

## THE HATSOPOULOS–GYFTOPOULOS RESOLUTION OF THE SCHRÖDINGER–PARK PARADOX ABOUT THE CONCEPT OF “STATE” IN QUANTUM STATISTICAL MECHANICS

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A seldom recognized fundamental difficulty undermines the concept of individual “state” in the present formulations of quantum statistical mechanics (and in its quantum information theory interpretation as well). The difficulty is an unavoidable consequence of an almost forgotten corollary proved by Schrödinger in 1936 and perused by Park, *Am. J. Phys.* **36**, 211 (1968). To resolve it, we must either reject as unsound the concept of state, or else undertake a serious reformulation of quantum theory and the role of statistics. We restate the difficulty and discuss a possible resolution proposed in 1976 by Hatsopoulos and Gyftopoulos, *Found. Phys.* **6**, 15; 127; 439; 561 (1976).

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### 1. Introduction

In 1936, Schrödinger<sup>1</sup> published an article to denounce a “repugnant” but unavoidable consequence of the present formulation of Quantum Mechanics (QM) and Quantum Statistical Mechanics (QSM). Schrödinger claimed no priority on the mathematical result, and properly acknowledged that it is hardly more than a corollary of a theorem about statistical operators that von Neumann proved five years earlier.<sup>2</sup>

Three decades later, Park<sup>3</sup> exploited von Neumann’s theorem and Schrödinger’s corollary to point out quite conclusively an essential tension undermining the logical conceptual framework of QSM (and of its Quantum Information Theory interpretation as well). Twenty more years later, Park returned to the subject in another magistral, but almost forgotten Ref. 4 in which he addresses the question of “whether an observer making measurements upon systems from a canonical ensemble can determine whether the systems were prepared by mixing, equilibration,

or selection”, and concludes that “a generalized quantal law of motion designed for compatibility with fundamental thermodynamic principles, would also provide a means for resolving paradoxes associated with the characteristic ambiguity of ensembles in quantum mechanics.”

Schrödinger’s corollary was “rediscovered” by Jaynes<sup>5,6</sup> and Gisin,<sup>7</sup> and generalized by Hughston, Jozsa, and Wootters<sup>8</sup> and Kirkpatrick.<sup>9</sup> Also some interpretation has been re-elaborated around it,<sup>10–15</sup> but unfortunately the original references have not always been duly cited. The problem at issue in this paper, first raised in Ref. 1, has been acknowledged “in passing” in innumerable other references (see, e.g., Refs. 16, 17 and references therein), but none has to our knowledge gone so deeply and conclusively to the conceptual roots as Refs. 3 and 4. For this reason it is useful once in a while to refresh our memory about the pioneering conceptual contributions by Schrödinger and Park. The crystal clear logic of their analyses should not be forgotten, especially if we decide that it is necessary to “go beyond”. Reference 1 has been cited by many others, but not about the problem we focus on here, rather because it also contains pioneering contributions to the questions of entanglement, EPR paradox and related nonlocal issues. References 1, 3 and 4 have often been cited also in relation to the projection postulate and the quantum measurement problem.

The tension that Park vividly brings out in his beautiful essay on the “nature of quantum states” is about the central concept of individual state of a system. The present formulation of QM and the standard interpretation of QSM imply the paradoxical conclusion that every system is “a quantum monster”: a single system can be thought as concurrently being “in” two (and actually even more) different states. We briefly review the issue below (as we have done also in Ref. 18), but we urge everyone interested in the foundations of quantum theory to read the original Refs. 3 and 4. The problem has been widely overlooked and is certainly not well known, in spite of the periodic rediscoveries. The overwhelming successes of QM and QSM understandably contributed to discourage or dismiss as useless any serious attempt to resolve the nevertheless unavoidable fundamental difficulty.

Here, we emphasize that a resolution of the tension requires a serious re-examination of the conceptual and mathematical foundations of quantum theory. We discuss four logical alternatives. We point out that one of these alternatives achieves a resolution of the fundamental difficulty without contradicting any of the successes of the present mathematical formalism in the equilibrium realm where it is backed by experiments. However, it requires an essentially new and different re-interpretation of the physical meaning of such successes. Moreover, in the nonequilibrium domain it opens to new discoveries, new physics compatible with the second law of thermodynamics, without contradicting QM, and resolving the Boltzmann paradox about irreversibility as well. Thermodynamics may thus play once again a key role in a conceptual advancement<sup>19–27</sup> which may prelude to uncovering new physics about far non-equilibrium dynamics.<sup>28–32</sup>

## 2. Schrödinger–Park Quantum Monsters

In this section, we review briefly the problem at issue. We start with the seemingly harmless assumption that every system is always in some definite, though perhaps unknown, state. We will conclude that the assumption is incompatible with the present formulation and interpretation of QSM/QIT. To this end, we concentrate on an important special class of systems that we call “strictly isolated”. A system is strictly isolated if and only if (a) it interacts with no other system in the universe, and (b) its state is at all times uncorrelated from the state of any other system in the universe.

The argument that “real systems can never be strictly isolated and thus we should dismiss this discussion as useless at the outset” is at once counterproductive, misleading and irrelevant, because the concept of strictly isolated system is a keystone of the entire conceptual edifice in physics, particularly indispensable to structure the principle of causality. Hence, the strictly isolated systems must be accepted, at least, as conceivable, in the same way as we accept within QM that a vector in Hilbert space may represent a state of a system. Here we take as an essential necessary requirement that, when applied to a conceivable system and in particular to an isolated system, the formulation of a physical theory like QSM must be free of internal conceptual inconsistencies.

In QM the states of a strictly isolated system are in one-to-one correspondence with the one-dimensional orthogonal projection operators on the Hilbert space of the system. We denote such projectors by the symbol  $P$ . If  $|\psi\rangle$  is an eigenvector of  $P$  such that  $P|\psi\rangle = |\psi\rangle$  and  $\langle\psi|\psi\rangle = 1$  then  $P = |\psi\rangle\langle\psi|$ . It is well known that different from classical states, quantum states are characterized by irreducible intrinsic probabilities. We give this for granted here, and do not elaborate further on this point.

Admittedly, the objective of QSM is to deal with situations in which the state of the system is not known with certainty. Such situations are handled, according to von Neumann<sup>2</sup> (but also to Jaynes<sup>5,6</sup> within the QIT approach) by assigning to each of the possible states of the system an appropriate statistical weight which describes an “extrinsic” (we use this term to contrast it with “intrinsic”) uncertainty as to whether that state is the actual state of the system. The selection of a rule for a proper assignment of the statistical weights is not of concern to us here.

To make clear the meaning of the words extrinsic and intrinsic, consider the following non-quantal example. We have two types of “biased” coins  $A$  and  $B$  for which “heads” and “tails” are not equally likely. Say that  $p_A = 1/3$  and  $1 - p_A = 2/3$  are the intrinsic probabilities of all coins of type  $A$ , and that  $p_B = 2/3$  and  $1 - p_B = 1/3$  those of coins of type  $B$ . Each time we need a coin for a new toss, however, we receive it from a slot machine that first tosses an unbiased coin  $C$  with intrinsic probabilities  $w = 1/2$  and  $1 - w = 1/2$  and, without telling us the outcome, gives us a coin of type  $A$  whenever coin  $C$  yields “head” and a coin of type  $B$  whenever  $C$  yields “tail”. Alternatively, we pick coins out of a box where

50% coins of type  $A$  and 50% coins of type  $B$  have been previously mixed. It is clear that for such a preparation scheme, the probabilities  $w$  and  $1 - w$  with which we receive (pick up) coins of type  $A$  or of type  $B$  have “nothing to do” with the intrinsic probabilities  $p_A$ ,  $1 - p_A$ , and  $p_B$ ,  $1 - p_B$  that characterize the biased coins we will toss. We therefore say that  $w$  and  $1 - w$  are extrinsic probabilities, that characterize the heterogeneity of the preparation scheme rather than features of the prepared systems (the coins). If on each coin we receive we are allowed only a single toss (projection measurement?), then due to the particular values ( $p_A = 1/3$ ,  $p_B = 2/3$  and  $w = 1/2$ ) chosen for this tricky preparation scheme, we get “heads” and “tails” which are equally likely; but if we are allowed repeated tosses (non-destructive measurements, gentle measurements, quantum cloning measurements, continuous time measurements?) then we expect to be able to discover the trick. Thus it is only under the single-toss constraint that we would not lose if we base our bets on a description of the preparation scheme that simply weighs the intrinsic probabilities with the extrinsic ones, i.e. that would require us to expect “head” with probability  $p_{\text{head}} = wp_A + (1 - w)p_B = 1/2 * 1/3 + 1/2 * 2/3 = 1/2$ .

For a strictly isolated system, the possible states according to QM are, in principle, all the one-dimensional projectors  $P$  on the Hilbert space  $\mathcal{H}$  of the system. Let  $\mathcal{P}$  denote the set of such one-dimensional projectors on  $\mathcal{H}$ . If we are really interested in characterizing unambiguously a preparation scheme that yields states in the set  $\mathcal{P}$  with some probability density, we should adopt a measure theoretic description as proposed in Ref. 18, and define a “statistical weight measure”  $\mu$  satisfying the normalization condition  $\mu(\mathcal{P}) = \int_{\mathcal{P}} \mu(dP) = 1$  and such that the expected value of an observable  $A$  (which on the base states is given by  $\text{Tr}(PA)$ ) is given by  $\langle A \rangle = \int_{\mathcal{P}} \text{Tr}(PA)\mu(dP)$ . As shown in Ref. 18, this description would not lead to the kind of ambiguities we are led to by adopting the von Neumann description, but it would not lead to the von Neumann density operator either.

Instead, following the von Neumann recipe, QSM and QIT assign to each state  $P_i$  a statistical weight  $w_i$ , and characterizes the extrinsically uncertain situation by a (von Neumann) statistical operator  $W = \sum_i w_i P_i$ , a weighted sum of the projectors representing the possible states ( $W$  is more often called the density operator and denoted by  $\rho$ , but we prefer to reserve this symbol for the state operators we define in the next section).

The von Neumann construction is ambiguous, because the same statistical operator is assigned to represent a variety of different preparations, with the only exception of homogeneous preparations (*proper* preparation in the language of Ref. 33) where there is only one possible state  $P_\psi$  with statistical weight 100% so that  $W = W^2 = P_\psi$  is “pure”. Given a statistical operator  $W$  (a non-negative, unit-trace, self-adjoint operator on the Hilbert space of the system), its decomposition into a weighted sum of one-dimensional projectors  $P_i$  with weights  $w_i$  implies that there is a preparation such that the system is in state  $P_i$  with probability  $w_i$ . The situation described by  $W$  has no extrinsic uncertainty if and only if  $W$  equals one

of the  $P_i$ 's, i.e. if and only if  $W^2 = W = P_i$  (von Neumann's theorem<sup>2</sup>). Then, QSM reduces to QM and no ambiguities arise.

The problem is that whenever  $W$  represents a situation with extrinsic uncertainty ( $W^2 \neq W$ ), then the decomposition of  $W$  into a weighted sum of one-dimensional projectors is not unique. This is the essence of Schrödinger's corollary<sup>1</sup> relevant to this issue (for a mathematical generalization see Ref. 9 and for interpretation in the framework of nonlocal effects see e.g. Ref. 10).

For our purposes, notice that every statistical (density) operator  $W$ , when restricted to its range  $\text{Ran}(W)$ , has an inverse that we denote by  $W^{-1}$ . If  $W \neq W^2$ , then  $\text{Ran}(W)$  is at least two-dimensional, i.e. the rank of  $W$  is greater than 1. Let  $P_j = |\psi_j\rangle\langle\psi_j|$  denote the orthogonal projector onto the one-dimensional subspace of  $\text{Ran}(W)$  spanned by the  $j$ th eigenvector  $|\psi_j\rangle$  of an eigenbasis of the restriction of  $W$  to its range  $\text{Ran}(W)$  ( $j$  runs from 1 to the rank of  $W$ ). Then,  $W = \sum_j w_j P_j$  where  $w_j$  is the  $j$ th eigenvalue, repeated in case of degeneracy. It is noteworthy that  $w_j = [\text{Tr}_{\text{Ran}(W)}(W^{-1}P_j)]^{-1}$ . Schrödinger's corollary states that, chosen an arbitrary vector  $\alpha_1$  in  $\text{Ran}(W)$ , it is always possible to construct a set of vectors  $|\alpha_k\rangle$  ( $k$  running from 1 to the rank of  $W$ ,  $\alpha_1$  being the chosen vector) which span  $\text{Ran}(W)$  (but are not in general orthogonal to each other), such that the orthogonal projectors  $P'_k = |\alpha_k\rangle\langle\alpha_k|$  onto the corresponding one-dimensional subspaces of  $\text{Ran}(W)$  give rise to the alternative resolution of the statistical operator  $W = \sum_k w'_k P'_k$ , with  $w'_k = [\text{Tr}_{\text{Ran}(W)}(W^{-1}P'_k)]^{-1}$ .

To fix ideas, consider the example of a qubit with the statistical operator given by  $W = p|1\rangle\langle 1| + (1 - p)|0\rangle\langle 0|$  for some given  $p$ ,  $0 < p < 1$ . Consistently with Schrödinger's corollary, it is easy to verify that the same  $W$  can also be obtained as a statistical mixture of the two projectors  $|+\rangle\langle +|$  and  $|a\rangle\langle a|$  where  $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ ,  $|a\rangle = (|+\rangle + |a-\rangle)/\sqrt{1 + a^2}$  (note that  $|a\rangle$  and  $|+\rangle$  are not orthogonal to each other),  $|-\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$ ,  $a = 1/(1 - 2p)$  and  $w = 2p(1 - p)$  so that  $W = w|+\rangle\langle +| + (1 - w)|a\rangle\langle a|$ . With  $p = 1/4$  this is exactly the example given by Park in Ref. 3.

QSM forces on us the following interpretation of Schrödinger's corollary. The first decomposition of  $W$  implies that we may have a preparation which yields the system in state  $P_j$  with probability  $w_j$ , therefore, the system is definitely in one of the states in the set  $\{P_j\}$ . The second decomposition implies that we may as well have a preparation which yields the system in state  $P'_k$  with probability  $w'_k$  and, therefore, the system is definitely in one of the states in the set  $\{P'_k\}$ . As both decompositions hold true simultaneously, the very rules we adopted to construct the statistical operator  $W$  allow us to conclude that the state of the system is certainly one in the set  $\{P_j\}$ , but concurrently it is also certainly one in the set  $\{P'_k\}$ . As the two sets of states  $\{P_j\}$  and  $\{P'_k\}$  are different (no elements in common), this would mean that the system “is” simultaneously “in” two different states, thus contradicting our starting assumption that a system is always in one definite state (though perhaps unknown). Little emphasis is gained by noting that, because the

possible different decompositions are not just two but an infinity, we are forced to conclude that the system is concurrently in an infinite number of different states! Obviously such conclusion is unbearable and perplexing, but it is unavoidable within the current formulation of QSM/QIT. The reason why we have learnt to live with this issue – by simply ignoring it – is that if we forget about interpretation and simply use the mathematics, so far we always got successful results that are in good agreement with experiments.

Also for the coin preparation example discussed above, there are infinite ways to provide 50% head and 50% tail upon a single toss of a coin chosen randomly out of a mixture of two kinds of biased coins of opposite bias. If we exclude the possibility of performing repeated (gentle) measurements on each single coin, then all such situations are indeed equivalent, and our adopting the weighted sum of probabilities as a faithful representation is in fact a tacit acceptance of the impossibility of making repeated measurements. This limitation amounts to accepting that the extrinsic probabilities ( $w$ ,  $1 - w$ ) combine irreducibly with the intrinsic ones ( $p_A$ ,  $p_B$ ), and once this is done there is no way to separate them again (at least not in a unique way). If these mixed probabilities are indeed all that we can conceive, then we must give up the assumption that each coin has its own possibly unknown, but definite bias, because otherwise we are led to a contradiction, for we would conclude that there is some definite probability that a single coin has at once two different biases (a monster coin which belongs concurrently to both the box of, say,  $2/3 - 1/3$  biased coins and to the box of, say,  $3/4 - 1/4$  biased coins).

### 3. Is There a Way Out?

In this section we discuss four main alternatives towards the resolution of the paradox, i.e. if we wish to clear our everyday, already complicated life from quantum monsters. Indeed, even though it has been latent for fifty years and it has not impeded major achievements, the conceptual tension denounced by Schrödinger and Park is untenable, and must be resolved.

Let us therefore restate the three main hinges of QSM which lead to the logical inconsistency:

- (1) a system is always in a definite, though perhaps unknown, state;
- (2) states (of strictly isolated systems) are in one-to-one correspondence with the one-dimensional projectors  $P$  on the Hilbert space  $\mathcal{H}$  of the system; and
- (3) statistics of measurement results from a heterogeneous preparation with extrinsic uncertainty (probabilities  $w_i$ ) as to which is the actual state of the system among a set  $\{P_i\}$  of possible states is described by the statistical operator  $W = \sum_i w_i P_i$ .

To remove the inconsistency, we must reject or modify at least one of these statements. But, in doing so, we cannot afford to contradict any of the innumerable successes of the present mathematical formulation of QSM.

A first alternative was discussed by Park<sup>3</sup> in his essay on the nature of quantum states. If we decide to retain statements (2) and (3), then we must reject statement (1), i.e. we must conclude that the concept of state is “fraught with ambiguities and should therefore be avoided.” A system should never be regarded as being in any physical state. We should dismiss as unsound all statements of this type: “Suppose an electron is in state  $\psi \dots$ ” Do we need to undertake this alternative and therefore abandon deliberately the concept of state? Are we ready to face all the ramifications of this alternative?

A second alternative is to retain statements (1) and (2), reject statement (3) and reformulate the mathematical description of situations with extrinsic uncertainty in a way not leading to ambiguities. To our knowledge, such a reformulation has never been considered. The key defect of the representation by means of statistical operators is that it mixes irrecoverably two different types of uncertainties: the intrinsic uncertainties inherent in the quantum states and the extrinsic uncertainties introduced by the statistical description.

In Ref. 18, we have suggested a measure-theoretic representation that would achieve the desired goal of keeping the necessary separation between intrinsic quantum uncertainties and extrinsic statistical uncertainties. We will elaborate on such representation elsewhere. Here, we point out that a change in the mathematical formalism involves the serious risk of contradicting some of the successes of the present formalism of QSM. Such successes are to us sufficient indication that changes in the present mathematical formalism should be resisted unless the need becomes incontrovertible.

A third alternative is the QIT approach proposed by Jaynes<sup>5,6</sup> and subsequent literature. The paradox is bypassed (rather than resolved) by introducing an *ad hoc* “recipe” whereby base states other than eigenstates of the statistical operator  $W$  are to be excluded as unconceivable, based on the belief that they do not represent “mutually exclusive events”.<sup>34</sup> We skip here the well-known details of the QIT *ad hoc* recipe<sup>5,6</sup> to obtain the maximal  $-\text{Tr}(W \ln W)$  statistical operator  $W$  which should provide the “best, unbiased description” of the statistics of measurement results. We need only point out, for the purpose of our discussion, that such recipe leads to the correct physical results (i.e. canonical and grand-canonical thermodynamic equilibrium distributions) only if (1) the experimenter is assumed to know the value of the energy of the system, not of some other observable(s); (2) the underlying pure components of the heterogeneous preparation are “mutually exclusive” in the sense that they are the eigenvectors of the Hamiltonian operator of the system. Then, QIT reduces to equilibrium QSM and expectation values are successfully computed (from the pragmatic point of view) by the formula  $\langle A \rangle = \text{Tr}(AW)$  where  $W = \exp(-\beta H)/\text{Tr}[\exp(-\beta H)]$  (or its grand-canonical equivalent).

However, from the conceptual point of view, the two *ad hoc* conditions just underlined are in clear conflict with the purely subjective interpretation assumed at the outset in the QIT approach, for they exclude choices that a truly unbiased

experimenter has no reason to exclude *a priori*. In other words, the fact that such conditions are necessary to represent the right physics, implies that they represent objective (rather than subjective) features of physical reality. In particular, they impose that among the many possible decompositions of the maximal  $-\text{Tr}(W \ln W)$  statistical operator  $W$ , which exist by Schrödinger's corollary, the observer is allowed to give a physical meaning only to the spectral decomposition, thereby being forced by the recipe to an extremely biased perspective. So, by ignoring and bypassing the Schrödinger–Park conceptual paradox, the QIT approach not only does not resolve it, but it opens up additional conceptual puzzles. For example, what should  $W$  be if the experimenter knows the value of a property other than energy, or is to describe statistics from a heterogeneous preparation which is a mixture of pure preparations corresponding to non-mutually-orthogonal QM states (non-mutually-exclusive events)? From the application point of view, practitioners in the chemical physics literature have devised successful modeling and computational recipes based on constrained maximal entropy<sup>35,36</sup> or rate-controlled constrained maximal entropy<sup>37,38</sup> in which the energy constraint is replaced by or complemented with suitably selected other constraining quantities, e.g., configurational averages<sup>35,36</sup> or potentials globally characterizing a class of slow rate-controlling reaction schemes.<sup>37,38</sup> But the empirical success of these approaches, in our view, corroborates the need for further discussions about the subjectivity-objectivity conceptual dilemma which remains unresolved.

A fourth intriguing alternative has been first proposed by Hatsopoulos and Gyftopoulos<sup>19–22</sup> in 1976. The idea is to retain statement (1) and modify statement (2) by adopting and incorporating the mathematics of statement (3) to describe the true physical states, i.e. the homogeneous preparations, and at the same time devoiding heterogeneous preparations (and, therefore, extrinsic statistics) of any fundamental role. The defining features of the projectors  $P$ , which represent the states for a strictly isolated system in QM, are:  $P^\dagger = P$ ,  $P > 0$ ,  $\text{Tr } P = 1$ ,  $P^2 = P$ . The defining features of the statistical (or density) operators  $W$  are  $W^\dagger = W$ ,  $W > 0$ ,  $\text{Tr } W = 1$ . Hatsopoulos and Gyftopoulos propose to modify statement (2) as follows:

- (2') (HG ansatz) States (of every strictly isolated system) are in one-to-one correspondence with the state operators  $\rho$  on  $\mathcal{H}$ , where  $\rho^\dagger = \rho$ ,  $\rho > 0$ ,  $\text{Tr } \rho = 1$ , without the restriction  $\rho^2 = \rho$ . We call these the “state operators” to emphasize that they play the same role that in QM is played by the projectors  $P$ , according to statement (2) above, i.e. they are associated with the homogeneous (or pure or proper) preparation schemes.

Mathematically, state operators  $\rho$  have the same defining features as the statistical (or density) operators  $W$ . But their physical meaning according to statement (2') is sharply different. A state operator  $\rho$  represents a state. Whatever uncertainties and probabilities it entails, they are intrinsic in the state, in the same sense as uncertainties are intrinsic in a state described (in QM) by a projector  $P = |\psi\rangle\langle\psi|$ . A



statistical operator  $W$ , instead, represents (ambiguously) a mixture of intrinsic and extrinsic uncertainties obtained via a heterogeneous preparation. In Refs. 19–22, all the successful mathematical results of QSM are re-derived for the state operators  $\rho$ . There, it is shown that statement (2′) is non-contradictory to any of the (mathematical) successes of the present QSM theory, in that region where theory is backed by experiment. However, it demands a serious re-interpretation of such successes because they now emerge no longer as statistical results (partly intrinsic and partly extrinsic probabilities), but as non-statistical consequences (only intrinsic probabilities) of the nature of the individual states.

In addition, statement (2′) implies the existence of a broader variety of states than conceived of in QM (according to statement (2)). Strikingly, if we adopt statement (2′) with all its ramifications, those situations in which the state of the system is not known with certainty stop playing the perplexing central role that in QSM is necessary to justify the successful mathematical results such as canonical and grand canonical equilibrium distributions. The physical entropy that has been central in so many discoveries in physics, would have finally gained its deserved right to enter the edifice from the front door. It would be measured by  $-k_B \text{Tr } \rho \ln \rho$  and, by way of statement (2′), be related to intrinsic probabilities, differently from the von Neumann measure  $-\text{Tr } W \ln W$  which measures the state of uncertainty determined by the extrinsic probabilities of a heterogeneous preparation. We would not be any more embarrassed by the inevitable need to cast our explanations of single-atom, single-photon, single-spin heat engines in terms of entropy, and entropy balances.

The same observations would be true even in the classical limit,<sup>25</sup> where the state operators tend to distributions on phase-space. In that limit, statement (2′) implies a broader variety of individual classical states than those conceived of in classical mechanics (and described by the Dirac delta distributions on phase-space). The classical phase-space distributions, that are presently interpreted as statistical descriptions of situations with extrinsic uncertainty, can be readily reinterpreted as non-statistical descriptions of individual states with intrinsic uncertainty. Thus, if we accept this fourth alternative, we must seriously reinterpret, from a new non-statistical perspective, all the successes not only of quantum theory but also of classical theory.

If we adopt the HG ansatz, the problem of describing statistics of measurement results from heterogeneous preparations loses the fundamental role it holds in QSM by virtue of statement (3). Nevertheless, when necessary, the problem can be unambiguously addressed as follows<sup>18</sup>:

- (3′) Preparations of a given system are in one-to-one correspondence with the normalized measures  $\mu$  that can be defined on the HG “quantal state domain of the system”,  $\mathcal{R}$ , i.e. the set of all possible state operators  $\rho$  on  $\mathcal{H}$  defined according to statement (2′) [the normalization condition is  $\mu(\mathcal{R}) = \int_{\mathcal{R}} \mu(d\rho) = 1$ ]. We call each such measure  $\mu$  a “statistical-weight measure over the quantal

phase-domain of the system”. Statistics of measurement results from a heterogeneous preparation with extrinsic uncertainty (probabilities  $w_i$ ) as to which is the actual state of the system among a discrete set  $\{\rho_i\}$  of possible states is described by the statistical-weight measure  $\mu = \sum_i w_i \mu_{\rho_i}$  where  $\mu_{\rho_i}$  is the Dirac measure “centered” at state  $\rho_i$ .<sup>a</sup>

The discussion of such description, first introduced in Ref. 18, is not essential here and will therefore be presented elsewhere (recently, some useful mathematical results have been developed along these lines, but in another context, in Refs. 40 and 41). For the present purpose it suffices to say that the Dirac measures are the only irreducible measures that can be defined over  $\mathcal{R}$ .<sup>18</sup> In fact, any other measure can be decomposed *in a unique way* into a “sum” of Dirac measures and is therefore reducible. The physical meaning of the uniqueness of the “spectral” resolution of any measure into its component Dirac measures is that the statistical descriptor  $\mu$  associated with any preparation is complete and unambiguous, because its unique “spectral” resolution identifies unambiguously every component homogeneous preparation through the support of the corresponding Dirac measure, as well as the respective statistical weight. As a result, this mathematical description of heterogeneous preparations does not lead to the Schrödinger–Park paradox and hence the concept of state is saved.<sup>b</sup>

#### 4. Concluding Remarks

In conclusion, the Hatsopoulos–Gyftopoulos ansatz, proposed three decades ago in Refs. 19–22 and follow up theory,<sup>23,26,27,30–32,42,43</sup> not only resolves the Schrödinger–Park paradox without rejecting the concept of state (a keystone of scientific thinking), but forces us to re-examine the physical nature of the individual states (quantum and classical), and finally gains for thermodynamics and in particular the second law a truly fundamental role, the prize it deserves not only for having never failed in the past 180 years since its discovery by Carnot, but also

<sup>a</sup>Among the measures that can be defined over  $\mathcal{R}$ , with every state operator  $\rho_o$  in  $\mathcal{R}$  we can associate a Dirac measure defined as follows.<sup>18,39</sup> Let  $E$  denote any subset of  $\mathcal{R}$ , then  $\mu_{\rho_o}(E) = 1$  if  $\rho_o \in E$  and  $\mu_{\rho_o}(E) = 0$  if  $\rho_o \notin E$ . The *support* of a measure is the subset of the domain  $\mathcal{R}$  for which the measure is nonzero. Clearly the Dirac measure  $\mu_{\rho_i}$  has a single-point support coinciding with the state operator  $\rho_i$ .

<sup>b</sup>Notice that within standard QM, where states of strictly isolated systems are one-to-one with the unit-norm vectors  $\psi$  in the Hilbert space  $\mathcal{H}$  of the system, a natural and unambiguous description of the statistics from a heterogeneous preparation can be obtained by using (instead of the von Neumann statistical operator  $W$ ) the normalized statistical-weight measures  $\mu$  defined on the set of all possible unit-norm (pure state) vectors  $\psi$  in  $\mathcal{H}$ . The uniqueness of the decomposition  $\mu = \sum_i w_i \mu_{\psi_i}$  into the component Dirac measures (in the discrete case) or its continuous version (Refs. 40 and 41) would not give rise to the Schrödinger–Park paradox. However, as we will show elsewhere, the maximal-statistical-uncertainty measures that would correspond to thermodynamic equilibrium according to standard QSM/QIT reasoning, would differ in general from the canonical and grand canonical distributions!

for having been and still being a perpetual source of reliable advice as to how things work in Nature.

In this paper, we restate a seldom recognized conceptual inconsistency which is unavoidable within the present formulation of QSM/QIT and discuss briefly logical alternatives towards its resolution. Together with Schrödinger<sup>1</sup> who first surfaced the paradox and Park<sup>3,4</sup> who first magisterially explained the incontrovertible tension it introduces around the fundamental concept of state of a system, we maintain that this fundamental difficulty is by itself a sufficient reason to go beyond QSM/QIT, for we must resolve the “essential tension” which has sapped the conceptual foundations of the present formulation of quantum theory for almost 80 years.

We argue that rather than adopting the drastic way out provokingly prospected by Park, namely, that we should reject as unsound the very concept of state of a system (as we basically do every day by simply ignoring the paradox), we may alternatively remove the paradox by rejecting the present statistical interpretation of QSM/QIT without nevertheless rejecting the successes of its mathematical formalism. The latter resolution is satisfactory both conceptually and mathematically, but requires that the physical meaning of the formalism be reinterpreted with care and detail. Facing the situation sounds perhaps uncomfortable because there seems to be no harmless way out, but if we adopt the Hatsopoulos–Gyftopoulos fundamental ansatz (of existence of a broader kinematics) the change will be at first mainly conceptual, so that practitioners who happily get results everyday out of QSM would basically maintain the *status quo*, because we would maintain the same mathematics both for the time-independent state operators that give us the canonical and grand-canonical description of thermodynamics equilibrium states, and for the time-dependent evolution of the idempotent density operators ( $\rho^2 = \rho$ ), i.e. the states of ordinary QM, which keep evolving unitarily. On the other hand, if the ansatz is right, new physics is likely to emerge, for it would imply that beyond the states of ordinary QM, there are states (“true” states, obtained from preparations that are “homogeneous” in the sense of von Neumann<sup>2</sup>) that even for an isolated and uncorrelated single degree of freedom “have physical entropy” ( $-k_B \text{Tr } \rho \ln \rho$ ) and require a non-idempotent state operator ( $\rho^2 \neq \rho$ ) for their description, and therefore exhibit the limitations imposed by the second law even at the microscopic level.

In addition, if we adopt as a further ansatz that the time evolution of these non-ordinary-QM states (the non-idempotent ones) obeys the nonlinear equation of motion developed by the present author,<sup>23,26,27,31,32,42,43</sup> then in most cases they do not evolve unitarily but follow a path that results from the competition of the Hamiltonian unitary propagator and a new internal-redistribution propagator that “pulls” the state operator  $\rho$  in the direction of steepest entropy ascent (maximal entropy generation) until it reaches a (partially) canonical form (or grand canonical, depending on the system). Full details can be found in Refs. 27 and 30.

The proposed resolution definitely goes beyond QM, and turns out to be in line with Schrödinger’s prescient conclusion of his 1936 article<sup>1</sup> where he writes: “My

point is that in a domain which the present theory does not cover, there is room for new assumptions without necessarily contradicting the theory in that region where it is backed by experiment.”

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## References

1. E. Schrödinger, *Proc. Cambridge Phil. Soc.* **32**, 446 (1936).
2. J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, Engl. transl. of the 1931 German edition by R. T. Beyer (Princeton Univ. Press, 1955), pp. 295–346.
3. J. L. Park, *Am. J. Phys.* **36**, 211 (1968).
4. J. L. Park, *Found. Phys.* **18**, 225 (1988).
5. E. T. Jaynes, *Phys. Rev.* **106**, 620 (1957).
6. E. T. Jaynes, *Phys. Rev.* **108**, 171 (1957).
7. N. Gisin, *Hel. Phys. Acta* **62**, 363 (1989).
8. L. P. Hughstone, R. Jozsa and W. K. Wootters, *Phys. Lett. A* **183**, 14 (1993).
9. K. A. Kirkpatrick, *Found. Phys. Lett.* **19**, 95 (2006).
10. N. D. Mermin, *Found. Phys.* **29**, 571 (1999).
11. O. Cohen, *Phys. Rev. A* **60**, 80 (1999).
12. O. Cohen, *Phys. Rev. A* **63**, 16102 (2001).
13. D. R. Terno, *Phys. Rev. A* **63**, 16101 (2001).
14. A. Amann and H. Atmanspacher, *Stud. Hist. Phil. Mod. Phys.* **29**, 151 (1998).
15. H. M. Wiseman and J. A. Vaccaro, *Phys. Rev. Lett.* **87**, 240402 (2001).
16. W. M. Elsasser, *Phys. Rev.* **52**, 987 (1937).
17. A. E. Allahverdyan and T. M. Nieuwenhuizen, *Phys. Rev. E* **71**, 066102 (2005).
18. G. P. Beretta, Sc.D. thesis, M.I.T., 1981, unpublished, quant-ph/0509116.
19. G. N. Hatsopoulos and E. P. Gyftopoulos, *Found. Phys.* **6**, 15 (1976).
20. G. N. Hatsopoulos and E. P. Gyftopoulos, *Found. Phys.* **6**, 127 (1976).
21. G. N. Hatsopoulos and E. P. Gyftopoulos, *Found. Phys.* **6**, 439 (1976).
22. G. N. Hatsopoulos and E. P. Gyftopoulos, *Found. Phys.* **6**, 561 (1976).
23. G. P. Beretta, in *Frontiers of Nonequilibrium Statistical Physics*, Proc. of the NATO Advanced Study Institute, Santa Fe, 1984, eds. G. T. Moore and M. O. Scully (Plenum Press, 1986), p. 205.
24. G. P. Beretta, in *The Physics of Phase Space*, Lecture Notes in Physics, Vol. 278, eds. Y. S. Kim and W. W. Zachary (Springer-Verlag, 1986), p. 441.
25. G. P. Beretta, *J. Math. Phys.* **25**, 1507 (1984).
26. G. P. Beretta, E. P. Gyftopoulos, J. L. Park and G. N. Hatsopoulos, *Nuovo Cimento B* **82**, 169 (1984).
27. G. P. Beretta, E. P. Gyftopoulos and J. L. Park, *Nuovo Cimento B* **87**, 77 (1985).
28. S. Gheorghiu-Svirschevski, *Phys. Rev. A* **63**, 022105 (2001).
29. S. Gheorghiu-Svirschevski, *Phys. Rev. A* **63**, 054102 (2001).
30. G. P. Beretta, quant-ph/0112046.
31. G. P. Beretta, *Mod. Phys. Lett. A* **20**, 977 (2005).
32. G. P. Beretta, *Phys. Rev. E* **73**, 026113 (2006).
33. B. d’Espagnat, *Conceptual Foundations of Quantum Mechanics*, 2nd edn. (Addison-Wesley, 1989).
34. E. Çubukçu, Sc.D. thesis, M.I.T., 1993, unpublished.

35. G. La Penna, *J. Chem. Phys.* **119**, 8162 (2003), and references therein.
36. G. La Penna, S. Morante, A. Perico and G. C. Rossi, *J. Chem. Phys.* **121**, 10725 (2004), and references therein.
37. J. C. Keck, *Progr. Energy Combust. Sci.* **16**, 125 (1990), and references therein.
38. D. Hamiroune, P. Bishnu, M. Metghalchi and J. C. Keck, *Combust. Theory Modell.* **2**, 81 (1998), and references therein.
39. G. Fano, *Mathematical Methods of Quantum Mechanics*, Engl. transl. of the 1967 edition (McGraw-Hill, 1971), p. 207.
40. R. R. Zapatrin, [quant-ph/0503173](#); [quant-ph/0504034](#); [quant-ph/0603019](#).
41. G. Parfionov and R. R. Zapatrin, [quant-ph/0603019](#); [quant-ph/0600614](#).
42. J. Maddox, *Nature* **316**, 11 (1985).
43. G. P. Beretta, *Found. Phys.* **17**, 365 (1987).
44. Available online at [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org).