

Article

Quantum Information: Systems, Their States, and the Use of Variances

Alain Deville ^{1,†}  and Yannick Deville ^{2,*,†} 

¹ Institut Matériaux Microélectronique et Nanosciences de Provence (IM2NP), Aix-Marseille Université, 13397 Marseille, France; alain.deville@univ-amu.fr

² Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse, 31400 Toulouse, France

* Correspondence: yannick.deville@irap.omp.eu; Tel.: +33-5-6133-2824

† These authors contributed equally to this work.

Abstract: Quantum information mobilizes the description of quantum systems, their states, and their behavior. Since a measurement postulate introduced by von Neumann in 1932, if a quantum system has been prepared in two different mixed states represented by the same density operator ρ , these preparations are said to have led to the same mixture. For more than 50 years, there has been a lack of consensus about this postulate. In a 2011 article, considering variances of spin components, Fratini and Hayrapetyan tried to show that this postulate is unjustified. The aim of the present paper is to discuss major points in this 2011 article and in their reply to a 2012 paper by Bodor and Diosi claiming that their analysis was irrelevant. Facing some ambiguities or inconsistencies in the 2011 paper and in the reply, we first try to guess their aim, establish results useful in this context, and finally discuss the use or misuse of several concepts implied in this debate.

Keywords: quantum pure state; mixed state; density operator; variance of an observable

1. Introduction

Quantum mechanics (QM) was essential in the development of both condensed matter physics and semiconductor electronics. The growth of telecommunications stimulated the appearance of the so-called second quantum revolution, particularly an opportunity for a reconsideration of some basic ideas of QM. Users of QM are familiar with the idea that if two mixed states, defined by different collections $\{p_i, |\varphi_i\rangle\}$ of pure (normed) states $|\varphi_i\rangle$ with probabilities p_i , are represented by the same density operator, they should be considered as the same mixed state. They are most often not aware that this is a consequence of a specific postulate introduced by von Neumann [1,2], according to which “the ρ matrix completely specifies all the properties of a quantum ensemble” (cf. Peres, pp. 75–76 of [3]). It is well known that John Bell criticized the place given to measurements in QM [4,5]. One may consider that a similar importance should be given to the concept of a preparation. And already in 1970, Zeh [6], considering the use of the axiom of measurement, spoke of a circular argument, and considered 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 with 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**” (here, and in subsequent citations, no part of the original text was stressed). Without any reference to that 1970 paper by Zeh, Nenashev recently claimed that the state of a system is fully described by its density matrix [7], but he did not explain why, if several paths (manipulations of a physical system



Citation: Deville, A.; Deville, Y. Quantum Information: Systems, Their States, and the Use of Variances. *Information* **2024**, *15*, 247. <https://doi.org/10.3390/info15050247>

Academic Editor: Luque Gabriel

Received: 1 April 2024

Revised: 18 April 2024

Accepted: 18 April 2024

Published: 25 April 2024



Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

initially in one or another state) lead to the same destination (described by identical results of measurements) and if one wishes to describe the whole story from the beginning of each journey, then keeping only this final common destination should be the right approach.

In the context of quantum information, a model for quantum computing with initially mixed states was proposed in 2011 [8]. In the same year, in the more general context of quantum mechanics, Fratini and Hayrapetyan (denoted as FH in what follows) published a paper entitled “Underlining some limitations of the statistical formalism in quantum mechanics” [9]. From the content of [9], FH appear to operate within the whole frame-postulates and concepts of QM and aim at showing how the point of view of QM may present limitations. In a 2012 ArXiv article, Bodor and Diosi [10] tried to show that the conclusions contained in [9] were unjustified. In their 2012 ArXiv reply [11], FH claimed that they had established that, in their specific instance, involving spins 1/2 and what they called ensembles \mathcal{A} and \mathcal{B} , “the variance obtained by analyzing one ensemble turned out to be different from the variance obtained by analyzing the other ensemble. On the other hand, the density matrices of both ensembles turned out to be the same”. That FH reply did not lead to a final agreement between these authors. The present paper tries to clarify the situation in order to help decide whether the conclusions from [9,11] should be kept.

It is first necessary to specify two points, which, in [9], are implicit. FH consider spins 1/2 and, in their thought experiment, make them cross “a Stern and Gerlach (SG) apparatus”. One should understand that particles with the same *magnetic moment* are manipulated, since, for instance, an atom with an electron spin 1/2 magnetic moment (e.g., a silver atom, as in the 1922 experiment by Stern and Gerlach) and an atom with a nuclear spin 1/2 (e.g., the isotope ^{19}F) behave quite differently in an SG device, the magnitudes of their magnetic moments being respectively of the order of μ_B , the Bohr magneton, and μ_N , the nuclear magneton ($\mu_B/\mu_N \simeq 1836$). In the following, when we speak of identical spins 1/2, this will implicitly mean identical magnetic moment operators, each one proportional to a spin 1/2 operator \vec{s} . An SG device was also introduced in [6] without this ambiguity because Zeh imagined a collection of *neutrons*.

FH also implicitly consider that these spins are distinguishable. If one mentally thinks of a collection of SG devices, e.g., “with the magnetic field along the \hat{x} direction” [9], the spins are distinguishable by the number given to the SG devices they cross. This is also true for “particles whose spin states are defined along the \hat{z} axis” [9]. This is not an academic distinction: the independent and undistinguishable electron spins of the conduction electrons in a metal give rise to the temperature-independent Pauli paramagnetism (the spin of the electron is a fermion), whereas in an ionic insulator, the paramagnetism of non-interacting electron spins 1/2 (distinguishable through the ion carrying the spin) follows a Curie law above typically a few Kelvins.

Following FH, we will be interested in a collection of an even number N of distinguishable, non-interacting, identical (magnetic moments associated with) spins 1/2. For brevity, we will call it the spin assembly.

In [9], FH use the concept of polarization without explicitly defining it. The degree of polarization of a spin 1/2 can be described by its polarization vector \vec{a} ([12], p. 173). The components of \vec{a} are real, such that $0 \leq |a| \leq 1$, and, in standard QM, the most general state of a spin 1/2 is described by the density operator $\rho = (1 + \vec{a} \cdot \vec{\sigma})/2$, where $\vec{\sigma}$ is the Pauli vector (its components are the Pauli operators $\sigma_x, \sigma_y, \sigma_z$) and 1 is a symbolic writing for the identity operator in the state space of the spin. The spin is in a totally unpolarized state when $\vec{a} = 0$, and then $\rho = 1/2$. If a collection of N distinguishable and independent spins is considered, total unpolarization is realized if and only if each spin is in its totally unpolarized state. This state is described with the density operator $I/2^N$ (I : unit operator in the state space of the spin assembly).

In Section 2, after a reminder about quantum systems and about the pure or mixed states of these systems, the so-called \mathcal{A} and \mathcal{B} ensembles introduced by FH will be presented. The way they are defined by FH somewhat mixes the concept of a quantum system and one of its possible pure or mixed states, and we will have to try and guess from the content

of [9], which states FH consider when calculating a variance. Then, a general result concerning mean values calculated with the statistical operator ρ will be recalled and justified. It has the important consequence that the difference found by FH in their variance calculations should *a priori* be either a false or an ill-interpreted result, which is a motivation for looking for the origin(s) of the difference they found in their variances.

In Section 3, mean values and variances of spin components will be calculated in several situations in order to facilitate the analysis of the results given by FH. The origin(s) of the differences found by FH in the calculation of the variances will be identified in Section 4. The question of the number of particles in the systems introduced by FH in the calculation of mean values and the presence of a reference made by FH to a book by Sakurai [13] will be discussed in Section 5 before a general conclusion about this debate.

2. Of Quantum Systems, Their Pure or Mixed States, and Mean Values in These States

We did not try to systematically keep the notations from [9], as some quantities used in our paper are absent in [9], and some notations in [9] are ambiguous (e.g., the distinction between the spin \vec{s}_i of spin i and the total spin $\vec{S} = \sum_i \vec{s}_i$ of the spin collection). The dimension of \mathcal{E} , the state space of the quantum system of interest Σ , is supposed to be finite, denoted as d , and a basis of orthonormal kets of \mathcal{E} will be denoted as the collection $\{|k\rangle\}$. The completeness relation is expressed as $\sum_k |k\rangle\langle k| = I$ (I : the identity operator acting in \mathcal{E}). A pure state of a spin 1/2 is usually written, in the Dirac formalism, as a ket $|\Phi\rangle = \alpha|+\rangle + \beta|-\rangle$ (an element of the state space of the spin, α and β being complex coefficients with $|\alpha|^2 + |\beta|^2 = 1$). When a collection of N identical distinguishable spins 1/2 is considered, then, in order to describe its possible pure states, the tensor product of the state space of each spin (with dimension $d = 2^N$) is introduced; it is a postulate that every ket of this space represents a pure state of the spin assembly. A mixed state of a quantum system (e.g., a single spin or this collection of spins) is a collection of unit-norm pure states $|\Phi_1\rangle, \dots, |\Phi_i\rangle, \dots$ of this system, with respective probabilities p_1, \dots, p_i, \dots (for each p_i , $0 \leq p_i \leq 1$, and $\sum p_i = 1$). With that mixed state, one may associate the statistical operator $\rho = \sum_i p_i |\Phi_i\rangle\langle\Phi_i|$; in the specific case of a pure state $|\Phi\rangle$, then $\rho = |\Phi\rangle\langle\Phi|$, the associated projector.

Before trying to go on clarifying the situations discussed by FH in [9], it is useful to make some comments about the concepts of pure and mixed states. The expressions “pure state” and “mixture” (reiner Fall, Gemenge), historically introduced by Weyl [14], were not used by von Neumann in his 1932 book (1955 English translation of [1,2]). von Neumann, having introduced the concept of a (pure) state and the probability content attached to it, presented that of a mixed state, writing (pp. 295–296 of [1,2]) 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 ϕ_1, ϕ_2, \dots with the respective probabilities w_1, w_2, \dots ($w_1 \geq 0, w_2 \geq 0, \dots, w_1 + w_2 + \dots = 1$) constitute the description” of the system of interest. The ket formalism, which will be used hereafter, was introduced by Dirac seven years later [15]. Some 80 years after von Neumann’s book, Weinberg used the same ideas when writing “Probabilities can enter in quantum mechanics not only because of the probabilistic nature of state vectors but also because (just as in classical mechanics) we may not know the state of a system. A system may be in any one of a number of states, represented by state vectors Ψ_n that are normalized but not necessarily orthogonal, with probabilities P_n satisfying $\sum_n P_n = 1$ ” ([16], p. 68). In the meantime, in his 1957 review [17], Fano had also explicitly used the concept of a pure state when introducing mixed states, writing that “to calculate the probability of finding a certain experimental result with a system in the mixed state, one must first calculate the probability for each of the pure states and then take an average, attributing to each of the pure states an assigned “weight””.

These passages from von Neumann and Weinberg contain an interpretation of the mixed state concept, implying an ignorance of the experimenter. A brief comment on its possible use in the context of [9] will be made in Section 5.

2.1. The Ensembles \mathcal{A} and \mathcal{B} Introduced by FH

FH define their ensemble \mathcal{A} as follows: “ N particles whose spin states are defined along the \hat{x} axis, $N/2$ of which are eigenstates of the spin operator \hat{S}_x with eigenvalue $+\hbar/2$, while the remaining $N/2$ are eigenstates of the same operator with eigenvalue $-\hbar/2$ ” (and FH define their ensemble \mathcal{B} just by replacing the \hat{x} axis by the \hat{z} axis and the total spin component along \hat{x} by the one along \hat{z}). This defines partly Σ and quite partly its quantum state. Σ is a collection of particles with spin $1/2$, and the rest of [9] indicates that FH consider only their spin. It is not explicitly written that they are distinguishable, but nowhere is any antisymmetry of the fermion states suggested, and their experimental conditions, with the use of an SG device, clearly suggest that they can be distinguished. This passage of [9] is ambiguous, as “states are defined along the \hat{x} axis” may just refer to the choice of a basis for the description of the spin states. Further in [9], FH give contradictory precisions on the nature of the state -pure or mixed- of the spin assembly, since they first claim that “both \mathcal{A} and \mathcal{B} are totally unpolarized ensembles. In the language of statistical quantum mechanics, which will be encountered in Section 4, **they are also said to be in a maximally mixed state**”. But it is quite difficult to suppose that experimental conditions not detailed in [9] have resulted in a totally mixed state because precisions then added in [9] rule out this supposition. More precisely, FH write: “we can pragmatically think of using, for example, a Stern and Gerlach (SG) apparatus with the magnetic field along the \hat{x} direction [20]. The SG apparatus would measure the spin of each single particle of the ensemble, so that the total spin of the ensemble would then be obtained as the sum of all the single-particle spin measurements.”, and “Because of the characteristics chosen for ensemble \mathcal{A} , the SG apparatus would exactly separate particle flux into two equal parts, or, what is the same, it will measure $N/2$ particles having spin along the $+\hat{x}$ direction and $N/2$ particles having spin along the $-\hat{x}$ direction. **The probability of registering the outcome $\pm\hbar/2$, when the spin along \hat{x} is measured on state $|S_x, \pm 1\rangle$, is in fact 1**”. The latter citation leaves no doubt: at the input of the SG device, each spin is either in its $|+x\rangle$ or $| -x\rangle$ state; this is still true at its output. And in their 2012 reply [11] to Bodor and Diosi [10], FH do insist that “These two ensembles are definitely not statistical ensembles”, adding “we considered prepared ensembles”. If in contrast one accepts to consider that the spin assembly is in the totally unpolarized state $\rho = I/2^N$, then Equation (8) of [9] is false (this equation states that, for what FH call their ensemble \mathcal{A} , the mean value and the variance of the component S_x of the total spin, which is denoted as S_x^A in [9], are both equal to 0, a result to be opposed to the true result established below in Section 3.3). Moreover, if one tries to suppose that FH improperly used their expression “unpolarized ensemble” for their ensemble \mathcal{A} in order to describe a pure state with a mean value of their S_x^A equal to 0, one has to give up this assumption when reaching Section 4 of [9], in which FH consider mixed states, not pure states, then making a confusion between states and particles when introducing their Equation (7) (think e.g., of a single spin $1/2$ in a mixed state). In Section 5.3, we will suppose that FH adopt the point of view of someone who *ignores* that their ensemble \mathcal{A} was prepared in a well-defined pure state and then decides *to assume* that the collection of N spins is in a mixed state where the 2^N states of the S_x eigenbasis all contribute with the same weight to the statistical mixture ($\rho = I/2^N$). We will then show that this approach should be discarded.

Faced with these ambiguities and inconsistencies, in Section 3, we will successively consider the spin assembly in pure or mixed states chosen for their interest in the analysis of the content of [9] without identifying specifically one of the results with what FH intended to do.

2.2. More on Pure or Mixed States

FH speak of the “total spin of ensemble \mathcal{A} ” [9]. Their definition of \mathcal{A} suggests us to introduce the observable $S_x = \sum_i s_{xi}$ (we use the standard definition for the \hat{z} axis), a linear Hermitian operator acting in the state space $\mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_2 \otimes \dots \otimes \mathcal{E}_N$, and s_{x1} is a condensed writing for $s_{x1} \otimes I_2 \otimes \dots \otimes I_N$, where e.g., I_2 is the identity operator acting in \mathcal{E}_2 . In

order to make more explicit what seems to have been FH’s aim, we imagine an experiment with a spin 1/2 crossing an SG device with the field gradient along the \hat{x} direction, its downward ($-1/2$) path being interrupted by the presence of a detector. If a spin 1/2 is sent into its input and no spin is then detected at the level of the interrupted path, in experimental conditions when the spin is not lost, one then knows that the spin arrived at the upward aperture and may say that this SG device prepared this spin in the $|+x\rangle$ state, where $s_x | +x \rangle = (1/2) | +x \rangle$ (we systematically use reduced units, here 1/2 and not $\hbar/2$). We now imagine a collection of N such independent SG devices (N even), each one able to prepare either in the $|+x\rangle$ or in the $|-x\rangle$ state the spin which crossed it, and N spins 1/2 simultaneously sent, one at the input of each SG device (the spins are then distinguishable through the number of the SG device they cross). Depending on the positions of the N detectors, one may obtain 2^N such (pure) product-states, each one an eigenstate of S_x . One of these 2^N product-states has all the spins in their $|+x\rangle$ state; one of them has all the spins in their $|-x\rangle$ state; and a number of them have $N/2$ spins in the $|+x\rangle$ state (as in the states in the ensemble \mathcal{A} of [9]), e.g., the one with the $N/2$ first ones in the $|+x\rangle$ state; the remaining ones in the $|-x\rangle$ state, the following state:

$$|1+x, 2+x, \dots, N/2-1+x, N/2+x, N/2+1-x, \dots, N-1-x, \dots, N-x\rangle, \quad (1)$$

a compact writing for the tensor product of N kets, each one defined by the number of the spin, the fact that it is an eigenstate of the x component of that spin, and the $+$ or $-$ state. We will call $|\Psi_{x\delta}\rangle$ the one corresponding to the specific ordered choice, called δ , of the N individual kets in a given product-state. When FH speak of their ensemble \mathcal{A} , composed of N spins (with N even), and simultaneously write that the result of the measurement of the \hat{x} component (of a spin) is surely $+\hbar/2$ or $-\hbar/2$, depending on the number i of the measured spin, and that the numbers of $+\hbar/2$ and $-\hbar/2$ results are both equal to $N/2$, this implicitly means that they consider that the assembly is in one of the pure states just denoted as $|\Psi_{x\delta}\rangle$, and that they do not tell us what specific ordered choice (of the $+$ and $-$ values) presently denoted as δ is implied.

Since FH also speak of a mixed state, we will also imagine, for the spin assembly, the mixed state $\{|\Psi_{x\delta_1}\rangle, N_{N/2}^{-1}, \dots, |\Psi_{x\delta_{N_{N/2}}}\rangle, N_{N/2}^{-1}\}$, each pure state implying $N/2$ spins with the $|+x\rangle$ state and $N/2$ with $|-x\rangle$, all with the same weight $N_{N/2}^{-1}$, where $N_{N/2} = N!/((N/2)!(N/2)!)$ is the number of distinct orderings of these N spin states (cf. [18], p. 352: if e.g., $N = 4$, $N_{N/2} = 6$). Such a mixed state therefore mobilizes the whole collection of distinct $|\Psi_{x\delta}\rangle$ pure states, all with the same weight in the mixture. Of course, the statistical operator ρ associated with this mixture is *not* equal to $I/2^N$, since only part of the eigenvectors of S_x are of the form $|\Psi_{x\delta}\rangle$ (e.g., the product-ket $\Pi_{\otimes i} |i, +x\rangle$, implying the $|+x\rangle$ state of each spin is not of that form). Consequently, while it is easy to imagine an experimental device enabling one to get the mixture described by the statistical operator $I/2^N$ (think of the collection of spins in an oven at temperature T , the whole being placed in a static magnetic field, and the Zeeman energy E_Z verifying $E_Z \ll kT$), getting the mixed state $\{|\Psi_{x\delta_1}\rangle, N_{N/2}^{-1}, \dots, |\Psi_{x\delta_{N_{N/2}}}\rangle, N_{N/2}^{-1}\}$ necessitates some selection among the pure states and therefore should be more elaborate.

2.3. A Consequence of the Definition of the Statistical Operator ρ

If Σ is in a pure state described by the normed ket $|\Phi\rangle$, the mean value of an observable \hat{O} acting on the kets of \mathcal{E} is the quantity $\langle\Phi|\hat{O}|\Phi\rangle$. If Σ is in a mixed state symbolically written $\{|\Phi_i\rangle, p_i\}$, a collection of normed (but not necessarily orthogonal) kets $|\Phi_i\rangle$, weighted by the respective probabilities p_i , the mean value of \hat{O} in that mixture is the quantity:

$$\sum_i p_i \langle\Phi_i|\hat{O}|\Phi_i\rangle = \sum_{i,k,k'} p_i \langle\Phi_i|k\rangle\langle k|\hat{O}|k'\rangle\langle k'|\Phi_i\rangle \quad (2)$$

where the completeness relation was used twice. This quantity may be written

$$\langle \hat{O} \rangle = \sum_{kk'} \rho_{k'k} O_{kk'} \tag{3}$$

with

$$O_{kk'} = \langle k | \hat{O} | k' \rangle, \tag{4}$$

and

$$\rho_{k'k} = \sum_i p_i \langle k' | \Phi_i \rangle \langle \Phi_i | k \rangle. \tag{5}$$

$O_{kk'}$ is a matrix element in the chosen basis of the observable \hat{O} , and $\rho_{k'k}$ a matrix element in the same basis of the statistical operator ρ (see e.g., [17]). The mean value may then be written:

$$\langle \hat{O} \rangle = \sum_{k'} (\rho \hat{O})_{k'k'} = \text{Tr}(\rho \hat{O}) \tag{6}$$

The statistical matrix may be written as $\rho = \sum_{k,k'} \rho_{kk'} | k \rangle \langle k' |$, and using Equation (5), one finally gets:

$$\rho = \sum_i p_i | \Phi_i \rangle \langle \Phi_i | \tag{7}$$

Therefore, if Σ is in a mixed state (or statistical mixture) $\{ | \Phi_i \rangle, p_i \}$, and if one is interested in the mean value $\langle \hat{O} \rangle$ or the variance $\langle (\hat{O} - \langle \hat{O} \rangle)^2 \rangle$ of \hat{O} or in the mean value of some function of \hat{O} , then, **as a consequence of the definition of the density operator ρ , the result calculated directly using the definition $\{ | \Phi_i \rangle, p_i \}$ of the mixed state and the result obtained using the statistical operator ρ and the trace are necessarily equal.** This well-known result, ignored in [9], will be explicitly used in Section 5.

For the definition of a variance in a quantum context, one can see e.g., [12] or [19]. Robertson, when introducing the variance in a quantum context in [20], called the square root of the variance *the uncertainty*.

3. Spin Components of the Spin Assembly: Useful Results

We now calculate mean values and variances of spin components of the spin assembly in some specific pure or mixed states. They will be used in the next section when trying to explain the origin of the differences found in the values of variances in the 2011 paper by FH.

3.1. Spin Assembly in the Pure State $| \psi_{X\delta} \rangle$

3.1.1. The S_x Component and Pure State $| \Psi_{X\delta} \rangle$

When the spin assembly is in the pure state $| \Psi_{X\delta} \rangle$, calculating the mean value and the variance of S_x is easy because: (1) S_x is the sum of all s_{xi} components, (2) $| \Psi_{X\delta} \rangle$ is a tensor product without partial entanglement, (3) each factor of the product is an eigenket of the corresponding s_{xi} , and the eigenvalues may be written $\varepsilon_i/2$, with $\varepsilon_i = \pm 1$. Consequently, for any ordering defined by δ :

$$S_x | \Psi_{X\delta} \rangle = \frac{1}{2} \sum_{j=1}^N \varepsilon_j | \Psi_{X\delta} \rangle = 0 \tag{8}$$

because, in the sum $\sum_{j=1}^N \varepsilon_j$, with $\varepsilon_j = \pm 1$, the values 1 and -1 both appear $N/2$ times. The mean value of the total spin S_x in any of these pure states is:

$$\langle S_x \rangle = \langle \Psi_{X\delta} | S_x | \Psi_{X\delta} \rangle = 0 \tag{9}$$

since $S_x | \Psi_{X\delta} \rangle$ is equal to zero. The variance of the total spin S_x in any of these pure states is:

$$\langle \Psi_{X\delta} | (S_x - \langle S_x \rangle)^2 | \Psi_{X\delta} \rangle = \langle \Psi_{X\delta} | S_x^2 | \Psi_{X\delta} \rangle = 0 \tag{10}$$

which results from the fact that presently: (1) $\langle S_x \rangle = 0$, (2) $S_x^2 | \Psi_{x\delta} \rangle = S_x(S_x | \Psi_{x\delta} \rangle)$, which equals 0, as $S_x | \Psi_{x\delta} \rangle = 0$.

Both the mean value and the variance of S_x are therefore equal to zero. To sum up, S_x has a zero variance because $| \Psi_{x\delta} \rangle$ is an eigenvector of S_x for the eigenvalue 0.

Calculating the mean value and the variance of S_x was easy, but it would be wrong to think that the assembly could be replaced by a single spin. $| \Psi_{x\delta} \rangle$ describes a pure state of an N spin 1/2 collection, and the just used sums $\sum_{j=1}^N s_{jx}$ and $\sum_{j=1}^N \epsilon_j$ mobilize the whole assembly. For instance, if $| \Psi_{x\delta} \rangle$ is a state with the first spin in the $| +x \rangle$ state, the mean value $\langle 1+x | s_{1x} | 1+x \rangle$ is equal to $+1/2$. This is true, in this specific case, for $\langle \Psi_{x\delta} | s_{1x} | \Psi_{x\delta} \rangle$. But $\langle \Psi_{x\delta} | S_x | \Psi_{x\delta} \rangle$, the mean value of the x component of the total spin is a sum of N such quantities, with $N/2$ of them being equal to $+1/2$ and the $N/2$ remaining ones being equal to $-1/2$.

3.1.2. The S_z Component, and Again Pure State $| \psi_{X\delta} \rangle$

We first consider a single spin 1/2 in the pure state $| \pm x \rangle$: when acting on $| \pm x \rangle$, the basis vectors of s_x, s_z generates the vectors $(1/2) | \mp x \rangle$, and its mean value in $| \pm x \rangle$ is

$$\langle \pm x | s_z | \pm x \rangle = \langle \pm x | s_z \frac{| + \rangle \pm | - \rangle}{\sqrt{2}} \rangle \tag{11}$$

$$= \langle \pm x | \frac{1}{2} \frac{| + \rangle \mp | - \rangle}{\sqrt{2}} \rangle = \frac{1}{2} \langle \pm x | \mp x \rangle = 0 \tag{12}$$

Its variance in this state is presently equal to the mean value of s_z^2 , i.e., to

$$\langle \pm x | s_z^2 | \pm x \rangle = \frac{1}{4} \tag{13}$$

as $s_z^2 | \pm x \rangle = s_z(s_z | \pm x \rangle) = s_z(1/2) | \mp x \rangle = (1/4) | \pm x \rangle$.

We now come to the mean value and variance of S_z in the pure state $| \Psi_{x\delta} \rangle$. The mean value of $S_z = \sum_j s_{jz}$ is a sum of N contributions, each one equal to 0, and therefore $\langle S_z \rangle = \langle \Psi_{x\delta} | S_z | \Psi_{x\delta} \rangle = 0$.

The variance of the total spin component S_z is:

$$\langle \Psi_{x\delta} | (S_z - \langle S_z \rangle)^2 | \Psi_{x\delta} \rangle = \langle \Psi_{x\delta} | S_z^2 | \Psi_{x\delta} \rangle \tag{14}$$

S_z^2 introduces two sorts of terms: the $s_{iz}s_{jz}(j \neq i)$ terms, which do not contribute, and the N terms of the form s_{iz}^2 , each one making a contribution equal to $1/4$:

$$\langle \Psi_{x\delta} | (S_z - \langle S_z \rangle)^2 | \Psi_{x\delta} \rangle = N/4$$

3.2. S_X and the Mixed State $\{ | \Psi_{X\delta 1} \rangle, N_{N/2}^{-1}, \dots, | \Psi_{X\delta N_{N/2}} \rangle, N_{N/2}^{-1} \}$

The spin assembly is now supposed to be in the mixed state $\{ | \Psi_{x\delta 1} \rangle, N_{N/2}^{-1}, \dots, | \Psi_{x\delta N_{N/2}} \rangle, N_{N/2}^{-1} \}$, with the way this mixed state was obtained not being described. As a first step in the calculation of the mean value and the variance of the total spin S_x , one has to consider the contribution of a single pure state $| \Psi_{x\delta} \rangle$ of the mixture to this mean value and to this variance. Here, the result is simple: from the result obtained in Section 3.1, both contributions are equal to zero for any δ ordering. Therefore, the mean value and the variance of S_x in this mixed state, the sum of the corresponding $N_{N/2}$ contributions, are again both equal to 0.

3.3. The Totally Unpolarized Mixture

If the spin assembly is in the totally unpolarized mixed state $\rho = I/2^N$, and if one wishes to calculate the mean value and the variance of S_x , this mixed state may be inter-

preted as made up of the 2^N tensor products $|1 \pm x \rangle \otimes |2 \pm x \rangle \otimes \dots \otimes |N \pm x \rangle$, a basis of eigenstates of S_x , all with the same weight $1/2^N$. The mean value of S_x is equal to 0 since: (1) S_x is a sum of N terms, each one implying a single spin, (2) the contribution of any such term to the trace of S_x , calculated in the eigenbasis of S_x , is 0, as there are $N/2$ diagonal elements equal to $1/2$ and $N/2$ diagonal elements equal to $-1/2$. The variance of S_x is here equal to $N/4$, as the $s_{xi}s_{xj}(j \neq i)$ terms do not contribute, and each of the N terms of the form s_{xi}^2 in the sum $\sum_i s_{xi}^2$ makes a contribution to the trace of ρS_x^2 equal to $(1/2^N)2^N(1/4)$. The same results are obtained for S_z , using the standard basis and the kets $|1 \pm \rangle \otimes |2 \pm \rangle \otimes \dots \otimes |N \pm \rangle$:

$$\text{If } \rho = \frac{I}{2^N} \text{ (totally unpolarized mixture): } \begin{cases} \text{mean value of } S_x = 0 \\ \text{variance of } S_x = \frac{N}{4} \end{cases}$$

and the same is true for S_z .

3.4. Exchanging the Roles of X and Z

The existence and use of the ensemble \mathcal{B} in [9] must be taken into account by considering quantum states, either pure or mixed, and observables (obtained from each situation already considered in this section) and by calculating the corresponding mean values and variances once the \hat{x} axis has been replaced by the \hat{z} axis and the total spin component S_z and the pure state $|\Psi_{z\delta}\rangle$ have replaced S_x and $|\Psi_{x\delta}\rangle$. Considering e.g., $|\Psi_{z\delta}\rangle$, for a similar reason to the one found with S_x and $|\Psi_{x\delta}\rangle$, now $S_z |\Psi_{z\delta}\rangle = 0$, and the mean value and the variance of S_z in a $|\Psi_{z\delta}\rangle$ state are equal to zero. Had a difference been found for the results for the \hat{x} axis with the total spin component S_x on one side and the \hat{z} axis with the total spin component S_z on the other, this would have meant that the isotropy of space was not respected.

4. The Origins of the Difference in the Values of Variances Found by FH

In Section 3, we found that the mean value and the variance of S_x are both equal to zero in both the pure state $|\Psi_{x\delta}\rangle$, for an arbitrary δ ordering, and the mixed state $\{|\Psi_{x\delta 1}\rangle, N_{N/2}^{-1}, \dots, |\Psi_{x\delta N_{N/2}}\rangle, N_{N/2}^{-1}\}$. The origin(s) of the difference in the values of variances claimed by FH must be identified and explained in some detail. This is not an easy task, as we showed that their paper [9] contains ambiguous and even contradictory elements. **We first consider the results they get in their Section 3.** FH calculate the variance of the same observable, first for their ensemble \mathcal{A} (their Equation (8)) and then for their ensemble \mathcal{B} (their Equation (13)), find that the values differ, and then write “We can certainly conclude that the two ensembles \mathcal{A} and \mathcal{B} are not equal”. Speaking of *ensembles that are not equal* is using an expression that is not defined within QM. In fact, two quantum systems may be identical or distinct, and if they are identical, they may be in the same state or not. In Section 1, we gave reasons why the system considered by FH in [9] is a collection of distinguishable, independent, identical magnetic moments associated with spins $1/2$. In Section 2.1, we stressed that [9,11] by FH contain ambiguities and inconsistencies. We then introduced a pure state of the spin assembly, which we called $|\Psi_{x\delta}\rangle$ and gave reasons why, when FH speak of *ensemble \mathcal{A}* , it should be understood that the system is in this pure state $|\Psi_{x\delta}\rangle$. In Section 3.1 of [9], FH speak of “the total spin of ensemble \mathcal{A} ” and the existence of their Equation (11) with the presence of N (the number of spins) clearly confirms that, whereas their notation is unclear, they are interested in the mean value and the variance of the x component of the total spin. It is then interesting to examine the following two situations: **one first considers their ensemble \mathcal{A} only** and the mean value and the variance of $S_z = \sum_i s_{zi}$ **in the pure state $|\Psi_{x\delta}\rangle$** : one gets (cf. Section 3)

$$\langle S_z \rangle = 0, \quad \langle (S_z - \langle S_z \rangle)^2 \rangle = \frac{N}{4}, \tag{15}$$

to be opposed to

$$\langle S_x \rangle = 0, \quad \langle (S_x - \langle S_x \rangle)^2 \rangle = 0 \tag{16}$$

One then considers their ensemble \mathcal{B} only: the roles of S_x and S_z have only to be exchanged, as explained in Section 3.4, and if one defines $|\Psi_{z\delta}\rangle$ by replacing the kets $|\pm x\rangle$ by the kets $|\pm\rangle$ (here keeping the usual notation), the mean values **in the pure state** $|\Psi_{z\delta}\rangle$ are respectively:

$$\langle S_x \rangle = 0, \quad \langle (S_x - \langle S_x \rangle)^2 \rangle = \frac{N}{4} \tag{17}$$

$$\langle S_z \rangle = 0, \quad \langle (S_z - \langle S_z \rangle)^2 \rangle = 0 \tag{18}$$

Therefore, the mean value and the variance of S_x , instead of those of S_z , are 0 and $N/4$, respectively, as can also be obtained using a projector and a trace (cf. Section 2.3). The difference has two origins: (1) S_x and S_z do not commute and play symmetrical roles; (2) one compares results in the pure state $|\Psi_{x\delta}\rangle$ and in the pure state $|\Psi_{z\delta}\rangle$.

We then conclude, or rather suggest, that: (1) \mathcal{A} and \mathcal{B} correspond to two *distinct pure states* of the collection of N (distinguishable, identical) spins, which we respectively denoted as $|\Psi_{x\delta}\rangle$ and $|\Psi_{z\delta}\rangle$, (2) the difference found by FH in their Section 3 is due to the fact that $|\Psi_{x\delta}\rangle$ is an eigenstate of S_x (see what they call their ensemble \mathcal{A}) but not of S_z , whereas $|\Psi_{z\delta}\rangle$ is an eigenstate of S_z (see what they call their ensemble \mathcal{B}) but not of S_x . And the value of the variance of S_z in the first case and of S_x in the second one, $N/4$, comes from the fact that $S_z = \sum_i s_{zi}$ and $S_x = \sum_i s_{xi}$ are two sums, implying N spin components, each related to a single spin. This value $N/4$ is an exact result, not an approximate one. If the spin assembly is in the state $|\Psi_{x\delta}\rangle$ and if one is interested in the mean of S_z then, focusing on the contribution of s_{zi} , one knows that in the tensor product, such as (1), one may write

$$|i, \pm x\rangle = \frac{|i, +\rangle \pm |i, -\rangle}{\sqrt{2}} \tag{19}$$

Then, when one measures s_{zi} , the *probability* of getting $+1/2$ is $1/2$ and $-1/2$ is also $1/2$. This expresses the principle of superposition in the present situation.

This being said, **one now has to examine the content and results of Section 4 of [9]**. FH denote the density operator ρ as \hat{P} . If they want to be consistent with what they did in their Section 3, they should consider, for their ensemble \mathcal{A} with (even) N spins, the *pure state* $|\Psi_{x\delta}\rangle$, and the result obtained with $|\Psi_{x\delta}\rangle \langle \Psi_{x\delta}|$ will be equal to the one obtained when using the ket $|\Psi_{x\delta}\rangle$ (cf. Section 2.3). Through their Equation (16), they instead consider a *single spin* in the *mixed state* written, with our notations, as

$$\left\{ \frac{1}{2}, | +x \rangle, \frac{1}{2}, | -x \rangle \right\}$$

Clearly, the mean value or the variance of s_x in this *mixed state of a single spin* has no reason why it should be equal respectively to the mean value or the variance of the *total spin component* $S_x = \sum s_{xi}$ in the *pure state* $|\Psi_{x\delta}\rangle$ of the collection of N spins. Their approach is therefore inconsistent, and when, after their Equation (19), they write that “These results are in stark contrast with Equations (8) and (13)”, their comparison is meaningless.

We are therefore justified in speaking of the origins, rather than the origin, of the difference in the values of variances found by FH, as there is a double inconsistency in their comparison: (1) a pure state versus a mixed state and (2) a spin assembly (N spins, with N even) and a single spin.

5. Discussion

In the previous sections, we started from the content of the 2011 FH paper [9] and tried to guess the aim of its authors. Some points that were then deferred will be addressed in the following discussion.

5.1. Calculations of Variances in a Pure State

Whereas the deep content of QM is still presently largely discussed, through the expression *interpretations of QM*, there is a consensus on the general rules of QM. We examine the following simple situation: a spin 1/2 in the pure state

$$|V\rangle = \frac{|+\rangle + i\sqrt{3}|-\rangle}{2}$$

If this spin is in a pure state and if one then measures s_y , the result is, in a random way, either $+1/2$ or $-1/2$. If the experiment consisting of a preparation in state $|V\rangle$, followed by the measurement of s_y , is repeated M times with $M \gg 1$, one can get (a reasonable estimation of) the probability of occurrence of the result $+1/2$ or $-1/2$. Using these probabilities in order to *calculate* the mean value $\langle V | s_y | V \rangle$ would implicitly mobilize the $\{|+\rangle, |-\rangle\}$ basis. In fact, calculations are often made *in a single chosen basis*. If one uses the standard basis $|+\rangle, |-\rangle$ and considers s_y , which is an observable that does not commute with s_z , then the following phenomenon is faced: when one has to calculate the mean value of s_y in state $|V\rangle$, it happens that the so-called interference terms $\langle + | s_y | - \rangle$ and $\langle - | s_y | + \rangle$ contribute to this mean value, a manifestation of the principle of superposition. One finally gets $\langle V | s_y | V \rangle = \sqrt{3}/4$.

The variance of s_y in this state is (cf. Section 2.3) the following mean value (in this state):

$$\langle V | (s_y - \langle s_y \rangle)^2 | V \rangle = \langle V | s_y^2 | V \rangle - (\langle V | s_y | V \rangle)^2 = \frac{1}{16}$$

If, keeping state $|V\rangle$ and the same basis, one calculates the mean value and the variance of s_z , diagonal in the $\{|+\rangle, |-\rangle\}$ basis, instead of those of s_y , no interference term appears. If Equation (4) from FH in [9] is valid for a first observable \hat{O} , then it cannot be used (keeping the same basis) for a second observable that does not commute with \hat{O} . For instance, given a pure state of a spin 1/2, e.g., $|V\rangle$, it cannot be used for both s_x and s_z .

If one must calculate the mean value or the variance of an observable attached to a system in a mixed state, each pure state of the mixture brings its own contribution, and the principle of superposition operates for each such pure state. The mean value or the variance may be calculated either by summing the contributions of all states in the mixture (and the calculation of each contribution mobilizes the weight affecting this pure state), or by using the density operator, a tool for this kind of calculation, as a result of its building up, as shown in Section 2.3. Then, if, in a given use, the two methods do not give the same results, at least one mistake has been made.

In [9], speaking of their ensembles \mathcal{A} and \mathcal{B} , FH write: “We shall focus on deriving, for both ensembles, the expectation value and the variance of the spin along the \hat{x} direction. Both of them are measurable quantities”. In fact, QM introduces so-called measurable quantities (observables), and associates Hermitian operators with them. s_x (or s_z) is (associated with) an observable. Given a pure or mixed state, the expectation value or the variance of s_x (or s_z) can be calculated (with the already recalled precautions), but they are not *measurable quantities*.

In their reply [11] to [10], FH insist that their “two ensembles are definitely not statistical ensembles”, and they add “we considered prepared ensembles, because we are basically free to decide which case study to investigate”. In that paper by FH, the expression “pure state” does not appear even once, but QM currently considers that a pure state results from some preparation act, and one should therefore understand that FH here claim that they consider a spin system in a pure state. It is now possible to comment on the fact that, in the same paper [11], in a note on page 3, FH add that “In Refs. [1,2], the variance has been computed by taking the quantum mechanical prediction on the single-particles measurements and by then applying Classical Statistics”. From what has been already detailed in our present paper: (1) applying classical statistics is meaningful only if one has a mixed

state, and if quantum calculations have first been performed at the level of each pure state. In [11], FH eliminate the case of mixed states; (2) in the pure states, which FH consider in [9], some spin operators have a variance containing a factor equal to N , which means that their system contains N spins and that the spin operator they consider is a component not of a single spin but of the total spin, which we denoted as $S_z = \sum_i s_{zi}$ or $S_x = \sum_i s_{xi}$. This being said, *it cannot be claimed* that in the calculation of the variance one should apply *Classical Statistics*. It is true that, given the pure states we called $|\Psi_{x\delta}\rangle$ and $|\Psi_{z\delta}\rangle$, the calculation of the mean value of S_z mobilizes a sum of N simpler quantities. But the calculation of each of them obeys the usual quantum rules rather than mobilizing classical probabilities.

5.2. FH and the Avogadro Number

We now consider the issue of the reference to the Avogadro number in the second paper by FH [11]. N is the number of (identical) particles in the physical system. The fact that the Avogadro number N_A is such that $\sqrt{N_A} \gg 1$ has well-known experimental consequences, and first in a non-quantum context, e.g., in the fact that fluctuations are very small, except near phase-transitions. And phenomenological thermodynamics considers macroscopic systems. Our theoretical results in Section 3 are obtained through considerations implicitly making use of probabilities, not estimations, and they are true even for $N = 2$ or 4. In their 2012 reply, FH write that “In realistic ensembles, N is of the order of the Avogadro Number ($\simeq 10^{23}$)” [11]. Two practical instances show that this is not true: in the case of electron spins and ESR experiments, already 50 years ago, under what was called standard conditions, (which implied diluted samples in order to have weak dipolar broadening and non-saturating conditions for the ESR signal), it was possible both to detect roughly 10^{13} spins at 300 K, and therefore even a weaker number of them at 4.2 K, and describe them theoretically with QM. And roughly 20 years ago, single-spin ESR through scanning tunneling spectroscopy was developed [21]. In the just mentioned passage from [11], FH add that (*in realistic ensembles*) “neither writing nor dealing with its N -particle density matrix is clearly feasible”. But precisely in the present paper, we did such calculations for both the mean value and the variance of spin components, which were possible because the spins were independent, and the results were exact. Two mixed states were considered: (1) the totally unpolarized case ($\rho = I/2^N$), (2) the mixed state $\{|\Psi_{x\delta 1}\rangle, N_{N/2}^{-1}, \dots, |\Psi_{x\delta N_{N/2}}\rangle, N_{N/2}^{-1}\}$ (or, of course, the one obtained by writing z instead of x). The density operator ρ operates in the 2^N -dimensional state space of the spin assembly, and should not be confused with a spin operator operating in the state space of a given spin, even in the specific case of total unpolarization: $\rho = I/2^N$ is then a (tensor) product of N identity operators acting in the state space of each spin. And, in the case of independent spins, calculations are possible without writing explicitly the matrix associated with $\rho = I/2^N$ in an arbitrary basis, in which ρ is diagonal.

5.3. Still Trying to Understand the Results from FH

We now come back to a question that was approached at the beginning of Section 2. In [9], FH describe a process clearly leading to a pure state, but, as mentioned in Section 2.1, they give contradictory indications on this question; they also suggest that their \mathcal{A} and \mathcal{B} are in a mixed state (cf. their writing “Both \mathcal{A} and \mathcal{B} ” ... “are also said to be in a maximally mixed state”). We may suppose that they adopt the point of view of someone who *ignores* that their ensemble \mathcal{A} was prepared in a well-defined pure state and then *supposes* that the collection of N spins is in a mixed state where the 2^N states of the S_x eigenbasis all contribute with the same weight to the statistical mixture ($\rho = I/2^N$). However, this supposition should be rejected, since, as mentioned in Section 2.1 it is inconsistent with Equation (8) of [9].

One may instead imagine a scientist who, ignoring that ensemble \mathcal{A} was prepared in an eigenstate of S_x with the eigenvalue 0, $|\Psi_{x\delta}\rangle$, decides that it is in a mixed state where the eigenstates of the S_x eigenbasis with this eigenvalue equal to 0 all contribute, with the same weight. Then, if he calculates the mean value of S_x and its variance

(cf. Section 3.2), he will *accidentally* find the same results as those obtained for the pure state $|\Psi_{x\delta}\rangle$ (cf. Section 3.1.1). If he starts from ensemble \mathcal{B} and $|\Psi_{z\delta}\rangle$, and similarly introduces the corresponding mixed state, the same can be said using S_z . One could assume that this reasoning was perhaps held by FH. If so, they confused the pure state $|\Psi_{x\delta}\rangle$ and a mixed state exclusively made up of states with the eigenvalue 0 of S_x , all with the same weight. But **this explanation cannot be kept** because, as written in Section 2.1 from their 2012 reply [11], FH insisted that, concerning their \mathcal{A} and \mathcal{B} ensembles: “These two ensembles are definitely not statistical ensembles”, adding “we considered prepared ensembles”, which may be read as meaning that they considered pure states.

5.4. FH and a Book from Sakurai

In both [9,11], FH refer to a book on quantum mechanics by Sakurai [13]. This fact necessitates a short incursion into a question belonging to the area of the interpretation(s) of quantum mechanics. It seems that, like Ballentine [12], Sakurai adopted what Ballentine calls the ensemble interpretation (for more details, see (Ballentine 1998)). Perhaps for personal pedagogical reasons, and contrary to Ballentine, in his book, Sakurai did not use the expression “pure state”. Instead, he spoke of a “state ket”, and introduced a “pure ensemble”, which he defined as “-a collection- of identically prepared physical systems, all characterized by the same ket $|\alpha\rangle$ ”. This led him to introduce the expression of the mean value of an observable A “taken with respect to state $|\alpha\rangle$ ” as the sum of measured values a' , each one multiplied by a quantity $|\langle a' | \alpha \rangle|^2$, interpreted as a probability (cf. his Equation (1.4.6), p. 25), a result obtained under the condition that the kets $|a'\rangle$ are (a basis of) eigenkets of A . **Therefore, if one considers two non-commuting observables, care must be taken, as this expression cannot be used for both of them with the same basis.** The approach followed by Sakurai has the effect, both an advantage and a risk, of avoiding the presence of interference terms. When reading Sakurai, one must also notice that if he was interested in a single spin 1/2, in a pure state $|\alpha\rangle$, he introduced the “number of dimensions, N , of the ket space”, equal to 2 for a spin 1/2, and not to be confused with the number of spins in the ensemble associated with this spin by Sakurai. In this context introduced by Sakurai, it is meaningless to speak of the total spin of this collection. Sakurai described mixed states in his Section 3.4. (p. 178). Then, what is the choice made by FH? They cite Sakurai in their two papers. They do not speak of a system in a pure state. They speak of an ensemble—their \mathcal{A} or \mathcal{B} ensemble—but not of a *pure ensemble* as Sakurai did; they do not follow Sakurai’s definition, since all the members of their ensemble have not been identically prepared. Moreover, they speak of the *total spin* of their ensemble, which is contradictory to what Sakurai did. The question is then: do FH, who cite Sakurai in their two papers, adopt his approach? If the answer is yes, they are speaking of a single spin 1/2; when they speak of a total spin, this is meaningless. Moreover, they are not allowed to consider a collection of spins not all in the same state. In spite of their reference to Sakurai, the answer seems to be no. As already said, the way they speak of their *ensemble* \mathcal{A} or \mathcal{B} is ambiguous. In the previous sections, we tried to give a meaning to both the system and its state, as possibly implicitly used by FH.

5.5. Before Concluding

Arriving here, it should be clear that, in the work proposed by FH, some major points are wrong, and others are ambiguous and then difficult to analyze. For instance a given result they obtain for the value of a variance may be exact by accident, or may be wrong either because the system and its state are ill-defined, and/or because the method they suggest (they use?) in the calculation of an expectation value and/or a variance is wrong. And there is a strong ambiguity as to what FH call \mathcal{A} or \mathcal{B} ensemble, as in their reply [11], they seem to insist upon the fact they consider what is usually called a pure state, but in contrast, in their previous paper, they wrote that they were unpolarized (cf. its Section 2: “Both \mathcal{A} and \mathcal{B} are totally unpolarized ensembles” and its Section 5: “the two ensembles considered in this paper are both unpolarized”), therefore *not* in a pure state.

Faced with this reality, and with the following passage from BD in [10]: “The mistake of FH has nothing to do with quantum mechanics rather it is a classical statistical misconception”, we consider that it would be quite hazardous to try and give a meaning to this passage from the reply [11] by FH: “By “statistical ensemble” is meant an ensemble whose populations of states are statistically determined by means of a certain statistical distribution that guarantees random mixing”, without any reference to pure states.

6. Conclusions

In his 1970 paper, Zeh stressed the existence of a possible weakness in the general postulates of QM when observing that the density matrix formalism cannot be a complete description of a statistical ensemble, as it may happen that this ensemble cannot be rederived from the density matrix. Some 40 years later, the 2011 paper by Fratini and Hayrapetyan (FH) was aimed at discussing possible limits of the density operator formalism in QM. But an idea is unfortunately weakened if advocated through the use of false arguments. In the present paper, it has been shown that the differences in the values of variances as claimed by FH are wrong results, partly as a consequence of ill-defined and/or contradictory situations in their definition of both a quantum system and its possible quantum states and partly as an undue comparison between results obtained in different situations and systems (e.g., one spin in a mixed state versus a spin assembly in a pure state). One interest of the paper [10] by Bodor and Diosi is the existence of reply [11]. In that paper, FH explicitly write “The analysis we carried out in [1] does not include nor mention statistical ensembles, as we explicitly define and refer only to “prepared ensembles””. If FH mean that they just manipulated pure states, this means that when using the density matrix formalism, they have to use projectors; any variance calculated through a projector has the same value as if calculated directly. In their 2012 reply, FH claim that “density matrices do not provide a complete description of ensembles of states in quantum mechanics”. This is perhaps true, but FH failed to show it; therefore, the 2011–2012 discussion initiated by Fratini and Hayrapetyan neither confirms nor invalidates the 1970 comment by Zeh. The reader interested in the Zeh problem may read [22], which shows that the use of higher-order moments of a well-chosen random variable helps solve the question asked by Zeh for the spin of a collection of neutrons in two statistical mixtures described by the same density operator.

Author Contributions: A.D.: methodology, original draft. Y.D.: formal analysis, review and editing. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding. A waiver was provided by MDPI for APC.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: No new data were created in this investigation.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. von Neumann, J. *Mathematical Foundations of Quantum Mechanics*; Princeton University Press: London, UK, 1955.
2. von Neumann, J. *Mathematische Grundlagen der Quantenmechanik*; Springer: Berlin/Heidelberg, Germany, 1932.
3. Peres, A. *Quantum Theory: Concepts and Methods*; Kluwer Academic Publishers: Dordrecht, The Netherlands, 1995.
4. Bell, J.S. Against “Measurement”. *Phys. World* **1990**, *3*, 33–41. [[CrossRef](#)]
5. Bell, J.S. Against “Measurement”. In *Proceedings of the NATO International School of History: “Sixty-Two Years of Uncertainty” Erice, August 5–15 1989*; NATO ASI Series B Physics; Miller, A.I., Ed.; Plenum Press: New York, NY, USA; London, UK, 1990; pp. 17–31.
6. Zeh, H.D. On the Interpretation of Measurement in Quantum Theory. *Found. Phys.* **1970**, *1*, 69–76. [[CrossRef](#)]
7. Nenashev, A.V. Why state of quantum system is fully defined by density matrix. *arXiv* **2016**, arXiv:1601.08205v1.
8. Siomau, M.; Fritzsche, S. Quantum computing with mixed states. *Eur. Phys. J. D* **2011**, *62*, 449–456. [[CrossRef](#)]
9. Fratini, F.; Hayrapetyan, A.G. Underlining some limitations of the statistical formalism in quantum mechanics. *Phys. Scr.* **2011**, *84*, 035008. [[CrossRef](#)]

10. Bodor, A.; Diósi, L. Comment on “Underlining some limitations of the statistical formalism in quantum mechanics” by Fratini and Hayrapetyan. *arXiv* **2012**, arXiv:1110.4549v1.
11. Fratini, F.; Hayrapetyan, A.G. Underlining some limitations of the statistical formalism in quantum mechanics: Reply to the Comment of Bodor and Diósi. *arXiv* **2012**, arXiv:1204.1071v1.
12. Ballentine, L.E. *Quantum Mechanics: A Modern Development*; World Scientific: Singapore, 1998.
13. Sakurai, J.J. *Modern Quantum Mechanics*, 2nd ed.; Maddison-Wesley: San Francisco, CA, USA, 1994.
14. Weyl, H. Quantenmechanik und Gruppentheorie. *Z. Phys.* **1927**, *46*, 1–46. [[CrossRef](#)]
15. Dirac, P.A.M. A new notation for quantum mechanics. *Math. Proc. Camb. Philos. Soc.* **1939**, *35*, 416–418. [[CrossRef](#)]
16. Weinberg, S. *Lectures on Quantum Mechanics*; Cambridge University Press: Cambridge, UK, 2013.
17. Fano, U. Description of States in Quantum Mechanics by Density and Operator Techniques. *Rev. Mod. Phys.* **1957**, *29*, 74–93. [[CrossRef](#)]
18. Mathews, J.; Walker, R.L. *Mathematical Methods of Physics*; Benjamin: New York, NY, USA, 1965.
19. Ohya, M.; Volovich, I. *Mathematical Foundations of Quantum Information and Computation and Its Applications to Nano- and Bio-Systems*; Springer: Berlin/Heidelberg, Germany, 2011.
20. Robertson, H.P. The Uncertainty Principle. *Phys. Rev.* **1929**, *34*, 13–164. [[CrossRef](#)]
21. Buchachenko, A.L.; Dalidchik, F.I.; Shub, B.R. Single spin ESR. *Chem. Phys. Lett.* **2001**, *340*, 103–108. [[CrossRef](#)]
22. Deville, A.; Deville, Y. Random-coefficient pure states, the density operator formalism and the Zeh problem. *arXiv* **2024**, arXiv:2201.03248v4.

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.