1 - \lambda)\alpha'$ the unique decomposition of $\beta \in S$ into the split face $\{\alpha\}$ and its complementary face $\{\alpha'\}$. It is clear that $u_\alpha(\alpha) = 1$, while $u_\alpha(\gamma) = 0$ for any $\gamma \in \partial S \setminus \{\alpha\}$. Hence α cannot be a coherent superposition of other pure states: indeed, should α be a coherent superposition of α_1, α_2 we would have $u_\alpha(\alpha_1) = u_\alpha(\alpha_2) = 0$ but $u_\alpha(\alpha) = 1$, a contradiction. Thus we have the following partial answer to the question (i) of Section 1:

Proposition 1. In a classical S there are no coherent superpositions.

The reverse does not hold: the absence of coherent superpositions in S does not imply that S is classical. Indeed, there are examples of compact convex sets which are not simplexes, but their extreme points are split faces so that there are no coherent superpositions (Asimov and Ellis, 1980, pp. 108–110). Thus there are possible nonclassical models without coherent superpositions.

In the convex approach the notion of orthogonality is usually defined by saying that α is orthogonal to β, with $\alpha, \beta \in \partial S$, whenever there is an effect $u \in [0, e]$ such that $u(\alpha) = 1$ and $u(\beta) = 0$. Hence, if S is classical then all its pure states are mutually orthogonal. The above mentioned examples show that the reverse does not hold: the mutual orthogonality of all pure states of a compact convex set S does not ensure that S is classical.

5. CLASSICAL STATES AND DISPERSION

There are three different roots for the appearance of a nonzero dispersion, or variance, of an observable at some state of the physical system. First, the state might be nonpure: the occurrence of dispersion is then common to both classical and quantum theories. Second, the observable might be not sharp: this possibility arises in our convex framework in which the notion of observable is more general than usual; it would not occur in standard classical mechanics nor in standard quantum mechanics where one deals only with sharp observables; in any case the occurrence of dispersion due to unsharpness of the observable is again common to both classical and quantum theories. Third, we might have dispersion even if the observable is sharp and the state is pure: this possibility, translating a basic probabilistic nature of a theory, is commonly accepted as a peculiar, distinguishing feature of the quantum case. It is precisely this last case that we want to pick up and formalize.

In view of the correspondence between observables and effect-valued measures on $\mathscr{B}(\mathbb{R})$, we can handle the notion of dispersion-free states, restricting our attention to those observables which are effects. The dispersion, or variance, of the effect $u \in [0, e]$ in the state $\alpha \in S$ is easily seen to be

$$V(u, \alpha) := u(\alpha) - u(\alpha)^2$$

and we have that, for fixed continuous u, $V(u, \alpha)$ is a weak* continuous and concave function on S so that, by the so-called Bauer Maximum Principle (see, e.g., Hartkämper and Neumann, 1974), it attains its minimum on ∂S, while, for fixed α, $V(u, \alpha)$ is a weak* continuous and concave function on $[0, e]$, so that it attains its minimum on the set $\partial[0, e]$ of extremal elements of $[0, e]$, i.e., at some sharp effect (this agrees with the so-called Alfsen Dispersion Theorem).

The above remarks confirm that in order to pick up the dispersion coming from the shape of S, i.e., the one irreducibly inherent in the given formal model, we have to restrict consideration to sharp effects and pure states.

The vanishing of the variance $V(u, \alpha)$ means $u(\alpha) = 0, 1$. In general, a sharp effect does not need to attain the values 0 and 1 on ∂S: when it does we shall say that it is definite. Then we are led to say that $\alpha \in \partial S$ is dispersion-free if $u(\alpha) = 0, 1$ for all sharp definite effects. Consequently, S will be called nondispersive if all its pure states are dispersion-free.

We come now to the question (ii) raised in Section 1, namely the connection between the classicality and the nondispersiveness of the set of states. Half of the question is answered by the following:

Proposition 2. If S is classical, then it is nondispersive.

Proof. First notice that in a Bauer simplex any norm-exposed face is split (Alfsen and Shultz, 1979, Proposition 1.6). If u is sharp and definite, then the splitting property of $u^{-1}(1)$ and $u^{-1}(0)$ implies $u(\alpha) = 0, 1$ for any $\alpha \in \partial S$, which means that the pure states are dispersion free, i.e., S is nondispersive. ■

The converse, however, is not true: the nondispersiveness of S does not imply that S is classical. We get the simplest counterexample by taking for S a square in $\mathbb{R}^2$ (Davies, 1972): the pure states are the vertices of the square, and they are dispersion-free, but S is clearly nonclassical. Less trivial counterexamples are provided by the prime simplexes (Alfsen, 1971, p. 164; Asimov and Ellis, 1980, p. 124), which are nondispersive but nonclassical; they occur in some models of algebraic statistical theories (Bratteli and Robinson, 1979, Example 4.3.26).

Thus the problem arises of seeing which additional conditions should be imposed on a nondispersive set of states to make it classical. To this purpose let us recall that $\alpha \in \partial S$ is said to be projective if there exists a P-projection P_α on $A^b(S_0)^*$ such that α is the only element of S which belongs to the image of P_α. The P-projections (Alfsen and Shultz, 1976, 1979; Asimov and Ellis, 1980) provide a direct generalization of the von Neumann–Lüders operations in the quantum measurement theory (Busch *et al.*, 1991), of filters in the operational approach (Bugajski and Lahti, 1980; Lahti and Bugajski, 1985), of the conditioning in the noncommutative probability theory (Edwards and Rüttimann, 1990), and of the Sasaki projections in orthomodular lattices (Alfsen and Shultz, 1979). Now we have:

Proposition 3. For a compact convex set S the conditions (i) S is nondispersive, (ii) S is the σ-convex hull of ∂S, and (iii) every element of ∂S is projective, are jointly sufficient to make it classical.

Proof. Conditions (ii) and (iii) imply that to every projective face $\{\alpha\}$, $\alpha \in \partial S$, is associated a definite sharp effect u_α (the projective unit associated to the P-projection P_α) such that $u_\alpha^{-1}(1) = \{\alpha\}$ (Alfsen and Shultz, 1976, Corollary 2.13). Then (i) implies that $\{\alpha\}$ has to be a split face. Let F be a norm-closed proper face of S. By (ii) we have that ∂F is nonempty and $\partial F = F \cap \partial S$, so that F is the σ-convex hull of ∂F. All split faces of a compact convex set form a complete Boolean lattice under set-inclusion ordering (Edwards, 1972, Proposition 3.10); therefore F is a split face, being the lattice join of the split faces $\{\alpha\}, \alpha \in \partial F$. This means that S is a simplex, since all its norm-closed faces are split (Alfsen and Shultz, 1979, Proposition 1.6). We have still to prove that S is a Bauer simplex. Any weak*-closed ("closed" for short) face is norm closed, hence it is split. Moreover, any closed face F defines a closed subset $F \cap \partial S$ of ∂S; conversely, the σ-convex hull of any closed subset of ∂S defines, by (ii), a closed face which is split. This one-to-one correspondence between closed split faces of S and closed subsets of ∂S means that the weak* (physical) topology of ∂S is equivalent to the so-called facial topology, which implies that S is a Bauer simplex (Alfsen, 1971, Theorem II.7.6). ■

Notice that the conditions (ii) and (iii) above are rather restrictive and we might ask whether they could be weakened; they are satisfied, however, by the state space of any atomic JBW-algebra (Alfsen and Shultz, 1978), in particular they are met in standard quantum mechanics.

6. CLASSICAL STATES AND BOOLEAN LOGIC

To handle the question (iii) of Section 1 we need a bridge from the "logical" to the "convex" description. To build the bridge starting from the side of the convex description, based on the set S of states, it would be natural to identify its *logic* with the poset $\partial[0, e]$, orthocomplemented by $u \mapsto u^\perp := e - u$. Notice that some other possibilities have been considered in the literature, e.g., identifying the logic associated to S with the set of projective units of $[0, e]$, or with the set of P-projections (filters) over $A(S)^*$. But for spectral convex sets (Alfsen and Shultz, 1976) these structures become isomorphic to $\partial[0, e]$, which acquires the property of being a complete orthomodular lattice.

If S is classical, then $A^b(S)$ is a Banach lattice, and it is easy to show (Hartkämper and Neumann, 1974, pp. 7, 8) that $\partial[0, e]$ is Boolean. However, the Boolean character of $\partial[0, e]$ is not enough to guarantee that S is classical: just remark that $A^b(S)$ is a Banach lattice (hence $\partial[0, e]$ is Boolean) for any simplex S, not necessarily a Bauer one. Nevertheless S is "nearly classical" since it is weak* dense in the base Σ of $A^b(S)^*$: every element of S is thus uniquely decomposable into the extreme points of the Bauer simplex Σ.

Let us now face the problem of the bridge between the logical and the convex descriptions, starting from the side of the former. Thus we take from the outset an orthomodular lattice $\mathscr{L}$ whose elements correspond to special two-valued observables of our physical system, and we denote by $S(\mathscr{L})$ the convex set of all probability measures, or states, on $\mathscr{L}$.

Every $a \in \mathscr{L}$ defines a real affine (bounded) function $u_a: S(\mathscr{L}) \to [0, 1]$ through $u_a(\alpha) := \alpha(a)$, $\alpha \in S$. The family of all such functions determines the weak topology on $S(\mathscr{L})$, to be called the $\mathscr{L}$-topology, with respect to which $S(\mathscr{L})$ is compact (Fischer and Rüttimann, 1978). The same family of functions, in short $\mathscr{L}$ itself, can thus be viewed both as a subset of the order interval $[0, e]$ of the Banach space $A^b(S(\mathscr{L}))$ of all real affine bounded functions on $S(\mathscr{L})$, and as a subset of the order interval $[0, e]_0$ of the Banach space $A(S(\mathscr{L}))$ of all real affine $\mathscr{L}$-continuous functions on $S(\mathscr{L})$. Now, $A^b(S(\mathscr{L}))$ is the second Banach dual of $A(S(\mathscr{L}))$, hence $A(S(\mathscr{L}))$ is canonically identified with a weak* dense, norm-closed subspace of $A^b(S(\mathscr{L}))$. In this way the *logical* pair $\mathscr{L}$, $S(\mathscr{L})$ generates the triple $S(\mathscr{L})$, $A(S(\mathscr{L}))$, and $A^b(S(\mathscr{L}))$ basic for the convexity models. This transition from the logical to the convex description is a special case of the linearization procedure worked out by Rüttimann (1993).

We can now handle the question (iii) of Section 1, which is answered by the following:

Proposition 4. If $S(\mathscr{L})$ is strongly ordering on $\mathscr{L}$, then $S(\mathscr{L})$ is classical (i.e., a Bauer simplex) if and only if $\mathscr{L}$ is Boolean.

Proof. Suppose $S(\mathscr{L})$ is a simplex. The strong ordering property of $S(\mathscr{L})$ implies that any $a \in \mathscr{L}$ is uniquely determined by $a^{(1)} := \{\alpha \in S(\mathscr{L}) | \alpha(a) = 1\} = \{\alpha \in S(\mathscr{L}) | u_a(\alpha) = 1\}$, and $a \le b \Leftrightarrow a^{(1)} \subseteq b^{(1)}$, $a, b \in \mathscr{L}$. Clearly $a^{(1)}$ is a closed exposed face of $S(\mathscr{L})$, and if $S(\mathscr{L})$ is a simplex, any $a^{(1)}$ is a split face (Asimov and Ellis, 1980, Theorem 2.7.2). Since the split faces of a compact convex set form a Boolean lattice, the mapping $a \mapsto a^{(1)}$ embeds $\mathscr{L}$ into the Boolean lattice of the split faces of $S(\mathscr{L})$ preserving the orhtomodular lattice structure of $\mathscr{L}$, hence $\mathscr{L}$ is Boolean. Conversely, assume that $\mathscr{L}$ is Boolean. The Stone representation theorem and the Stone–Weierstrass theorem (Asimov and Ellis, 1980, Theorems 6.14 and 6.9) lead us now to identify $A(S(\mathscr{L}))$ with $C(\partial S(\mathscr{L}))$, the Banach space of real continuous functions on the extreme boundary of $S(\mathscr{L})$. This implies that $S(\mathscr{L})$ is homeomorphic and affinely isomorphic to $M_1^+(\partial S(\mathscr{L}))$, which is a Bauer simplex. ■

Notice that if $S(\mathscr{L})$ is a simplex and is strongly ordering, then $\mathscr{L}$ becomes represented by a subset of $\partial[0, e]$ (Alfsen and Shultz, 1976, Proposition 10.2 and Corollary 2.13). The problem of identifying the elements of $\mathscr{L}$ with sharp effects in $\partial[0, e]$ in a more general context has been examined by Cook (1978), Cook and Rüttimann (1985), and Keller (1989).

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