Random-coefficient pure states and statistical mixtures

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Within the field of quantum information processing, the development of Blind Quantum Source Separation and Blind Quantum Process Tomography has led, within the formalism of the Hilbert space, to the introduction of the concept of a random-coefficient pure state. This paper describes an experimental situation necessitating its introduction. Links between a random-coefficient pure state and a statistical operator ρ are established. The meaning of these links is dependent upon the meaning given to ρ, and the two usual ways for introducing the ρ concept are first examined. The interest of the random-coefficient pure states is briefly introduced.

I. INTRODUCTION

In modern science, the information concept was implicitly introduced in the field of Physics, when Boltzmann gave a microscopic interpretation of entropy [1], 2] and when, more than fifty years later, Szilard used the entropy concept together with his intelligent beings [3]. The developments of Telecommunications and Electronics then led to the birth and growing of a Theory of Information (see e.g. the appearance of the so-called Shannon entropy). All the corresponding activities took place in a classical context. The correspondence principle allows us to see these concepts, theories, and associated physical objects as a limit of some quantum tools, and quantum information (QI), quantum computation and QI Processing (QIP) have been developing for several decades.

The present paper uses the standard Hilbert space framework, i.e. standard Quantum Mechanics (QM): as a result of its postulates, including the existence of a principle of superposition (of states), then, given a quantum system Σ, one introduces its state space E, a Hilbert space. It is considered that when a measurement is started, Σ may be found in a pure state (described by a ket in the Dirac formalism), as a result of a preparation act, and that less specific states of Σ may be described with the mixed state or statistical mixture (of states) concept. Both pure states and statistical mixtures may be formally described with a density operator ρ. The time behavior of an isolated system obeys the Schrödinger equation. The standard Hilbert space framework is used by both the so-called standard (or "orthodox") interpretation of QM and by the statistical one (Einstein, Blokhintsev, Ballentine), more or less implicitly accepted by many users of QM. The formal constructions and possible results from mathematical physicists involved in quantum field theory or trying to build general quantum theories aiming e.g. at unifying general relativity and QM are out of the scope of the present paper. We therefore stress that we presently non exhaustively eliminate such approaches as: 1) the one initiated by Segal ([4], 1947), with his introduction claiming "Hilbert space plays no role in our theory", an approach then developed by Haag and Daniel Kastler, and known as the C*-algebra formulation of QM, 2) the one from Mielnik ([5], 1974) and again Haag, together with Bannier [6]. These approaches are not even mentioned in the book by Laloé devoted to the interpretations of QM [7], which just testifies to the vastness of the existing debate about the foundations of QM.

Working in the field of Quantum Information Processing (QIP) for some fifteen years, we have been led first to extend the classical field of Blind Source Separation (BSS) [8],[9] to a quantum version, namely Blind Quantum Source Separation (BQSS) [10], [11], [12], [13]. More recently we introduced the field of Blind Quantum Process Tomography (BQPT), an extension of Quantum Process Tomography [14], [15],[16], [13]. In these contexts, we were led not to use the ρ formalism, but to introduce what is hereafter called a Random-Coefficient Pure State (RCPS); Σ being an isolated quantum system, E its state space, with dimension d, and \{{\mid k >}\} an orthonormed basis of E, it is supposed that at some time t, Σ may be in a random-coefficient pure state

\[
\mid \Psi > = \sum_{k} c_k \mid k > , \tag{1}
\]

where the c_k are Random Variables (RV), with the constraint \(\sum_k |c_k|^2 = 1\). In contrast, the coefficients of the development of the usual pure states are deterministic quantities. Our present aim is to stabilize the RCPS concept, and is neither a historical review of QM aspects nor a discussion of the foundations of QM. However, the content given to the concept of a statistical mixture is still linked to its historical origins, which can’t be completely forgotten if this concept is to be examined, in order to better identify possible links between an RCPS
II. ABOUT THE STATISTICAL MIXTURE CONCEPT

With a physical observable quantity $O$ attached to $\Sigma$, QM associates a linear Hermitian operator $\hat{O}$ acting on the states of $\Sigma$. The mean value of $\hat{O}$ when $\Sigma$ is in the pure (normed) state $|\Psi\rangle$ is a quantity that reads $<\Psi | \hat{O} | \Psi>$ in the Dirac formalism. If $\Sigma$ is in a mixed state described synthetically as $\{p_i, |\varphi_i\rangle\}$, where the normed pure state $|\varphi_i\rangle$ contributes with a weight $p_i$ to the statistical mixture (for any $i$, $0 < p_i < 1$ and $\sum_i p_i = 1$), the mean value of $\hat{O}$ is equal to $\sum_i p_i <\varphi_i | \hat{O} | \varphi_i>$. The writing $\{p_i, |\varphi_i\rangle\}$ is considered ambiguous, as it may happen that two apparently different so-defined mixed states may lead to the same mean value for $\hat{O}$, and this for any observable $O$, and this ambiguity is eliminated by introducing the statistical operator $\rho = \sum_i p_i | \varphi_i \rangle \langle \varphi_i |$, acting linearly on the (hereafter assumed to be normed) states of $\Sigma$. $\rho$ is Hermitian, positive (its eigenvalues are all non-negative) and its trace is equal to 1. The eigenvalue spectrum of a Hermitian positive operator with finite trace is entirely discrete, a result of Hilbert space theory ([117], page 335). When an isolated system is in a statistical mixture, $\rho$ obeys the Liouville-von Neumann equation. In the special case when $\Sigma$ is in a pure state $|\Psi\rangle$, its statistical operator is the projector $\rho = |\Psi \rangle \langle \Psi |$. The statistical operator $\rho$ obeys the relation $Tr \rho^2 \leq Tr \rho$, and the equality is verified iff $\rho$ is a projector, i.e. if and only if $\rho$ describes a pure state.

There are presently two ways of introducing the concept of a mixed state or statistical mixture. The first one was developed by von Neumann in his 1932 canonical book [18], after his 1927 paper [19]. In his book, von Neumann, having considered the probability content attached to a pure state [20], adds "the statistical character may become even more prominent, if we do not even know what state is actually present - for example when several states $\varphi_1$, $\varphi_2$, ... with the respective probabilities $w_1$, $w_2$, ... ($w_1 \geq 0$, $w_2 \geq 0$, ..., $w_1 + w_2 + ... = 1$) constitute the description" of the system of interest ([18], pages 295-296). $S$ being his quantum system of interest, von Neumann moreover considers (cf. [18], page 298) "great statistical ensembles which consist of many systems $S_1$, ..., $S_N$, i.e., $N$ models of $S$, $N$ large", adopting the so-called frequency interpretation of probabilities and referring to von Mises [21], [22]. Similarly, at the beginning of his Chapter V, devoted to thermodynamical questions, von Neumann introduces a mental ensemble of identical systems in which he measures some operator $R$, now separating this ensemble into sub-ensembles according to the result of the measurement. Von Neumann started Ch. IV of [18] saying that in his previous chapter he had "succeeded in reducing all assertions of quantum mechanics" to a formula expressing that the mean value of a physical quantity $O$ when the system is in the state $|\Psi\rangle$ is equal to a quantity written, with our notations, as $<\Psi | \hat{O} | \Psi >$. But he had rather postulated it in his Ch. III [23]. Consequently, given a system $\Sigma$ in a statistical mixture described by $\rho$ and $\hat{O}$ attached to an observable $O$ of $\Sigma$, the assertion that everything should be contained in the expression $E(\hat{O}) = Tr (\rho \hat{O})$ expresses a postulate.

The second way of introducing the statistical mixture concept also appeared in 1927, in a paper by Landau [24]. In the following decades, the books by Kemble on QM ([25], 1937) and by Tolman on Statistical Mechanics ([26], 1938), the synthetic papers by F. London and Bauer ([27], 1939) and by Fano ([28], 1957) [29] all referred to von Neumann, and none cited Landau, possibly for two reasons: 1) the conditions of its publication (Landau was 19 years old, he was from the USSR and international relations were under tension), 2) a difference between Landau's and von Neumann's points of view: the first section of [24], short and explicitly devoted to this subject, is entitled "Coupled systems in wave mechanics", and Landau writes: "A system cannot be uniquely defined in wave mechanics; we always have a probability ensemble (statistical treatment). If the system is coupled with another, there is a double uncertainty in its behaviour". But if some operator is then introduced through a Partial Trace procedure in the presence of such a coupling, this operator does not obey the Liouville-von Neumann equation, and calling it a statistical or density operator may lead to some confusion. Already in 1935, but in a different context - discussions about entanglement after the EPR paper - Schrödinger was led to examine two systems which "enter into temporary physical interaction due to known forces between them, and" ... "after a time of mutual influence" ... "separate again" [30]. However, in Volume III of their Course of Theoretical Physics (English translation of the second edition, [31]) Landau and Lifshitz first supposed that a "closed system as a whole is in some state described by a wave function $\Psi(q, x)$, where $x$ denotes the set of coordinates of the system considered, and $q$ the remaining coordinates of the system considered". Through an integration over the $q$ variables, corresponding to the introduction of a partial trace, they introduced an operator which they again called a density matrix (thus keeping the difference with its now well-accepted meaning resulting from the von Neumann approach). Then, in a second step only, they "suppose that the system" (of interest) "is closed, or became so at some time".
The possibility of a confusion resulting from the use of the expression density matrix (or statistical operator) by both von Neumann and Landau under different assumptions (the possible existence of a coupling of the system of interest with a second system in Landau’s approach) was eliminated, at least in principle, by Feynman when, in Chapter 2 entitled *Density matrices* of his 1972 inspiring treatise *Statistical Mechanics* [32], he used an approach which, instead of following von Neumann and his postulate, improved Landau’s treatment, leading to what we will call *The Landau-Feynman definition of a statistical mixture*. Feynman considers a system $\Sigma$ composed of two parts, the system of interest, $\Sigma_1$, and $\Sigma_2$, the rest of the universe. He explicitly writes “it is unknown whether or not the rest of the universe is in a pure state”. In the following, as in [13], $\Sigma_2$ will be the collection of systems with which $\Sigma_1$ may interact at the chosen time scale, the whole system $\Sigma$ being isolated at this time scale. This restricted meaning used for $\Sigma_2$ should be accepted by most physicists, if the concept of the preparation of $\Sigma_2$ into a pure state, to be used shortly, is to be meaningful.

At a time $t_0$ when $\Sigma_1$ and $\Sigma_2$ are uncoupled, $\Sigma_1$ and $\Sigma_2$ are separately prepared, each in a pure state, $\Sigma$, the global system, is therefore in a pure state $|\Psi(t_0)\rangle$. In a situation when, after this preparation act, an internal coupling exists between $\Sigma_1$ and $\Sigma_2$, and this until some time $t_1$, one is interested in the behaviour of one’s system of interest $\Sigma_1$ for $t \geq t_1$, i.e. at the time when this coupling disappears or after this time, the system of interest being then isolated, at the chosen time scale.

Feynman, in a thorough, concise, rarely cited analysis, first observes that for $t > t_0$ the whole system obeys the Schrödinger equation, and then, for $t \geq t_1$, i.e. after the disappearance of this internal coupling, he calculates the mean value of $\hat{O}$ for an arbitrary observable $\hat{O}$ of $\Sigma_1$, his system of interest. He shows that:

1) this mean value at $t_1$ is equal to $\text{Tr}_1\{\rho_1(t_1)\hat{O}\}$, where $\rho_1(t_1) = \text{Tr}_2\rho(t_1)$, $\rho(t_1)$ being the projector $|\Psi(t_1)\rangle < |\Psi(t_1)\rangle$, and $|\Psi(t_1)\rangle >$ the ket describing $\Sigma$ at $t_1$, according to the Schrödinger equation. $\text{Tr}_1$ (resp. $\text{Tr}_2$) is a trace calculated over the kets of an orthonormed basis of $\Sigma_1$ (resp. $\Sigma_2$).

2) $t_1$ being replaced with $t$, result 1) keeps true for any time $t > t_1$.

3) For $t \geq t_1$, the partial trace $\rho_1(t)$ obeys the Liouville-von Neumann equation. The use of the Schrödinger equation for $t \geq t_1$ for the establishment of this property implies that when $t \geq t_1$, $\Sigma_1$ may be submitted to time-dependent forces giving birth to a time-dependent Hamiltonian, the sources of these forces (e.g. an oscillating magnetic field acting on a spin magnetic moment) being then included in this system of interest $\Sigma_1$. In the rest of this paper, when it is spoken of an isolated system, the system will possibly include such a source.

One may then say that, once $\Sigma_1$ is uncoupled to $\Sigma_2$, if one is interested in the mean value of the Hermitian operator attached to an observable of $\Sigma_1$ only, everything happens as if $\Sigma_1$ were in a statistical mixture (of states) described by the statistical operator $\rho_1(t)$ (it can be verified that $\rho_1(t)$ verifies all the properties of a statistical operator).

While the existence of a statistical mixture is a postulate in von Neumann’s approach, a significant interest of Feynman’s treatment is that it proposes a possible origin of a statistical mixture, only using already existing quantum postulates, and specifically the fact that the mean value of $\hat{O}$ in state $|\Psi\rangle$ is $<\Psi|\hat{O}|\Psi\rangle$.

The assumptions made, and when $t \geq t_1$, the obtained results may be read by claiming that the system of interest $\Sigma_1$ keeps a memory of its past coupling with $\Sigma_2$, and once this has been said the existence of $\Sigma_2$ should be forgotten. The way $\rho_1(t_1)$ is introduced shows that this claimed memory is a manifestation of the (so-called quantum) correlations created by the $\Sigma_1 - \Sigma_2$ coupling which did exist between $t_0$ and $t_1$ and created an entangled state.

Of course, someone could take $\Sigma_2$ as the system of interest, and introduce his own so-called reduced statistical operator $\rho_2(t)$. But nothing allows him to add that the state of $\Sigma$ is $\rho_1(t) \otimes \rho_2(t)$, and starting speaking of some ignorance interpretation will not change the situation. This should be obvious, since $\Sigma$ is in a pure state $|\Psi(t)\rangle$, while $\rho_1(t) \otimes \rho_2(t)$ generally corresponds to a statistical mixture.

Since the existence of this book by Feynman, it may be considered that the von Neumann and the Landau-Feynman approaches have both their own interest. And e.g. QPT often considers a composite system made up of the system of interest (state space $\mathcal{E}_1$) and its environment (state space $\mathcal{E}_2$) and introduces a partial trace over (a basis of) $\mathcal{E}_2$ (see e.g. Ch. 8 of [33], and [34]).

In 1966 B. d’Espagnat had called a statistical mixture as defined by von Neumann a proper mixture, and one defined through partial tracing an improper mixture [35]. The 1972 clarification by Feynman eliminated the relevance of this distinction, since the expression improper mixture may suggest that a Landau-Feynman mixture has a poorer quality than a von Neumann one, whereas its existence is just a consequence of the postulates of quantum mechanics. Unhappily, d’Espagnat kept his distinction after 1972 [36], with, consequently, controversies about its relevance (see e.g. [37]).

### III. RANDOM-COEFFICIENT PURE STATES

We first recall an experimental situation which necessitates the Random-Coefficient Pure State (RCPS) concept. We then establish links between an RCPS and a statistical mixture as described by a density operator $\rho$. 

A. An experimental situation with a system in an RCPS

We recall a simple situation - detailed, in the context of BQSS, in [13] - when the random-coefficient pure state concept is meaningful. \( \Sigma \) consists of the magnetic moment \( \vec{\mu} \) of an electron spin \( 1/2 \), with \( \vec{\mu} = -G \vec{s} \) (isotropic tensor), in a static field \( \vec{B}_0 = B_0 \vec{Z} \) with amplitude \( B_0 \). Writing the Zeeman Hamiltonian as \( h = -\vec{\mu} \cdot \vec{B}_0 = GB_0 s_Z \) indicates that while the spin is a quantum object, the magnetic field is treated classically. Someone (the Writer) first prepares the spin in the \(| + Z \rangle \) eigenstate of \( s_Z \) (eigenvalue \(+1/2\)). The moment is then received by a second person (the Reader), who ignores the direction of \( \vec{B}_0 \), chooses some direction \( z \) (unit vector \( \vec{u}_z \)) attached to the Laboratory as the quantization direction and introduces a Laboratory-tied cartesian frame \( x y z \), used to define \( \theta_E \) and \( \varphi_E \), the Euler angles of \( \vec{Z} \). Since the field is treated classically, \( \theta_E \) and \( \varphi_E \) behave as classical variables, while \( s_Z \) is an operator. The Reader measures \( s_z = \vec{s} \cdot \vec{u}_z \) (eigenstates: \(+\) and \(-\)), and is interested in the probability \( p_{+z} \) of getting \(+1/2\). An elementary calculation indicates that, when the time writing and reading may be neglected:

\[
| + Z \rangle = r|+\rangle + \sqrt{1-r^2} e^{i\varphi}|-\rangle, \tag{2}
\]

with

\[
r = \cos \frac{\theta_E}{2}, \quad \varphi = \varphi_E. \tag{3}
\]

and therefore \( p_{+z} = \cos^2 \theta_E/2 \). Once the direction of \( \vec{B}_0 \) has been chosen, state \(| + Z \rangle \) is then unambiguously defined. If this direction has a deterministic nature, \( r \) and \( \varphi \) are deterministic variables, and \(| + Z \rangle \), usually called a pure state, may be called a deterministic-coefficient pure state. If \( \theta_E \) and \( \varphi_E \) obey probabilistic laws, one may consider that the quantum quantities \( r \) and \( \varphi \), which depend upon the classical Random Variables (RV) \( \theta_E \) and \( \varphi_E \), do possess the properties of conventional, i.e., classical, RV. We are not strictly facing the quantum equivalent of a classical situation here. Rather, the stochastic character of the field direction, with classical nature, is reflected in the random behavior of the quantum state expressed through Eq. (2). While random operators are well known e.g. in NMR (see Ch. VIII of [38]), we here meet a random-coefficient pure state. And the probability \( p_{+z} \), equal to \( \cos^2 \theta_E/2 \), is therefore itself a random variable.

In the field of probability theory, a vector whose components are random variables is called a random vector (see e.g. page 243 of [39]). In Eq. (2), \(| + Z \rangle \), with its random coefficients \( r \) and \( \varphi \), may therefore be called a random ket, or as describing a random pure state (of the spin \( 1/2 \)), and since our 2007 paper [10], we always used these expressions with this meaning. However, in the present paper, instead of speaking of a random pure state we introduce the expression random-coefficient pure state, specifically because already in 1990 Wootters spoke of three possible kinds of what he called random pure states [40].

B. From random-coefficient pure state to statistical operator

We now consider an isolated quantum system \( \Sigma \), \( E \) its state space, with dimension \( d \), and an orthonormed basis \(| k \rangle \) of \( E \). At some time \( t \), \( \Sigma \) is supposed to be in an arbitrary random-coefficient pure state

\[
| \Psi > = \sum_k c_k | k >, \tag{4}
\]

where the \( c_k \) are RV, with the constraint \( \sum_k | c_k |^2 = 1 \). One is interested in the mean value then taken by the scalar Hermitian operator \( \hat{O} \) associated with some observable of \( \Sigma \). One first considers a given choice of the value of each RV \( c_k \). The contribution of this specific, then deterministic-coefficient, pure state, denoted as \( | \Psi_s > \), is, from the rules of QM:

\[
< \Psi_s | \hat{O} | \Psi_s > = \sum_{k,l} c_k^* c_l < k | l > c_l, \tag{5}
\]

The mean value of \( \hat{O} \) when \( \Sigma \) is in this RCPS is defined as the expected value, or mathematical expectation, of this quantity:

\[
E\{< \Psi_s | \hat{O} | \Psi_s >\} = \sum_{k,l} E\{c_k^* c_l\} \hat{O}_{kl} \tag{6}
\]

\[
= \sum_{k,l} r_{lk} \hat{O}_{kl} \tag{7}
\]

\[
= Tr(r \hat{O}), \tag{8}
\]

where, in the chosen basis, \( \hat{O}_{kl} = < k | \hat{O} | l > \) and

\[
r_{lk} = < l | r | k >= E\{c_k^* c_l\} \tag{9}
\]

\[
r = \sum_{k,l} r_{kl} | k > < l |. \tag{10}
\]

In the following, \( E\{c_k^* c_l\} \), also called the mean value of \( c_k^* c_l \) (cf. pages 47-48 and 326-327 of [26]), will be denoted as \( < c_k^* c_l > \), as often done in the field of QM (see e.g. Eq. (3.3.36) of [41]). The introduction of the linear operator \( r \) with matrix elements \( r_{lk} \) in the \{ \(| k > \) \} basis, and that of a trace, are the consequences of the superposition principle and of the fact that the expectation of the sum is equal to the sum of the expectations. \( r \) has the following properties, resulting from a transposition of the usual arguments in the presence of a statistical mixture to the present situation, i.e. an arbitrary RCPS (cf. also the Appendix):

1) for any pair \((k,l)\), \( r_{lk} = r_{kl}^* \): the operator \( r \) is Hermitian,
2) in a basis \(\{|i\rangle\}\) in which the Hermitian operator \(r\) is diagonal, its diagonal elements are its eigenvalues; being of the form \(E\{c_i|c_i|^2\} = p_i\), they are all non-negative (\(r\) is a positive operator), and their sum is equal to 1,

3) for any ket \(|u\rangle\), \(<u|r|u\rangle \geq 0\), since it is equal to \(\sum_i p_i |<i|u\rangle|^2\).

4) \(H\) being the Hamiltonian of \(\Sigma\), for each choice of the \(c_k\) values the corresponding ket \(|\Psi_s\rangle\) obeys the Schrödinger equation, and from \(t_r\) on, \(r\) follows the Liouville-von Neumann equation \(i\hbar dr/dt = [H, r]\).

This operator \(r\) has all the properties of a statistical operator. This result had been suggested, for a qubit, in [13]. The case when a statistical operator \(\rho\) is first given will be examined in the next subsection.

C. From a statistical operator to random-coefficient pure states

We now come to the situation found when a statistical mixture is described by a statistical operator \(\rho\), and examine whether it is possible to find at least one or possibly more than one random-coefficient pure state with which one may associate the same statistical operator \(r\) equal to \(\rho\). The present situation may be called the inverse problem of the one discussed in Subsection III B. Starting with system \(\Sigma\) and its state space \(\mathcal{E}\), it is assumed that \(\Sigma\) is in a statistical mixture described by a statistical operator \(\rho\). In an orthonormed basis of \(\mathcal{E}\), \(\{|i\rangle\}\), in which \(\rho\) is diagonal:

\[
\rho = \sum_i p_i |i\rangle\langle i| \tag{11}
\]

where the \(p_i\) are probabilities. We are first able to show that at least some well-chosen RCPS \(|\Psi_1\rangle = \sum_i c_i |i\rangle\), developed over this basis and the \(c_i\) being RV, may be associated with a statistical matrix \(r\) equal to that representing \(\rho\) in that basis, even while the following strong conditions have been imposed upon the coefficients \(c_i\):

1) the RV \(c_i\) are real, which avoids considering complex RV.

2) RV \(c_d\) obeys \(c_d = \delta \sqrt{1 - \sum_{i=1}^{d-1} c_i^2}\), \(\delta\) being an RV taking the values +1 and −1, each with probability 1/2, and \(\delta\) is statistically independent from all the \(c_i\) with \(i < d\).

3) All the \(c_i, c_j \neq i\) pairs with \(i < d\) and \(j < d\) are statistically independent. 4) each RV \(c_i\) with \(i < d\) obeys a centered, truncated \(|c_i| \leq 1\) Gaussian probability density function, with a variance equal to \(p_i\). As a consequence of these assumed properties, if \(i < d\), \(j < d\) and \(i \neq j\), then \(r_{ij} = <c_j|c_i> > 0\), and if \(i < d\) and \(j = d\), then \(r_{id} = <c_d|\sqrt{1 - \sum_{i=1}^{d-1} c_i^2}\) and, as \(\delta\) is independent from the \(c_i\) and \(c_d\) is a centered RV, \(r_{id} = 0\); the same is true for \(r_{ij}\) with \(j < d\). Therefore, the non-diagonal matrix elements of \(r\), the statistical matrix associated with this random-coefficient pure state in the chosen basis, namely the mean values \(r_{ij} = <c_j|c_i>\), with \(j \neq i\), are all equal to 0: in the orthonormed basis \(|i\rangle\) both \(r\) and \(\rho\) are diagonal matrices. And, from 4), \(r_{ii} = p_i\).

Therefore, starting from a statistical mixture described by a density operator \(\rho\), it has been possible to build a random-coefficient pure state with a matrix \(r\) equal to \(\rho\).

We will say that \(|\Psi_1\rangle >\) may be associated with \(\rho\).

A second possible random-coefficient pure state \(|\Psi_2\rangle\), again written as in Eq. (4) (the \(c_i\) are again RV), may be supposed to obey assumptions 1), 2), 3), whereas 4) is now replaced by the following condition 4') each RV \(c_i\) with \(i < d\) has a centered truncated \(|c_i| \leq 1\) Laplace probability density function, again with a variance equal to \(p_i\). Then \(|\Psi_2\rangle >\) may be associated with \(\rho\).

A third possible random-coefficient pure state \(|\Psi_3\rangle\), again written as in Eq. (4) (the \(c_i\) are again RV) may be built, which is supposed to obey the following conditions: assumptions 1) and 2) are kept, but it is now assumed that: 3') \(i < d\), \(j < d\) and \(i \neq j\), any mean value \(r_{ij} = <c_j|c_i>\) is equal to zero and 4") for any value of \(i, c_i\) obeys \(c_i^2 > p_i\). Then \(|\Psi_3\rangle >\) may be associated with \(\rho\).

At first sight, the existence of more than one random-coefficient pure state possibly associated with a given statistical operator \(\rho\) is reminiscent of the well-known situation briefly mentioned in Section II in the context of statistical mixtures. If, for instance, first using the von Neumann definition of a statistical mixture, and considering a spin 1/2 and either the standard basis \(|\{|+, -\rangle\}\) or the basis \(|\{|+\rangle, |-\rangle\}\) in which \(s_z\) is diagonal, one then introduces the following two mixtures:

\[
|+\rangle, p_+ = \frac{1}{2}, |-\rangle, p_- = \frac{1}{2}; \tag{12}
\]

\[
|+\rangle, p_{x+} = \frac{1}{2}, |-\rangle, p_{x-} = \frac{1}{2}. \tag{13}
\]

they are both associated with the same statistical operator \(\rho = I/2\ (I: \text{identity operator})\), and this keeps true for any other direction than \(x\). In fact, since the statistical operator associated with the first mixture may be expressed introducing the projectors \(P_+ = |+\rangle\langle+| \text{ and } P_- = |-\rangle\langle-|\), then writing this statistical operator as

\[
\rho_z = \frac{1}{2}(P_+ + P_-), \tag{14}
\]

and doing similarly with the second mixture, introducing successively \(P_{x+}, P_{x-}, P_x\), one finally finds that \(\rho_z = \rho_x = I/2\), and this is true for any direction. In this well-known case, whereas the physical processes for obtaining e.g. the first mixture (standard basis) and the second one (\(s_z\) basis) have been different, the same statistical operator \(\rho = I/2\) is then mobilized. Peres ([42], page 75) proposes an instance of a statistical mixture of three pure states, while \(d = 2\). This statistical mixture may of course be written as a sum implying two projectors. The present situation, with RCPS, is however different from the one usually found in QM, just illustrated with the instance given with Eqs. (12) and (13) and the introduction of the projectors \(P_+, P_-, P_{x+}, \text{ and } P_{x-}\), finally leading to the same density operator \(\rho = I/2\). If
one thought of presently operating similarly, one could think of introducing the concept of a random projector $| \Psi > < \Psi |$ associated with a random-coefficient pure state $| \Psi >$, as opposed to the usual projector, associated with a deterministic-coefficient pure state. In the orthonormed basis $\{| k >\}$, this random projector would be represented by a matrix with elements $P_{ij} = c_{i}^{*}c_{j}$, with a random nature. But doing this can’t help in clarifying the content of the random-coefficient pure state concept, since a random projector would precisely start from that concept.

IV. DISCUSSION

If the spectrum of the Hermitian operator $\hat{O}$ associated with an observable of $\Sigma$ is discrete, with eigenvalues $\omega_{i}$ in finite number and without degeneracies, and if $\{| \omega_{i} >\}$ is a basis of $\mathcal{E}$ made up of eigenkets of $\hat{O}$, then, if $\hat{O}$ is measured while $\Sigma$ is in the pure (deterministic) state $| \Psi > = \sum_{i}c_{i}|\omega_{i} >$, all $c_{i}$ being complex deterministic coefficients with $\Sigma_{i}|c_{i}|^{2} = 1$, QM postulates that the only possible results are the $\omega_{i}$, obtained with the probabilities $|c_{i}|^{2}$. In this paper, considerations about the foundations of QM are limited to those directly linked with the subject under discussion. The question of the nature of the mathematical object $\rho >$, discussed by Laloë asking ”Does it describe ensembles of systems only (statistical description), or one single system as well (single events)” [7], is out of our scope. When some ambiguity could perhaps exist, we called $| \Psi >$ a deterministic-coefficient pure state, as opposed to the random-coefficient pure states considered in this paper. One should however at least mention Bell’s strong reluctance in giving a place to the operation of measurement in the foundations of QM [43]. His question ”Was the wavefunction of the world waiting to jump for thousands of millions of years until a single-celled living creature appeared? Or did it have to wait a little longer, for some better qualified system … with a PhD?” is well-known. It may be said that his question was provocative, but this is a statement about the question, not an answer. This question may in the long term affect the content given to the statistical mixture concept.

In Section III the usual point of view was adopted, according to which two different preparations, leading to mixtures first respectively called $\rho_{x}$ and $\rho_{y}$, in fact should be identified with the same statistical mixture, namely $I/2$. But if one accepts the place measurements do presently occupy in the foundations of QM, the question is: why should the role of preparations be simultaneously minimized? One then should not ignore Zeh’s position, who claimed [44] that ”the density matrix formalism cannot be a complete description of the ensemble, as the ensemble cannot be rederived from the density matrix.”.

With these reservations, we accept the place presently given to the measurement process. Having chosen the Hilbert space machinery, we however do not promote the idea that, within this formalism, an isolated quantum system should be either in a (deterministic-coefficient) pure or in a mixed state, and this for two different reasons as commented hereafter.

The first reason is the fact that the way one speaks of a statistical mixture may introduce a confusion. Undoubtedly, when von Neumann spoke (his note 156, page 298 of [18]) of the so-called collectives introduced by von Mises, he was thinking of a statistical behavior. When, before an election, statisticians introduce some mean citizen who is to vote for candidate A with a $x\%$ probability, everybody understands that they speak of a mental object, not of a true citizen [45]. But already in the 1939 paper [27], the title of Section 4, Mélanges et cas purs (mixtures and pure cases), if taken literally, could be understood as referring to the same quantum physical object, able to be either in a pure state or in a mixture of pure states. And similarly, an implicit use of some economy of thought process is probably a reason for saying that a quantum system $\Sigma$ isolated from its neighbours may be either in a pure state or in a statistical mixture (cf. our Section I), but may be in fact a source of confusion, if taken literally. Therefore, when, in the Lectures on quantum Mechanics from Steven Weinberg, one reads ([41], page 69) ”As far as calculating expectation values is concerned, we can” … ”say that the system is in any of the states $\Psi_{n}$ with probabilities $P_{n}$,” (we are not interested here with the rest of the sentence), one should understand that when calculating some expectation value, everything happens as if the system were in these states with these probabilities, an idea quite compatible with the fact that it truly is in a given pure state. It should therefore be kept in mind that the statistical operator $\rho$, which is said to describe both a pure state and a statistical mixture, is a synthetic tool which subsumes the corresponding distinct realities - the physical system, the mental statistical object - through a single state space, in which $\rho$ operates.

The second reason is the core of this paper. In Subsection III A an experimental situation was described leading to the existence of Random-Coefficient Pure States, this within the formalism of the Hilbert space and with the usual postulates of QM, except, of course, any possible one eliminating more or less implicitly the existence of RCPS. The formalism of the statistical operator $\rho$ usually only manipulates mean values of observables (and possibly some function of these observables, e.g. a dispersion with a link to the Heisenberg inequalities), in connection with the results obtained when measuring these observables. The fact that with a given statistical operator $\rho$ one may associate more than one RCPS suggests the possibility that, given a RCPS, and using adequate statistical methods, more information could be obtained from this random-coefficient pure state than the one which can be obtained through the formalism of the statistical operator $\rho$. Treating a simple case, we have very recently been able to show that this is precisely the case, a result
established and presented in a separate paper [46].

V. CONCLUSION

Quantum mechanics, within the standard Hilbert space framework, considers that the physical system may exist in a (deterministic-coefficient) pure state, as the result of some preparation act, and that, more generally the state of an isolated system may be described as a statistical mixture, both accepting a description with the statistical operator $\rho$. In the development of Quantum Information Processing and more specifically of Blind Quantum Source Separation (BQSS) and Blind Quantum Process Tomography (BQPT), the use of the concept of a random-coefficient pure state has been found useful. In the present paper it was established that with a given random-coefficient pure state one may associate a single, well-defined, density operator, and that with a given density operator one may associate more than one random-coefficient pure state. Speaking of a statistical mixture one may associate more than one random-coefficient pure state of the present paper it was established that with a given density operator one may associate a single, well-defined, density operator, and that with a given density operator one may associate more than one random-coefficient pure state. In contrast, the manipulation of a random-coefficient pure state makes an explicit use of random quantities, the coefficients of its development over a basis of the state space, with a more informative content, through their statistical laws.

Appendix A: Properties of the operator $r$

A justification of some properties obeyed by the operator $r$ associated with a random-coefficient pure state, introduced in Subsection III B, is given here, using the notations of that section. $r$ acts on the (deterministic-coefficient) states of $E$, the state space of $\Sigma$. For instance, when considering $r|\Psi_s\rangle$, $r$ acts on the (deterministic-coefficient) state $O|\Psi_s\rangle$ resulting from the action of $O$ on the (deterministic-coefficient) state $|\Psi_s\rangle$.

Property 1: hermiticity of $r$. If $X$ is a complex random variable with $X = A + iB$, $A$ and $B$ being real random variables, then $(E\{X\})^* = E\{A\} - iE\{B\} = E\{X^*\}$ (expectation and complex conjugation commute). Therefore, considering the matrix with elements

$$r_{lk} = E\{c^*_lc_l\}$$

in the chosen basis, then $r^*_{kl} = (E\{c^*_lc_k\})^* = E\{c^*_lc_k\} = r_{lk}$. Therefore, the matrix with elements $r_{lk}$ and the operator $r$ are Hermitian.

Property 3: $< u | r | u > = < u | \sum_i p_i | i > < i | u > = \sum_i p_i | < i | u >|^2 \geq 0$.

Property 4: $\Sigma$ has been assumed to be isolated, with Hamiltonian $H$. Once a (deterministic-coefficient) pure state $|\Psi_s\rangle$ has been defined, its time evolution is well-defined, following the Schrödinger equation. If a random-coefficient quantum state is defined at some time $t_r$ (reference), as $|\Psi_{rk}\rangle = \sum_k c_k | k >$, its time behaviour is therefore defined by this Hamiltonian and by the probability laws associated with the random variables $c_k$ defined at time $t_r$. Consequently:

$$\frac{d}{dt} r = \sum_{k,l} \frac{dr_{kl}}{dt} | k > < l |$$

$$= \sum_{k,l} \frac{dE\{c^*_lc_k\}}{dt} | k > < l |$$

$$= \sum_{k,l} E\{\frac{d(c^*_lc_k)}{dt}\} | k > < l |$$

$$= \sum_{k,l} E\{\frac{d^*_lc_k + c^*_l \frac{dc_k}{dt}}{dt}\} | k > < l | \quad (A5)$$

Since $ih \sum_k (dc_k/dt) | k >= \sum_k c_k H | k >$, then

$$i\hbar \frac{d}{dt} r = \sum_{k,l} E\{-c_k c^*_l | k > < l | H + c^*_l c_k H | k > < l | \}$$

$$= -r H + H r$$

$$= [H, r]. \quad (A6)$$

$r$ therefore obeys the Liouville-von Neumann equation.

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Today, probability theory is generally treated with Kolmogorov’s axiomatic approach. In this 1939 letter, Kolmogorov considers the meaning of his approach, stressing that when probabilities are used in a practical situation, the mathematical treatment should be seen as an idealization, and he refers to von Mises and his frequentist description.

See property $E_2$ in page 203 of the 1932 book by von Neumann, and in its page 210: “we recognize $P.$ (or $E_2$ .) as the most far reaching pronouncement on elementary processes”. And von Neumann has first written: “We shall now assume this statement $P.$ to be generally valid” (page 201), and “We shall now deduce $E_3.$ from $P.$, and $E_2.$ from $E_1.$.” (page 203).

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Presently, it is generally considered that the statistical operator $\rho$ (which von Neumann denoted as $U$), obeys the Liouville-von Neumann equation, and we keep the idea that any definition of $\rho$ should be compatible with this property. We then follow Fano, when, in Section 3 of his 1957 paper, he introduces “an incoherent superposition of a number of pure states $\psi_i^{(i)}$ with statistical weights $p_i^{(i)}$” and a density operator which he denotes $\rho$, a procedure compatible with the von Neumann approach. We do not follow him when, after starting Section 11 with the following observation: “When two systems $a$ and $b$ interact, or have been in interaction for a certain period of time, practical interest often centers in the resulting state of a only, irrespective of what has become of $b$”, and being interested in a situation when a is still coupled to $b$, and wanting to treat what is seen as an irreversible process, he focuses upon $a$, and calls $\rho^{(a)}$, the operator which he obtained through a partial trace over $b$ states, explicitly noting that this operator does not obey his Eq. (3.12), the Liouville-von Neumann equation (which he calls the Schrodinger equation).

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