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Solving the Zeh Problem About the Density Operator with Higher-Order Statistics

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Abstract: Since a 1932 work from von Neumann, it has been considered that if two statistical mixtures are represented by the same density operator ρ, they should, in fact, be considered as the same mixture. In a 1970 paper, Zeh introduced a thought experiment with neutron spins, and suggested that, in that experiment, the density operator could not tell the whole story. Since then, no consensus has emerged yet, and controversies on the subject still presently develop. In his 1995 book, speaking of the use of the density operator, Peres spoke of a von Neumann postulate. In this paper, keeping the random variable used by von Neumann in his treatment of statistical mixtures, but also considering higher-order moments of this random variable, it is established that the two mixtures imagined by Zeh, with the same ρ, should however be distinguished. We show that the rejection of that postulate, installed on statistical mixtures for historical reasons, does not affect the general use of ρ, e.g., in quantum statistical mechanics, and the von Neumann entropy keeps its own interest and even helps clarifying that confusing consequence of the postulate identified by Peres.

Keywords: statistical mixture; density operator; von Neumann postulate; von Neumann entropy; higher-order statistics

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1. Introduction

The developments of Physics, Communications and Electronics have led to the birth and growing of a Theory of Information, first in the classical context (see, e.g., the appearance of the Shannon entropy [1]) and, for several decades, in the quantum domain (see, e.g., the *Feynman Lectures on Computation* [2], and *Quantum Computation and Quantum Information* by Nielsen and Chuang [3]). A second quantum revolution is now spoken of, which also stimulates a reflection on some basic ideas of Quantum Mechanics (QM). A question asked by Zeh more than fifty years ago [4] about the content of the density operator ρ, which we will call *the Zeh problem*, is still waiting for an answer. In the field of quantum Information Processing (QIP), it has been possible, in a given context, not to use the density operator formalism (see, e.g., [5–8] and the explanations in [8]). In the following pages, the Zeh problem is discussed and solved.

The present paper uses standard Quantum Mechanics (QM). As a result of its postulates, including the existence of a principle of superposition (of states), which the late Nobel Laureate Steven Weinberg called the first postulate of QM [9], then, given a quantum system Σ, and its state space $\mathcal{E}$, a Hilbert space, any vector of $\mathcal{E}$ (defined up to a phase factor

$e^{i\varphi}$, φ being a real quantity) represents a possible state of Σ called a pure state. This standard Hilbert space framework is used by both the Copenhagen approach (Bohr, Heisenberg, Pauli, Rosenfeld) and by the statistical interpretation (Einstein, Schrödinger, Blokhintsev, Ballentine), with the meaning given by Ballentine [10] to the latter expression; one of these interpretations is more-or-less implicitly accepted by many users of QM. Weinberg has stressed that "quantum field theory is based on the same quantum mechanics that was invented by Schrödinger, Heisenberg, Pauli, Born, and others in 1925–26, and has been used ever since in atomic, molecular, nuclear, and condensed matter physics" ([11], p. 49).

A state of the Hilbert space—pure state—used in QM, and described by a ket in the Dirac formalism [12], obeying the Schrödinger equation if Σ is isolated, can be obtained from a preparation act, and if an observable O attached to Σ is *measured* while Σ is in the pure (normed) state $\mid \Psi\rangle$, the mean value of the result is the quantity $\langle\Psi \mid \widehat{O} \mid \Psi\rangle$ (with $\widehat{O}$ being the Hermitian operator attached to O).

The questions on the meaning of the pure state concept, of the principle of superposition (of pure states) and of the probabilistic content of the quantity $\langle\Psi \mid \widehat{O} \mid \Psi\rangle$ are presently still debated, through the so-called problem of the foundations of QM. From the beginning of this paper, *the reader is urged to keep in mind that this paper is NOT devoted to the problem of the foundations of QM and its so-called interpretation (the interested reader may consult [13]), but to a far more modest question.*

We start from the fact that von Neumann [14,15] considered a more general situation than the one described by a pure state, the one called a mixed state or statistical mixture (of states). Since von Neumann's work, it is considered that if two so defined statistical mixtures are represented by the same density operator, they must be seen as the same statistical mixture, and it is more generally considered that ρ completely describes the properties of a statistical mixture. Already in 1970, Zeh, in a paper devoted to the question of the measurement in QM, imagined a thought experiment with neutrons, and wrote that "the statistical ensemble consisting of equal probabilities of neutrons with spin up and spin down in the x direction cannot be distinguished by measurement from the analogous ensemble having the spins parallel or antiparallel to the y direction. Both ensembles, however, can be easily prepared by appropriate versions of the Stern–Gerlach experiment. One is justified in describing both ensembles by the same density matrix as long as the axiom of measurement is accepted. However, the density matrix formalism cannot be a complete description of the ensemble, as the ensemble cannot be rederived from the density matrix" [4]. We call this situation for neutrons proposed by Zeh *the Zeh problem*. Since then, no consensus has emerged. Recently, for instance, a controversy appeared after a 2011 paper by Fratini and Hayrapetyan [16] claimed that they had established limits in the statistical operator formalism, through considerations about variances, followed by a paper from Bodor and Diosi [17] asserting that their analysis was irrelevant, without any final agreement [18]. We recently showed [19] that the use of variances made in [16,18] was wrong. The question from Zeh, therefore, still keeps its own interest.

Peres, in his 1995 book [20], when he writes that "the ρ matrix completely specifies all the properties of a quantum ensemble" (p. 76), has first spoken of a "fundamental postulate" (p. 75). In Section 2, considering the content of [14], we first confirm that von Neumann proposed a postulate when introducing the density operator ρ. We point out that the use of the ρ formalism, which certainly facilitates the calculations may, however, hide the probabilistic content then manipulated. In Section 3, we come to the Zeh problem, with a spin $1/2$ and *the two von Neumann mixed states considered by Zeh*, described by the same density operator. Using the density operator formalism, we calculate the mean value of the s_x component of the neutron spin, successively for the first and second mixtures, leading to the same result. This is just the first moment of the Random Variable (RV) considered by von Neumann in the presence of his statistical mixture. Disregarding the von Neumann postulate, we then calculate the successive moments of that RV, and show that at least one of these moments differs when comparing their values for the two mixtures considered by Zeh, which allows us to differentiate between these two mixed states. Section 4 is devoted to a discussion, before a conclusion in Section 5. In a short Appendix A, any reader wishing to access the 1970 paper by Zeh is invited not to confuse the von Neumann postulate considered in this paper and what Zeh, in his 1970 paper, called the measurement axiom.

2. von Neumann Statistical Mixture and Postulate

In the following, we keep the notations introduced in Section 1, which, e.g., imply that any pure state is normed, and that the mean value of observable O in pure state $\mid \Psi\rangle$ is $\langle\Psi \mid \widehat{O} \mid \Psi\rangle$. In his 1932 book (see also his 1927 paper [15]), von Neumann used the language of the wave function, and obviously not the ket formalism, introduced by Dirac seven years later [12]. In this section, we consequently both respect his own writing and, when commenting passages from [14], keep the notations introduced in Section 1.

In order to avoid any misunderstanding for a reader unfamiliar with the wave function language, we first recall the definition of a (von Neumann) mixed state, or statistical mixture, given by Cohen-Tannoudji et al. in [21] (p. 300): in such a situation, "*the state of this system may be either the state* $\mid \psi_1\rangle$ *with a probability* p_1*, or the state* $\mid \psi_2\rangle$ *with a probability* p_2, etc. Obviously: $p_1 + p_2 + ... = \sum_k p_k = 1$". The experiment imagined by Zeh (see Section 3) gives two instances of such mixtures. In Note 156 from [14], with his reference to von Mises, von Neumann indicates that he uses what is now called the frequentist interpretation of probability (see also, e.g., [22]).

If Σ is in pure state $\mid \Psi\rangle$, and observable O is then measured, the result of the measurement is random, and, at the beginning of the present section, it was recalled that the mean value of the (result of the) measurement, obeying specific (so-called quantum) rules, is the quantity $\langle\Psi \mid \widehat{O} \mid \Psi\rangle$. On page 296 of [14], von Neumann, in the presence of a statistical mixture $\{\mid \psi_i\rangle, p_i\}$, introduces an expectation value "in the sense of the generally valid rules of the calculus of probabilities". Considering an observable O and that statistical mixture, he introduces the following RV: the quantity $\langle\psi_i \mid \widehat{O} \mid \psi_i\rangle$, associated with pure state $\mid \psi_i\rangle$ of the mixture. von Neumann then defines the following quantity, which is here denoted as m_1:

$$m_1 = \sum_i p_i \langle\psi_i \mid \widehat{O} \mid \psi_i\rangle. \quad (1)$$

The latter quantity, called the mean value of (the result of the measurement of) O by physicists, and its expectation by people from the field of probability, is presently written as m_1, since it is the first moment of the considered RV. More generally, the *nth* moment of this RV, denoted as m_n (we have adopted the notation used by Papoulis in his treatise on probability; see page 109 of [23]), and not considered in von Neumann's book, is the following quantity:

$$m_n = \sum_i p_i (\langle\psi_i \mid \widehat{O} \mid \psi_i\rangle)^n \quad (2)$$

and the summation is over all the pure states of the statistical mixture.

Equation (2) should be commented on. Any user of QM knows well that when a quantum system is in a pure state, the result of the measurement of an observable has a random character. The bra–ket formalism and rules of calculation allow him, e.g., to know the mean value of an observable while respecting the superposition principle and the possible existence of so-called quantum interference terms. Faced with a (von Neumann) statistical mixture, he uses the density operator formalism, without any explicit use of the general laws of probability. Reading Equation (2), he should, however, notice the following:

once the von Neumann postulate has been given up, Equation (2) is just respecting the fact that von Neumann first defined a statistical mixture *using the general concepts of probability theory, and then took the quantity* $\langle \psi_i \mid \widehat{O} \mid \psi_i \rangle$ *(associated with a randomly drawn pure state* $\mid \psi_i \rangle$ *of the mixture) as the random variable*.

The difficulty in mentally manipulating mixed states may be subsumed through the following observation: One applies the general laws of the probability theory to a quantum quantity, $\langle \psi_i \mid \widehat{O} \mid \psi_i \rangle$. Anybody who has first accepted to give up the von Neumann postulate, but then refuses the definition of the moments as expressed in Equation (2), must successively deny the existence of the first moment (i.e., the mean value) of an observable in the presence of the statistical mixture, then deny the concept of a density operator, and finally deny the very existence of a statistical mixture as introduced by von Neumann, whereas the thought experiment from Zeh does exist (think also of thermal equilibrium).

In the context of QIP, if somebody (the writer) prepares a statistical mixture $\{\mid \psi_i \rangle, p_i\}$ and gives access to that mixture to someone (the reader), without telling him which the $\mid \psi_i \rangle$ and their probabilities p_i are, then, if the reader wants to identify this mixture, his task is to determine the states of the mixture, i.e., the $\mid \psi_i \rangle$, and their probabilities, p_i. The measurement of the $\langle \psi_i | \widehat{O} | \psi_i \rangle$ for some O is just a tool for this work.

The introduction of the density operator $\rho = \sum_i p_i \mid \psi_i \rangle \langle \psi_i \mid$, a linear operator acting on the elements of $\mathcal{E}$ attached to Σ, allows one to write m_1 as a Trace, a quantity which is independent of the chosen basis: $m_1 = Tr \rho \widehat{O}$.

When Peres speaks of a fundamental postulate (*and we will speak of the von Neumann postulate*), he is considering a *statistical mixture,* and the fact that von Neumann, introducing the concept of a statistical mixture, then adds that the density operator expresses the whole content of that statistical mixture. One has to refer here to the beginning of Ch. IV in [14]: von Neumann, having considered the probability content attached to a pure state, adds (pp. 295–296) that "the statistical character may become even more prominent, if we do not even know what state is actually present—for example when several states $\phi_1, \phi_2, ...$ 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 quantum system of interest, which he denotes as S. He then introduces the expectation value of the observable O in the mixed state, the quantity $\Sigma_i w_i \langle \phi_i \mid \widehat{O} \mid \phi_i \rangle$, writing it as a Trace: $Tr\{\rho \widehat{O}\}$ (where the density operator is denoted as U in [14]). And, on page 296, having just introduced the density operator and that Trace, and concerning this operator, von Neumann adds: "Hence, it characterizes the mixture of states just described completely, with respect to its statistical properties". Consequently, given a system Σ in a statistical mixture described by ρ, and $\widehat{O}$ attached to an observable O of $\sum$, the assertion that everything should be contained in the expression $E\{\widehat{O}\} = Tr\{\rho \widehat{O}\}$ and, hence, in ρ expresses a postulate, as stressed by Peres. However, this fact is not always identified, a result of von Neumann's authority. A significant instance in the field of quantum information is found in the already-cited book by Nielsen and Chuang, in the version [3] published ten years after the appearance of the book from Peres: its authors, on page 98, consider a quantum system "in one of a number of states $\mid \psi_i \rangle$, where i is an index, with respective probabilities p_i". But on page 97, without any proof or at least reference, they have claimed that "the density operator" formalism "is mathematically equivalent to the state vector approach".

The density operator $\rho = \Sigma_i p_i \mid \varphi_i \rangle \langle \varphi_i \mid$ is Hermitian, and is positive-definite (all of its eigenvalues are non-negative; see, e.g., [24]). The eigenvalue spectrum of a Hermitian positive-definite operator with a finite trace is entirely discrete, a result of Hilbert space theory ([24], p. 335). When an isolated system is in a statistical mixture, ρ obeys the Liouville–von Neumann equation. In the special case when Σ is in a pure state $\mid \Psi \rangle$, ρ is a projector: $\rho = \mid \Psi\rangle\langle\Psi \mid$. The relation $Tr\rho^2 \leq Tr\rho$ is obeyed by ρ, the equality being verified iff ρ is a projector, i.e., if and only if ρ describes a pure state. $\rho^2 = \rho$ iff ρ is a projector.

3. The Zeh Problem and the Use of Higher-Order Moments

The problem identified by Zeh through his thought experiment manipulating neutrons was presented in Section 1. Zeh introduces Stern–Gerlach (SG) equipment. In their 1922 experiment, Stern and Gerlach used silver atoms placed in a furnace heated to a high temperature, leaving the furnace through a hole and propagating in a straight line. They then crossed an inhomogeneous magnetic field and condensed on a plate (see [21], p. 394). As they have no electric charge, they were not submitted to the Laplace force, but they have an electronic permanent magnetic moment. In a classical approach, one should then observe a single spot, *whereas two spots* were observed, which could only be explained, later on, as the result of a quantum behavior: a silver atom has a spin 1/2. Zeh considers the random emission of neutrons by a neutron source. It is well-established that a neutron has a nuclear spin 1/2, here denoted as $\overrightarrow{s}$ (it is usually written as $\overrightarrow{I}$, with the symbol $\overrightarrow{s}$ being kept for spins with electronic origin) and a magnetic moment $\mu = -1.913047\ \mu_N$ (μ_N: nuclear magneton) proportional to its spin. The force acting on the magnetic moment of the successive neutrons deflects them into two well-identified beams, with one beam corresponding to the spin quantum state $\mid +z\rangle$ and one beam corresponding to the spin quantum state $\mid -z\rangle$. The letter z is reminiscent of the fact that the field gradient and the force on the spin were directed along z in Figure 1, on page 395 of [21]. $+$ indicates that the state is an eigenstate of s_z, for the eigenvalue $+1/2$.

As the neutrons are emitted one by one (no interaction between them), interact only with the magnetic field before being collected on the plate, and are not each identified when leaving the furnace, but are only counted when arriving on the plate, with the same total number $N/2$ in the two packets, one may say (strictly speaking, in the limit $N \longrightarrow \infty$) that one has prepared the following (von Neumann) statistical mixture: $\mid +z\rangle$, $\frac{1}{2}$, and $\mid -z\rangle$, $\frac{1}{2}$. This mixture is the one compatible with the SG equipment in reference [21]. Following up the question from Zeh in [4], we now consider a spin 1/2, and successively its state in

$$\text{Mixture 1: } \mid +x\rangle,\ 1/2 \ \text{ and } \quad \mid -x\rangle,\ 1/2 \tag{3}$$

$$\text{Mixture 2: } \mid +y\rangle,\ 1/2 \ \text{ and } \quad \mid -y\rangle,\ 1/2 \tag{4}$$

with $\mid +x\rangle$ and $\mid -x\rangle$ being the eigenkets of s_x for the values $+1/2$ and $-1/2$, respectively, and $\mid +y\rangle$ and $\mid -y\rangle$ those of s_y for the values $+1/2$ and $-1/2$, respectively.

The density operator associated with both mixtures is $\rho = I/2$ (I: identity operator in the state space of the spin). We decide to forget the existence of the von Neumann postulate (as called by Peres), which suggests that both mixtures are the same, and which therefore would discourage us from undertaking what follows. We choose to use, instead of the ρ formalism, the very definition of these mixtures. And, in order to try and clarify the Zeh problem, keeping the RV used by von Neumann (see Section 2) in the presence of a statistical mixture, we decide to use the moment m_n of an arbitrary order introduced in Section 2, and not only the mean value, and then, in both mixtures, measure the s_x component of the neutron spin.

Just before the plate, at the level of each arriving beam, we therefore introduce equipment able to measure the s_x component of each neutron, and to store the result. von

Neumann wrote that the mean value of the result of this measurement, written in the Dirac formalism, is

$$\frac{1}{2} \quad \langle \quad +x \mid s_x \mid +x\rangle + \frac{1}{2}\langle -x \mid s_x \mid -x\rangle \text{ for mixture 1} \tag{5}$$
$$\frac{1}{2} \quad \langle \quad +y \mid s_x \mid +y\rangle + \frac{1}{2}\langle -y \mid s_x \mid -y\rangle \text{ for mixture 2.} \tag{6}$$

As detailed in Section 2, after Equation (2), for any value of the non-negative integer n, when measuring s_x, the corresponding nth moment, which we will note m_{n,s_x}, has the following value for mixture 1:

$$\begin{aligned} \text{mixture 1: } m_{n,s_x} &= \frac{1}{2}(\langle +x \mid s_x \mid +x\rangle)^n + \frac{1}{2}(\langle -x \mid s_x \mid -x\rangle)^n \\ &= \frac{1}{2}(\frac{1}{2})^n + \frac{1}{2}(-\frac{1}{2})^n. \end{aligned} \tag{7}$$

Therefore, in statistical mixture 1, any odd moment m_{n,s_x} has a value equal to 0*, and any even moment is equal to* $1/2^n$.

We now come to mixture 2. In practice, one uses a large number of independent neutron spins. Due to the just-explained behavior of the Stern–Gerlach apparatus (and here transposed to a field along direction y, hence with two beams, associated with states $\mid +y\rangle$ and $\mid -y\rangle$, respectively), one separately accesses two well-identified subsets of neutron spins; respectively, those in state $\mid +y\rangle$ and those in state $\mid -y\rangle$. One can then separately obtain estimates of $\langle +y \mid s_x \mid +y\rangle$ and of $\langle -y \mid s_x \mid -y\rangle$ and then derive an estimate of the nth moment (of the von Neumann RV, which we have decided to keep), m_{n,s_x}, which has the following value:

$$\text{mixture 2: } m_{n,s_x} = \frac{1}{2}(\langle +y \mid s_x \mid +y\rangle)^n + \frac{1}{2}(\langle -y \mid s_x \mid -y\rangle)^n. \tag{8}$$

We recall the developments of $\mid +y\rangle$ and $\mid -y\rangle$ within the standard basis,

$$\mid +y\rangle = \frac{\mid +\rangle + i \mid -\rangle}{\sqrt{2}} \quad \text{and} \quad \mid -y\rangle = \frac{\mid +\rangle - i \mid -\rangle}{\sqrt{2}}.$$

The quantity $\langle +y \mid s_x \mid +y\rangle$ is equal to zero, as the diagonal quantities $\langle + \mid s_x \mid +\rangle$ and $\langle - \mid s_x \mid -\rangle$ are both equal to 0, and the sum of the interference terms is equal to zero. The same result is obtained for $\langle -y \mid s_x \mid -y\rangle$.

Therefore, in statistical mixture 2, any moment m_{n,s_x} is equal to 0.

We have therefore established that each even-order moment of the RV introduced by von Neumann for the (result of the) measurement of s_x possesses different values in Zeh mixtures 1 and 2, a result that allows one to say that the two Zeh mixtures should be distinguished.

One guesses that if, in contrast, for the same mixtures being considered, one measures s_z instead of s_x, and then follows the same approach, the difference found for the moments m_{n,s_x} should disappear, since the choice of s_z introduces a new symmetry, and an inability for the von Neumann RV to distinguish between the two mixtures through the use of the moments of s_z. We choose to examine this question explicitly. One first considers the values of the moments m_{n,s_z} when the spin is in mixture 1. The developments of $\mid +x\rangle$ and $\mid -x\rangle$ in the standard basis are, respectively,

$$\mid +x\rangle = \frac{\mid +\rangle + \mid -\rangle}{\sqrt{2}} \quad \text{and} \quad \mid -x\rangle = \frac{\mid +\rangle - \mid -\rangle}{\sqrt{2}}.$$

The value of $\langle +x \mid s_z \mid +x\rangle$, calculated through a development of $\mid +x\rangle$ in the standard basis, is obtained as the sum of its interference terms, each equal to zero, and of the diagonal terms, with the sum of their contributions being equal to 0. Therefore, $\langle +x \mid s_z \mid +x\rangle = 0$. For the same reason, $\langle -x \mid s_z \mid -x\rangle = 0$. Therefore, any moment m_{n,s_z} in mixture 1 now has a value equal to 0. Following the same approach, one obtains the same result for mixture 2. As expected, considering measurements of s_z and the moments of the associated von Neumann RV, one is unable to establish any difference between Zeh mixtures 1 and 2. This result, however, does not change the previous conclusion, which corresponds to a sufficient condition: considering the two mixtures introduced by Zeh, possessing the same density operator, we first chose s_x as the observable to be measured. The mean value of the result when the spin is in a pure state $\mid \varphi\rangle$ is $\langle \varphi \mid s_x \mid \varphi\rangle$. Then, considering the two Zeh mixtures, we calculated m_{1,s_x}, the mean value of the result of the measurement, following the method introduced by von Neumann, which can be interpreted as the calculation of the first moment of his RV of interest. We then calculated the value of any moment m_{n,s_x} of that RV for both mixtures, which showed that at least one moment, and even all the even-order moments, have different values in mixtures 1 and 2, which allows one to establish a distinction between Zeh mixtures 1 and 2.

Before ending this section, one imagines someone who, in the presence of the first Zeh mixture, first decides to calculate $\langle +x \mid s_x^n \mid +x\rangle$ (n: integer where $n \geq 1$), i.e., the mean value of s_x^n in the pure state $\mid +x\rangle$, and then calculates

$$\frac{1}{2}\langle +x \mid s_x^n \mid +x\rangle + \frac{1}{2}\langle -x \mid s_x^n \mid -x\rangle = \begin{bmatrix} \frac{1}{2^n} \text{ if } n \text{ is even} \\ 0 \text{ if } n \text{ is odd} \end{bmatrix}. \tag{9}$$

He then performs the same calculation for the second Zeh mixture, and obtains an identical result. This just means that, faced with a von Neumann statistical mixture, instead of keeping the RV introduced by von Neumann and using the collection of its moments m_{n,s_x}, he focused on each pure state, considering s_x^n instead of s_x, and first its mean value in the chosen pure state and, secondly, its *mean value* in the mixture, an approach focused on mean values in a given pure state, which introduces no direct link with the content of a given mixed state, and which, therefore, had no reason for why it should be successful.

4. Discussion

In this paper, the fact that the mean value of an observable O in a pure state $\mid \Psi\rangle$ is $\langle \Psi \mid \widehat{O} \mid \Psi\rangle$ is accepted, and its meaning is not discussed. As stressed in the introduction, the subject of this paper, far more modest, starting once the existence of mixed states has been accepted is, however, still under debate (cf. Section 1).

von Neumann first accepted the existence of mixed states, using the usual probability concept, through its so-called frequency interpretation (cf. Section 2). When the state of the system of interest is described by a mixed state, von Neumann then decided to calculate the expectation value of an observable attached to the system, "in the sense of the generally valid rules of the calculus of probabilities" (page 296 of [14]). This led him to introduce a density operator ρ. Then, instead of considering that ρ is a tool useful for the calculation of a mean value, truly an answer to an important question, he tried to interpret ρ as describing the state of the system; therefore, giving up his first definition of the situation through his original definition of a mixed state and, finally, redefining the state of the system through its associated density operator ρ.

In his 1970 paper, Zeh focused on the spin of neutrons and Stern–Gerlach equipment, and on two statistical mixtures chosen so that both mixtures have the same density operator, $\rho = I/2$. Zeh observed that the description with ρ should not tell the whole story for these mixtures, since it forgets the initial preparation process of these mixtures. We have (1) decided to ignore the von Neumann postulate (cf. Section 3); and (2) kept the RV used by von Neumann, considered a well-chosen observable (s_x, not s_z), and calculated not only its mean (or expectation) value m_{1,s_x}, but the collection of its moments m_{n,s_x}. We then established that the even moments have different values in mixture 1 and mixture 2. This result allows us to say that, contrary to what is claimed when accepting the von Neumann postulate, the two Zeh mixtures should be distinguished. Their associated density operator, certainly an important tool, does not contain the whole information contained in the mixture $\{| \varphi_i\rangle, p_i\}$, which confirms an intuition from Zeh.

In our discussion of the Zeh problem, we did use the fact that, when $\sum$ is in the pure (normed) state $| \Psi\rangle$, the mean value of an observable O is the quantity $\langle\Psi | \widehat{O} | \Psi\rangle$. What we did not use is the von Neumann postulate itself (as called by Peres), and its consequence that ρ should contain all the information contained in the definition of a statistical mixture as the $\{| \varphi_i\rangle, p_i\}$ collection. This giving up of the von Neumann postulate does not affect the use of ρ and its importance, e.g., in quantum statistical mechanics. von Neumann proposed the quantity $S = -k_B\langle ln\rho\rangle = -k_B Tr\{\rho ln\rho\}$ (k_B: Boltzmann constant) as a definition of the entropy and, similarly, this is not affected by the giving up of the von Neumann postulate. And, the use of the von Neumann entropy, moreover, helps us to identify a consequence of the introduction of the von Neumann postulate. In [14], when examining the question of the quantum analog of the classical entropy, von Neumann first established that all pure states have the same entropy, which he took as the origin of entropy. In an interpretation of the entropy as a measure of disorder, this entropic behavior is understood as the fact that all pure states present the same quantity of disorder. We have shown that the two neutron mixtures introduced by Zeh should be distinguished and, since they do possess the same density operator ρ, they have the same value of their entropy and, therefore, the same degree of disorder. Introducing the von Neumann postulate and, therefore, claiming that they are the same mixture introduces a confusion between degree of disorder and true existence.

When manipulating mixed states in numerical simulations in the context of QIP, the use of moments with $n > 1$ may be limited by the efficiency of the computation software and/or the quantity of available data. In the context of an experiment, if, e.g., a system at thermal equilibrium is described by the quantum version of the Gibbs law, $\rho \propto \exp(-H/kT)$, it is not presently suggested to give up the use of ρ. It is just suggested to accept the idea that when manipulating ρ, one manipulates the mean value, or first moment, of the RV introduced by von Neumann, i.e., to answer a specific question asked by Zeh, when he stressed that the ρ tool was unable to describe the difference between the distinct mixtures he had prepared.

It is important to identify the reason that led von Neumann to introduce his postulate. In the preface of [14], von Neumann wrote that, at the time of its writing, "the relation of quantum mechanics to statistics and to the classical statistical mechanics" was "of special importance". And, 25 years later, Fano [25] stressed that "the name density matrix itself relates to the correspondence between ρ and the distribution function $\rho(p,q)$ in the phase space of classical statistical mechanics", and noted that, in that time interval, "States with less than maximum information, represented by density matrices ρ, have been considered primarily in statistical mechanics and their discussion has been influenced by the historical background in this field". In the previous development of classical statistical mechanics, Gibbs had introduced a probability density (within the phase space), denoted as $\rho(p,q)$, used for the calculations of mean values. In contrast, what corresponds to what is now called higher-order moments (see, e.g., their use in [5]) had not been explicitly considered in physics. Therefore, when von Neumann introduced his postulate, this he could implicitly consider not to be responsible for a loss of information, as compared with that contained in the definition of a statistical mixture through the explicit consideration of the $\{|\varphi_i\rangle, p_i\}$ collection. And, more importantly, in the context of a building of quantum statistical mechanics, the indiscernability of identical particles had already been identified, which led to distinguishing between their mathematical Hilbert space and a subspace built from either symmetrical states in the exchange of two particles (bosons) or antisymmetrical states (fermions) and, moreover, to build the quantum Maxwell–Boltzmann statistics for independent but distinguishable particles, e.g., electron spins diluted in ionic solids (cf. more generally Chapter X of [26]).

Within a given theory, postulates generally play an essential function in its building, i.e., their suppression would threaten the whole building. The situation is quite different with the present von Neumann postulate. In this paper, it was explained that its elimination does not affect the use of the density operator. The postulate has to just be replaced by acknowledging the fact that the density operator is introduced for the calculation of mean values, and, if desired and possible in the considered context, by using the information content present in a statistical mixture $\{|\varphi_i\rangle, p_i\}$, but not in its density operator.

5. Conclusions

In his 1970 paper, Zeh considered neutron spins prepared in two different statistical mixtures described by the same density operator ρ. Zeh stressed that ρ could not tell the whole story, as it ignored the result of the preparation step. This situation, which we call the Zeh problem, arises as a consequence of a postulate introduced by von Neumann in his treatment of statistical mixtures, and identified by Peres. That postulate says that, in the presence of a statistical mixture $\{| \varphi_i\rangle, p_i\}$, because the mean value of an observable O is $\sum_i p_i\langle\varphi_i \mid \hat{O} \mid \varphi_i\rangle$, the whole information contained in the mixture is also contained in its associated density operator $\rho = \sum_i p_i \mid \varphi_i\rangle\langle\varphi_i \mid$. The contents of the 1932 book by von Neumann indicates that its author, in the presence of a statistical mixture $\{| \varphi_i\rangle, p_i\}$, when interested in an observable O, chooses as the RV of interest the mean value of the observable O when the system is in a given pure state. He then focuses on the expectation value of that RV in the considered mixed state, i.e., its first moment. Disregarding that von Neumann postulate, we have calculated the value of the different moments m_{n,s_x} of the RV chosen by von Neumann, for the s_x spin component, for both Zeh mixtures, and thus established that at least one of these moments does not have the same value in both Zeh mixtures. It was then shown that the two Zeh mixtures have the same degree of order.

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Appendix A. For a Reader of the 1970 Paper by Zeh

Any reader of the 1970 paper by Zeh should avoid confusion between the following:

- What Peres called a fundamental postulate [20], a postulate which was given up in the present paper,
- What Zeh called the measurement axiom, which stipulates that when Σ is in a pure state, namely $\mid \Psi\rangle$, then if O is measured [21,24]: (A) the result is necessarily one of the eigenvalues of $\widehat{O}$; (B) $\mid \Psi\rangle$ being developed over the eigenstates of $\widehat{O}$, $\mid \Psi\rangle = \Sigma_i c_i \mid \varphi_i\rangle$ (in the simple case with no degeneracy), the probability of obtaining the eigenvalue λ_i associated with eigenket $\mid \varphi_i\rangle$ is $\mid c_i \mid^2$; and (C) if the result of the measurement is λ_i, then, at the end of the measurement, Σ is in the pure state $\mid \varphi_i\rangle$. Speaking of that axiom, Zeh wrote that it leads to a circular argument. From Section 1, we stressed that the question of the meaning of this measurement axiom, as called by Zeh, which is a part of the discussions about the foundations of QM, is strictly outside the scope in this paper, which accepts (A) and (B) of this measurement axiom, and does not address the question of the relevance of (C).

For that reason, we have chosen not to even cite the passages from the canonical von Neumann 1932 book where this major question is discussed. Just in contrast, we focused on its passages where von Neumann introduces the concept of a mixed state.

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