The Schrödinger-Park paradox about the concept of "state" in quantum statistical mechanics and quantum information theory is still open. One more reason to go beyond?

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A seldom recognized fundamental difficulty undermines the concept of individual "state" in the present formulations of quantum statistical mechanics and quantum information theory. The difficulty is an unavoidable consequence of an almost forgotten corollary proved by Schrödinger in 1936 and perused by Park in 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 alternatives towards its resolution.

1. Introduction

In 1936, Schrödinger [1] 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 proved by von Neumann [2] five years earlier.

Thirty years later, Park [3] exploited von Neumann's theorem and Schroedinger's corollary to point out quite conclusively an essential tension undermining the logical conceptual framework of QSM (and of Quantum Information Theory, QIT, as well).

Schrödinger's corollary was "rediscovered" by Jaynes [4] and Gisin [5], and generalized by Hughston, Jozsa, and Wooters [6] and Kirkpatrick [7]. Also some interpretation has been re-elaborated around it [8, 9], but unfortunately not always the original references have been duly cited. For this reason it is useful once in a while to refresh our memory about the pioneering 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".

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 QSM implies the paradoxical conclusion that every system is "a quantum monster": a single system concurrently "in" two (and actually even more) different states. We briefly review the issue below (as we have done also in Ref. 11), but we urge everyone interested in the foundations of quantum theory to read the original reference [3]. The problem has been widely overlooked and is certainly not well known, in spite of its 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 conceptual 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 three logical alternatives. We point out that one of these alternatives achieves a fundamental resolution of the difficulty without contradicting any of the successes of the present mathematical formalism. However, it requires an essentially new and different re-interpretation of the physical meaning of the successes of the mathematics of QM and QSM. If such re-interpretation will motivate new fundamental experimental tests and prove successful, once again Thermodynamics will have played a key role in a major step beyond. [12–23]

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, therefore, the following discussion should be dismissed as useless 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. It is therefore an essential necessary requirement that, when restricted to such systems, the formulation of a physical theory like QSM be free of internal 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 differently 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.

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 [2] (but also to Jaynes [4] 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 the coins of type A, and that $p_B = 2/3$ and $1 - p_B = 1/3$ those of the 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". It is clear that, for such a preparation scheme, the probabilities w and $1 - w$ with which we receive 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 every 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?) then we expect to be able to discover the trick. Thus, it is only under the one-toss constraint that we would not loose, 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_i on the Hilbert space of the system. QSM/QIT assigns to each state P_i a statistical weight w_i, and characterizes the extrinsically uncertain situation by a (von Neumann) statistical (or density) operator $W = \sum_i w_i P_i$, a weighted sum of the projectors representing the possible states.

This construction is ambiguous, because the same statistical operator is assigned to represent a variety of different preparations, with the only exception of homogeneous preparations where there is only one possible state P_ψ with statistical weight equal to 1, so that $W = P_\psi$ is "pure". Given a statistical operator W (a nonnegative, unit-trace, hermitean 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, to which the QSM/QIT von Neumann construction would assign the statistical operator $W = \sum_i w_i P_i$. 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 [2]). 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 [1] relevant to this issue (for a mathematical generalization see Ref. 7 and for interpretation in the framework of non-local effects see e.g. Ref. 8).

For our purposes, notice that every statistical (density) operator W, when restricted to its range $\mathrm{Ran}(W)$, has an inverse that we denote by W^{-1}. If $W \neq W^2$, then $\mathrm{Ran}(W)$ is at least two-dimensional, i.e., the rank of W is greater than 1. It follows that the restriction of the identity operator I to $\mathrm{Ran}(W)$ can be resolved into a sum of one-dimensional projectors in an infinite number of different ways. Let $\{P_j\}$ and $\{P'_k\}$ denote two different sets (no elements in common) of one-dimensional projectors such that, on $\mathrm{Ran}(W)$, $I = \sum_j P_j = \sum_k P'_k$ (j and k run from 1 to the rank of W). Then, $W = \sum_j w_j P_j = \sum_k w'_k P'_k$ where $w_j = [\mathrm{Tr}_{\mathrm{Ran}(W)}(W^{-1}P_j)]^{-1}$ and $w'_k = [\mathrm{Tr}_{\mathrm{Ran}(W)}(W^{-1}P'_k)]^{-1}$.

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 for sure 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 for sure in one of the states in the set $\{P'_k\}$. Because both decompositions hold true simultaneously, the very rules we adopted to construct statistical operators W allow us to conclude that that the state of the system is certainly one in the set $\{P_j\}$, but concurrently it is also certainly one in the set $\{P'_k\}$. Because 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, than 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 extrinsic probabilities (w,$1-w$) combine irreducibly with 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 lead 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 the box of, say, 3/4 – 1/4 biased coins).

3. Is there a way out?

In this section we discuss three main alternatives towards the resolution of the paradox, that is, 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) situations with extrinsic uncertainty as to which is the actual state of the system are unambiguously described by the statistical operators W. The decomposition $W = \sum_i w_i P_i$ implies that the state is P_i with statistical weight w_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 [3] 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 ψ . . . " 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. 11, we have suggested a measure-theoretic representation that would achieve the desired goal of keeping the necessary separation between intrinsic quantal 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 intriguing alternative has been first proposed by Hatsopoulos and Gyftopoulos [12] in 1976. The idea is to retain statement (1) and modify statement (2) by adopting the mathematics of statement (3) to describe the states. The defining features of the projectors P, which represent the states for a strictly isolated system in QM, are: $P^\dagger = P$, $P > 0$, $\mathrm{Tr}P = 1$, $P^2 = P$. The defining features of the statistical (or density) operators W are $W^\dagger = W$, $W > 0$, $\mathrm{Tr}W = 1$. Hatsopoulos and Gyftopoulos propose to modify statement (2) as follows:

(2') States (of every strictly isolated system) are in one-to-one correspondence with the state operators ρ on $\mathcal{H}$, where $\rho^\dagger = \rho$, $\rho > 0$, $\mathrm{Tr}\rho = 1$, 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 ρ 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 ρ 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 Ref. 12, all the successful mathematical results of QSM are re-derived for the state operators ρ. 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 $-k_{\mathrm{B}}\mathrm{Tr}\rho\ln\rho$ and by way of statement (2') and be related to intrinsic probabilities, differently from the von Neumann measure $-\mathrm{Tr}W \ln W$ which measures the state of uncertainty determined by the extrinsic probabilities of a heterogeneous preparation. We would not be anymore 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 [14], 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 third alternative, we must seriously reinterpret, from a new non-statistical perspective, all the successes not only of quantum theory but also of classical theory.

4. Concluding remarks

In conclusion, the Hatsopoulos-Gyftopoulos ansatz, proposed thirty years ago in Ref. 12 and follow up theory [13,15,16,18,21–23], 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 for having been and still being a perpetual source of reliable advise 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 [1] who first surfaced the paradox and Park [3] who first magistrally 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 resolves the "essential tension" which has sapped the conceptual foundations of the present formulation of quantum theory for almost eighty 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 the states of ordinary QM, there are states ("true" states, obtained from preparations that are "homogeneous" in the sense of von Neumann [2]) that even for an isolated and uncorrelated single degree of freedom "have physical entropy" ($-k_{\rm B}{\rm Tr}\rho\ln\rho$) and require a non-idempotent state operator ($\rho^2 \neq \rho$) for their description, and therefore exhibit even at the microscopic level the limitations imposed by the second law,

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 [12, 13, 15, 16, 18, 22, 23], 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 ρ 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. 21, 24.

The proposed resolution definitely goes beyond QM, and turns out to be in line with Schrödinger's prescient conclusion of his 1936 article [1] when 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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