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Mutually Exclusive and Exhaustive Quantum States

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The identification of a set of mutually exclusive and exhaustive propositions concerning the states of quantum systems is a cornerstone of the information-theoretic foundations of quantum statistics; but the set which is conventionally adopted is in fact incomplete, and is customarily deduced from numerous misconceptions of basic quantum mechanical principles. This paper exposes and corrects these common misstatements. It then identifies a new set of quantum state propositions which is truly exhaustive and mutually exclusive, and which is compatible with the foundations of quantum theory.

1. LOGICAL SPECTRA AND STATISTICAL PHYSICS

In recent years the abstract principles of information theory have been superposed upon the fundamental laws of mechanics in order to erect the old discipline of statistical mechanics on a basis more plausible, rational, and systematic than has historically been the case. These efforts must be regarded as very successful, if for no other reason than that they have clarified better than ever before just what really are the essential foundations of statistical mechanics. Nevertheless, the present state of those foundations remains shaky in the realm of quantum statistics because quantum mechanics itself is beset by numerous controversial misunderstandings. As we shall see in detail below, many of these common misinterpretations of quantum physics have been absorbed uncritically into the fabric of information-theoretic statistical mechanics, with the result that quantum statistics is not yet truly as well grounded as a cursory survey might suggest.

To apply information theory to any situation, the first step consists

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in identifying a list of relevant propositions concerning that situation. The list must be *mutually exclusive* (no two propositions can simultaneously be true) and *exhaustive* (one of the propositions is certainly true). Such a set of mutually exclusive and exhaustive propositions has sometimes been called a *logical spectrum*, and we shall, for brevity, adopt that terminology.[1]

Suppose now that we confront in a physical laboratory a complex system that has been prepared for study in some specified manner. (A classic example would be one mole of helium occupying a one-liter enclosure in thermal equilibrium at a specified temperature.) There are two kinds of logical spectra that might conceivably arise in the quantal analysis of the system. One is related to the quantum states or *preparations* of the system; the other concerns the possible data that would emerge from subsequent *measurements* of observables of interest.

The logical spectrum associated with measurement of an observable A is obviously just the list of propositions of this form: "Measurement of A yields the datum a." In fact this logical spectrum of propositions concerning the results of A-measurements is indexed by the eigenvalue spectrum $\{a_n\}$ of the observable A. It is customary to regard the projection operator onto the subspace belonging to a_n as the mathematical representative in quantum theory of that proposition of the above form which is indexed by a_n. None of this is problematical.

The logical spectrum associated with the possible quantum states, on the other hand, is not so immediately identifiable. It is, however, the one which is of greatest interest in statistical physics, where the central problem is to make the best possible state assignment compatible with whatever meager physical information can be extracted from a description of the means employed in the laboratory to prepare the system of interest. We shall find that the problem of selecting such a logical spectrum of quantal state preparations leads almost at once into that thicket of quantal misunderstandings mentioned earlier.

There is of course an orthodox choice for the logical spectrum of quantum states. It has been entrenched for decades in all treatises on quantum statistics, and has been, as we shall see, willingly adopted also by the protagonists of the information-theoretic school. To construct that logical spectrum, let $\{\psi_n\}$ denote a *specific* complete orthonormal set of state vectors. The *standard logical spectrum* for states in quantum statistics consists of all propositions of this form: "The system is in the state ψ_n." Thus it is asserted that such a set of pure states is a mutually exclusive and exhaustive list of possibilities.

We maintain that this traditional choice of a logical spectrum for quantum statistics is a fundamental error, reflecting the imbuement of a host of common misconstruals of the foundations of quantum mechanics itself. The fact that this orthodox spectrum leads nevertheless to empirically correct results in equilibrium statistical mechanics is no defense from the standpoint of foundations research. Indeed we shall demonstrate in future publications that the same established formulas of statistics can also be derived from the more rational choice of a logical spectrum of quantum states to be developed here.

2. SEVEN QUANTAL MISUNDERSTANDINGS

Before embarking on a detailed investigation of the better arguments in behalf of the standard logical spectrum, we digress to record for future reference seven popular statements of quantum dogma the influence of which has, as we shall see below, retarded progress in the foundations of statistical mechanics. All of the statements have been discredited or disproved in previous papers [(2–13)] by us and by other writers. Yet they are all still taken literally by many uncritical theorists, and comprise, along with a few other quantum shibboleths, the conventional parlance of quantum physics.

In this section we present the statements with a minimum of commentary, saving until later certain intricate criticisms particularly germane to the problem of choosing a logical spectrum.

(A) Every quantum system at any time "is in" or "has" a pure quantum state $|\Psi\rangle$.

(B) Immediately after a measurement of some nondegenerate observable A, the measured system is in the state $|\alpha_n\rangle$, where $A|\alpha_n\rangle = a_n|\alpha_n\rangle$, a_n being the datum that emerged in the act of measurement.

Statement (B) is of course the infamous projection postulate, often invoked in theoretical discussions of filtration *Gedanken*experiments in order to establish the individual pure state assignments mandated in (A). We shall not dwell upon (B) in this paper. Let it be noted, however, that (B) has been assiduously scrutinized on both physical and philosophical grounds, with the conclusion that it is, at best, a statement that is rarely correct in any sense whatever. Logically it is therefore false; moreover, when (A) is repudiated and replaced (cf. Section 4) by a correct statement concerning quantal state preparation, (B) then becomes, if taken literally, an irrational attribution of an ensemble property to an individual element of the ensemble.

(C) If a measurement of A is performed upon a system in the state $|\Psi\rangle$, the probability that the system will be found in state $|\alpha_n\rangle$ immediately after the measurement is $|\langle\alpha_n|\Psi\rangle|^2$.

It is apparent at once that (C) is compatible with (A) and (B) and that it will be left dangling inconsistently among the quantum axioms when (A) and (B) are renounced. Fortunately, the essential physical content of (C) can be preserved by a modification we shall discuss later.

(D) Consider these two state propositions about a given system $\mathscr{S}$:

(1) $\mathscr{S}$ is in the state ψ_1.

(2) $\mathscr{S}$ is in the state ψ_2.

These propositions are mutually exclusive if and only if $\langle\psi_1, \psi_2\rangle = 0$.

We shall discover below that this statement is commonly used in arguments leading to the standard logical spectrum in quantum statistics. Supposedly it follows, or at least acquires a measure of reasonableness, from the (erroneous) statement (C).

(E) The spectral expansion of a density operator,

$$\rho = \sum_n w_n \mid \psi_n\rangle\langle\psi_n \mid$$

has this physical interpretation: The true state $\mid \Psi\rangle$ is unknown, but is believed to be one among the mutually exclusive possibilities in the orthogonal eigenvector set $\{\mid \psi_n\rangle\}$. The eigenvalues $\{w_n\}$ are (subjective) probabilities reflecting degrees of rational belief in the respective alternatives $\{\mid \psi_n\rangle\}$.

There is a limited sense in which this statement, carefully interpreted, could be true; but as a general principle, (E) is unacceptable because it incorporates (erroneous) statements (A) and (D). Moreover, it denies to the density matrix its fundamental status in quantum theory by regarding its eigenvalues only as probabilities of the subjective type used in information theory and statistical physics. Thus the density matrix becomes a construct which displays a blend of the "subjective" probabilities $\{w_n\}$ and of the "objective" probabilities which inhere in the pure quantum states $\{\psi_n\}$. This makes the density matrix appear to be a fixture of quantum statistical mechanics but not of quantum mechanics itself, a view to which we shall take exception below.

(F) If A is measured upon a system in state $\mid \Psi\rangle$ but the result is not yet known, then this postmeasurement state of ignorance may be expressed by the density operator

$$\rho = \sum_n |\langle\alpha_n \mid \Psi\rangle|^2 \mid \alpha_n\rangle\langle\alpha_n \mid$$

This is just a theorem which follows immediately from the (erroneous) statements (B), (C), and (E).

(G) The quantal counterparts to various key mathematical constructs of classical statistical mechanics are given by these associations:

Construct	Classical representative	Quantal counterpart
I. System	Phase space	Hilbert space
II. State of system	Phase point (q, p)	Ray $\mid \Psi\rangle$
III. Observable	Function of phase	Hermitian operator with complete orthonormal eigenvector set
IV. Ignorance of true state	Gibbsian coefficient of probability of phase $\rho(q, p)$	Density operator $\rho = \sum_n w_n \mid \alpha_n\rangle\langle\alpha_n \mid$

These correspondences have long been used to motivate the traditional formulation of quantum statistical mechanics as a theory analogous to the original Gibbsian statistics. Such an analogical approach based on Gibbs[14] is an excellent idea, but only if the analogies are the correct ones. That this is not the case in the conventional tabulation given above may be seen by observing that analogy II reiterates statement (A) and analogy IV embodies the contents of statements (D) and (E). In Section 4 we present a corrected set of analogs.

This completes our somewhat iconoclastic summary of the common misstatements of quantal principles which have become embedded in the foundations of quantum statistics. We turn next to the literature of information-theoretic statistical mechanics in order to show just how these misunderstandings have contributed to the traditional choice of a logical spectrum in quantum statistics.

3. DERIVATIONS OF THE STANDARD LOGICAL SPECTRUM

The standard logical spectrum of propositions which assert that the system is in a state $\mid \psi_n\rangle$, the $\{\mid \psi_n\rangle\}$ constituting a complete orthonormal set, is derived in the literature from considerations based upon various combinations of the statements (A)–(G). To expose clearly the extent to which these statements have been implanted in the foundations of statistics, we review in this section the lines of reasoning of four contemporary writers who have attempted to develop those foundations with admirable rigor. All of these authors base statistical mechanics on information theory, and with that general point of view we have no quarrel. Indeed we believe with them that the information-theoretic approach is the best foundation for statistical physics, both rationally and didactically, in that it captures the essence of that discipline without resorting to inconclusive, even irrelevant arguments about ergodicity and time averages.

Jaynes,[15–17] the founder of information-theoretic statistical physics, selected the standard logical spectrum only after a very thorough analysis of the density matrix. In his original paper on quantum statistics, that analysis began with the explicit assertion that,[16] "it is possible to maintain the view that the system is at all times in some definite but unknown pure state...." This is of course just the statement we called (A). Jaynes then considered expansions of the density operator which are not necessarily spectral and which he termed "arrays." (Years before, Schrödinger[19] had also studied such expansions in an investigation of tremendous, if not widely recognized, significance for the foundations of quantum mechanics.)

An array can be represented by a density operator in the form

$$\rho = \sum_i w_i \mid \psi_i \rangle\langle \psi_i \mid \tag{1}$$

where $\{\mid \psi_i\rangle\}$ is not necessarily an orthogonal set but all $w_i \geqslant 0$ and $\sum_i w_i = 1$. Jaynes interpreted such an expansion as an elegant means for describing a set of alternative pure states $\{\mid \psi_i\rangle\}$, one of which was tacitly regarded as the true unknown state, the corresponding $\{w_i\}$ being the information-theoretic probabilities for the various alternatives. This is essentially statement (E) generalized to nonspectral expansions.

Finally, Jaynes discarded all but the spectral expansions, in effect adopting statement (E) as given above. The reasons given for doing this revolved around his search for a suitable expression for information-theoretic entropy I in quantum mechanics. In general, once a logical spectrum is chosen, I is defined in terms of the associated set of probabilities w_i by the formula

$$I \equiv -\sum_i w_i \ln w_i \tag{2}$$

But, according to Jaynes,[18] this procedure "would not be satisfactory because the w_i are not in general the probabilities of mutually exclusive events. According to quantum mechanics, if the state is known to be ψ_i, then the probability of finding it upon measurement to be ψ_j, is $|\langle \psi_j \mid \psi_i \rangle|^2$. Thus, the probabilities w_i refer to independent, mutually exclusive events only when the states ψ_i of the array are orthogonal to each other, and only in this case is the expression (2) for entropy satisfactory."

Thus Jaynes arrived at the standard logical spectrum of orthogonal pure states by an argument based on statement (D) as derived from statement (C). It should perhaps also be mentioned for completeness that Jaynes appended to this chain of reasoning the interesting aesthetic observation that (2) attains its minimum value when (1) is a spectral expansion, so that an orthogonal set $\{\psi_i\}$ "provides, in the sense of information content, the most economical description of the freedom of choice implied by a density matrix."[18]

Katz, in his fine monograph on statistical mechanics, strongly exploits the set of analogies described in statement (G). The choice of the standard logical spectrum of orthogonal states is quickly disposed of in one terse paragraph,[20] which invokes in sequence the quantal misstatements we have labeled (A), (C), and (D). Immediately thereafter the density operator is introduced, with an interpretation of the kind described in statement (E).

Another noteworthy book devoted to the information-theoretic foundations of statistical mechanics is by Hobson, who also makes much of the analogies in statement (G). His thorough analysis[21] of quantum mechanics, which culminates in the standard logical spectrum, is based upon every one of the conventional but erroneous tenets (A)–(F), including in particular the projection postulate (B). Hobson recognizes two quantal situations to which information theory might be applied. In case 1, $|\Psi\rangle$ is unknown, the observable A is measured, and the measurement yields some data D. There is a semantic difficulty here, for if in fact A were *measured*, the result would be some datum a_n. However, presumably there has been an A-measurement complete with the projection process (B), but for some reason a_n is not known though some evidence D has become available to aid in guessing at the measurement result. Statement (B) thus serves to provide the standard logical spectrum of orthogonal states, in this instance the orthogonal eigenvectors of the measured (?) observable A. In case 2, $|\Psi\rangle$ is known, A is measured, and the measurement yields nothing. Here the density operator chosen to represent such a state of ignorance is the one given in statement (F), the post-measurement, precognizance density operator of traditional measurement theory. Again the logical spectrum turns out to be the standard one, again provided by the projection postulate (B).

We conclude this review of arguments leading to the standard logical spectrum with a look at the excellent textbook by Baierlein. To our knowledge this is the only book on information-theoretic quantum statistics that has been written for students new to statistical physics. Thus the argument[22] by which Baierlein introduces the standard logical spectrum is necessarily simplified. He simply announces that thermal equilibrium is of special interest and posits that the eigenstates of energy, being stationary, constitute the natural list of mutually exclusive and exhaustive alternatives. However, since degeneracy in the Hamiltonian would lead to an infinity of nonorthogonal eigenstates, Baierlein is forced to augment this line of reasoning by the statement (D) in order to obtain the standard logical spectrum. As always, the statement (A) is lurking in the background.

4. THE SEVEN MISSTATEMENTS CORRECTED

Having established that the seven misstated "principles" of quantum mechanics are taken quite literally in even the best modern discussions of quantum statistics, we next consider the quantally correct versions of these statements. It will then become possible to make a very natural and rational decision as to what set of quantum state propositions should be the logical spectrum in quantum statistical mechanics. In the following analysis, the correction or nearest related replacement for each of the original misstatements will be denoted by the corresponding primed letter.

We have reported elsewhere[6] the details of one investigation of the theoretical consistency of statement (A). The conclusion that (A) cannot be upheld has also been reached independently by others[8–11] for various reasons. A significant clue to the irrationality inherent in (A) is the fact that *physically* $|\Psi\rangle$ is a catalogue which lists an arithmetic mean value for each of the quantal observables associated with the system of interest. That makes the true *empirical* referent of $|\Psi\rangle$ not an individual system but a statistical ensemble of identically prepared systems. This essential quantal ensemble is not an imaginary Gibbsian ensemble of replicas, but an actual collection of repetitions of an experiment that can be reproducibly prepared. Thus in the final analysis $|\Psi\rangle$ is not associated directly with a single system; instead it describes a reproducible mode of *preparation* for systems. But this point, which some may take to be merely semantic, is only the beginning of the trouble with (A); for there exist reproducible preparation schemes which can generate ensembles whose quantal mean values cannot be summarized by any single $|\Psi\rangle$ whatever. For example, consider the use of an oven with a small aperture as a molecular beam source. The collection of molecules emerging from the orifice constitutes a quantal ensemble which must be described as a Maxwell–Boltzmann mixture nonequivalent to any one state vector. Similarly, the ensemble of electrons generated by a hot filament cannot be characterized by any single $|\Psi\rangle$. Hence there are both theoretical and empirical reasons for replacing (A) with a statement (A′) that admits preparations characterized by a $|\Psi\rangle$ only as an interesting, probably seldom realized, special case:

(A′) With every repeatable empirical method of *preparation* of a system, there is associated a density operator ρ, the quantum state.

With regard to the projection postulate (B), there is really no correct *universal* statement that can replace it; and none is needed for complete and consistent treatments of either basic quantum mechanics or quantum statistics. However, the following statement could be regarded as an innocuous, but at least correct, substitute for (B):

(B′) It is conceivable that measurement of a nondegenerate observable A might be performable in such a way as to leave the postmeasurement ensemble of measured systems prepared in the manner characterized by the density operator

$$\rho = \sum_n \langle \alpha_n \mid \rho_0 \mid \alpha_n \rangle \mid \alpha_n \rangle\langle \alpha_n \mid \tag{3}$$

where ρ_0 is the density operator of the premeasurement preparation.

Statement (C) occurs, with the phraseology exactly as given in Section 2, in so many places that the reader may find our declaration that (C) is wrong to be radically eccentric. After all, is not statement (C) the most widely used of all quantum principles, the indispensable link between formalism and data that makes the theory physically meaningful? Is it not the basis, for example, of all calculations concerning scattering cross sections and spectral intensities?

To these rhetorical objections, we would reply first that the phrase "will be found in the state $\mid \alpha_n \rangle$ immediately after measurement" has become theoretically inconsistent with the replacement of (A) by (A′), since state vectors are not attributable to individual systems. Furthermore, the phrase is easily seen on reflection to be physically meaningless anyhow because experimenters do not apprehend Hilbert vectors; they gather *numerical data*. Thus statement (C), taken literally as it was in arguments leading to the standard logical spectrum, cannot possibly be the link between theory and experiment, or the basis for cross-section computations. The statement that actually plays this role in quantum physics is the following:

(C′) If a measurement of A is performed upon a system prepared in the manner characterized by quantum state ρ, the probability that the measurement will yield numerical datum a_n is $\langle \alpha_n \mid \rho \mid \alpha_n \rangle$.

The famous formula given in (C) is of course also a corollary of (C′): if $\rho = \mid \Psi \rangle\langle \Psi \mid$, $\langle \alpha_n \mid \rho \mid \alpha_n \rangle = |\langle \alpha_n \mid \Psi \rangle|^2$. [Like (C), (C′) is easily generalized to include degenerate eigenvalues.] Statement (C′) is related in an obvious way to the general trace formula for quantal mean values: $\bar{A} = \mathrm{Tr}(\rho A)$.

The reason that the difference between (C) and (C′) is rarely emphasized seems to be that in ordinary applications of quantum mechanics either statement induces the practical physicist to perform the same calculations anyway.

Nevertheless our insistence upon the distinction between (C) and (C′) is not meticulous pedantry; for that distinction will be seen to have a profound impact upon the foundations of quantum statistics.

Statement (D), grounded as it is in the discredited literal interpretation of (C), is now insupportable. A corrected version would read as follows:

(D′) Consider these two state propositions about a given system $\mathscr{S}$:

(1) $\mathscr{S}$ is prepared in the manner characterized by ρ_1.

(2) $\mathscr{S}$ is prepared in the manner characterized by ρ_2.

These propositions are mutually exclusive if and only if $\rho_1 \neq \rho_2$.

This revision of (D) is a drastic one which requires further analysis. We shall return to this point in Section 5 when we formulate a new logical spectrum for quantum statistics.

Statement (E) embraces what might be called the *ignorance interpretation* of the density operator. According to this view, the density operator lacks the fundamental status in quantum theory that is granted in statement (A′) but is instead merely an artifice useful in coping with situations where the true $|\Psi\rangle$ is unknown. A full critique of this ignorance interpretation of ρ would involve in effect all of the same arguments given in investigations referred to above in connection with the overthrow of (A) by (A′). Here we shall consider only one illustration, drawn from statistical physics, of the difficulties encountered when (E) is taken to be a general principle.

Suppose we know, concerning a certain laboratory preparation scheme for a system of interest, that a measurement of energy H following such a preparation invariably yields the eigenvalue h. Let h be ω-fold degenerate; its associated eigenspace will then be ω-dimensional and spanned therefore by any set of ω orthogonal eigenvectors belonging to the eigenspace. Let $\{\psi_n\}$ be such a set. It is an established principle in statistical mechanics that the density operator

$$\hat{\rho} = \frac{1}{\omega} \sum_{n=1}^{\omega} |\psi_n\rangle\langle\psi_n| \tag{4}$$

is the "best" quantum state assignment to make under these circumstances. This we do not challenge. Consider, however, the usual reasoning given to justify (4). The argument is based on (A), (D), and (E): The system has some state $|\Psi\rangle$; since the same energy is always measured, that state must be in the corresponding eigenspace; only ω elements of that eigenspace can be mutually exclusive; in the absence of additional knowledge, information theory assigns equal probability to each mutually exclusive alternative; and this state of ignorance is represented by (4).

Even if we neglect momentarily to replace (A) by (A′), the abandonment only of (D) demolishes this traditional derivation of (4). To see this, let $\{\chi_n\}$ denote another orthogonal set spanning the eigenspace of h; we then have two expansions of $\hat{\rho}$:

$$\hat{\rho} = \frac{1}{\omega} \sum_{n=1}^{\omega} | \psi_n \rangle \langle \psi_n | = \frac{1}{\omega} \sum_{n=1}^{\omega} | \chi_n \rangle \langle \chi_n | \tag{5}$$

If we now apply the ignorance interpretation (E), we must already wonder if it is entirely consistent to say that each ψ_n has subjective probability $1/\omega$ of being the true state while at the same time it can be said, with the same justification, that each χ_n has also subjective probability $1/\omega$ of being the true state. As long as (D) is believed, it is more or less plausible to argue that these two contradictory ignorance interpretations of $\hat{\rho}$ cannot properly be considered simultaneously. However, we have seen above that (D), having been based upon a literal reading of (C) rather than on the actual quantum mechanical principle (C′), is itself indefensible. Therefore the Pandora's box of nonspectral expansions of $\hat{\rho}$ may now be opened, with the consequence that (E) quickly becomes unpalatable.

For example, let W_1, W_2 be unequal fractions whose sum is unity. We may then write

$$\hat{\rho} = \frac{W_1}{\omega} \sum_{n=1}^{\omega} | \psi_n \rangle \langle \psi_n | + \frac{W_2}{\omega} \sum_{n=1}^{\omega} | \chi_n \rangle \langle \chi_n | \tag{6}$$

The ignorance interpretation must now be that ψ_n has subjective probability W_1/ω and χ_n has a different subjective probability W_2/ω; but this is the *same* $\hat{\rho}$ that was supposed to represent $1/\omega$ probability for each ψ_n, or for each χ_n

These waters of (E) sans (D) may be muddied still further by applying an almost forgotten theorem due to Schrödinger.[19] If a spectral expansion of ρ is given by

$$\rho = \sum_m p_m | \psi_m \rangle \langle \psi_m | \tag{7}$$

then the same density operator may also be resolved into (not generally orthogonal) constituents as follows:

$$\rho = \sum_n w_n | \phi_n \rangle \langle \phi_n | \tag{8}$$

where

$$w_n = \sum_k p_k | g_{nk} |^2 \qquad \text{and} \qquad \phi_n = \sum_k \frac{g_{nk} \sqrt{p_k}}{(\sum_l p_l | g_{nl} |^2)^{1/2}} \psi_k \tag{9}$$

The quantity g_{nk} is the nth component of a vector $\mathbf{g}_k$; the set $\{\mathbf{g}_k\}$ contains one element for each nonzero p_m and it is orthonormal. For every such set $\{\mathbf{g}_k\}$ there is an expansion of the form (8), wherein the associated coefficients

$\{w_n\}$ are positive fractions summing to unity and hence representing, in an ignorance interpretation, the subjective probabilities for corresponding states $\{\phi_n\}$. The $\{g_k\}$ may be of any dimensionality sufficiently high to permit formation of an orthonormal set with the requisite number of elements.

Let us apply this theorem now to the density operator given in (4). Consider the simple case $\omega = 2$, so that $p_m = 1/\omega = 1/2$. As a typical example, we choose the following components for $\mathbf{g}_1$ and $\mathbf{g}_2$:

$$\mathbf{g}_1\text{:}\quad \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix},\qquad \mathbf{g}_2\text{:}\quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\end{pmatrix} \tag{10}$$

Obviously these are orthonormal vectors, as required. Substituting into (8), (9), we obtain immediately an alternative expansion for $\hat{\rho}$:

$$\hat{\rho} = (1/6)\,|\,\phi_1\rangle\langle\phi_1\,| + (5/12)\,|\,\phi_2\rangle\langle\phi_2\,| + (5/12)\,|\,\phi_3\rangle\langle\phi_3\,| \tag{11}$$

where

$$\phi_1 = \psi_1\,,\qquad \phi_2 = \sqrt{\frac{2}{5}}\,\psi_1 + \sqrt{\frac{3}{5}}\,\psi_2\,,\qquad \phi_3 = \sqrt{\frac{2}{5}}\,\psi_1 - \sqrt{\frac{3}{5}}\,\psi_2$$

For comparison, the spectral expansion of $\hat{\rho}$ has in this special case the form

$$\hat{\rho} = \tfrac{1}{2}\,|\,\psi_1\rangle\langle\psi_1\,| + \tfrac{1}{2}\,|\,\psi_2\rangle\langle\psi_2\,| \tag{12}$$

The state vectors $\{\phi_n\}$ are not orthogonal, but without (D) they must be regarded as three distinct alternatives. According to the ignorance interpretation of $\hat{\rho}$, (11) would mean that the subjective probability for ϕ_1 $(=\psi_1)$ to be the true state is 1/6 while (12) leads instead to the assignment of subjective probability 1/2 to the very same state ψ_1 $(=\phi_1)$. Moreover, it should be noted that this single $\hat{\rho}$ seems to represent, in the ignorance interpretation, equal probabilities for one set of alternatives and unequal probabilities for another set of alternatives. Yet this $\hat{\rho}$ has the form (4) whose traditional "derivation" sketched above purported to assign equal probability to every mutually exclusive alternative.

The escape from this quagmire of contradictions is remarkably straightforward. All that is needed is the abandonment of the ignorance interpretation of the density operator. In this way the density operator attains its proper place in the hierarchy of quantal constructs as expressed in statement (A′). In the short the density operator is the fundamental state construct in basic quantum mechanics, not a fixture of statistical physics to be used to describe a lack of knowledge. This leaves the question as to what correct quantal statement should replace (E). Here is the closest possibility:

(E′) The mathematical resolution of a density operator ρ,

$$\rho = \sum_n w_n \rho_n \tag{13}$$

where each ρ_n is a density operator and the $\{w_n\}$ are positive fractions summing to unity, has this physical interpretation: An ensemble characterized by ρ may be prepared by combining subensembles characterized by the $\{\rho_n\}$ with respective weights $\{w_n\}$. Conversely, it is at least formally possible to regard a given ρ ensemble as being divisible into subensembles $\{\rho_n\}$ with respective weights $\{w_n\}$.

It is apparent from our considerations based on Schrödinger's theorem that the ensemble decompositions contemplated in (E′) are not unique. We must also underscore the qualifier "formally" in the converse portion of (E′). The mere mathematical existence of a decomposition (13) does not imply that there are actual selection procedures by which an ensemble generated by repeatable preparation of the type ρ could in fact be partitioned into those theoretical subensembles individually generated by repeatable preparations $\{\rho_n\}$. Whether such a partitioning scheme actually exists in any given situation is a profound question that has seldom been recognized; to our knowledge, it is being carefully studied by only a few scholars.[23]

In any case, (E′) has little to do with statistical mechanics, since the quantities $\{w_n\}$ are no longer interpreted as subjective probabilities for a logical spectrum of alternative states. This does not mean, however, that density operator expansions are useless to statistical physics. In fact, even in the absence of (E) as a quantal principle, there are distinctly statistical applications for the density operator formalism. We shall explore this point in a subsequent paper devoted to new information-theoretic foundations for quantum statistics.

We come next to the erroneous theorem (F), which was based on (B), (C), and (E). The correct substitute for (F) is the same as that for (B) since (A′) relates the quantum state to the ensemble rather than to the individual system:

(F′) Same as (B′).

In light of (E′), it would now be possible to augment (B′) so that it refers to mathematically conceivable decompositions of the postmeasurement ensemble into pure $|\alpha_n\rangle\langle\alpha_n|$ subensembles. In this way, (B′) could be made to resemble its incorrect antecedent (B) a bit more closely; but this would be an uninteresting accomplishment in the present context.

Finally there remains the analogical statement (G). To obtain (G′), the quantal counterparts column must be modified to reflect the true structure of modern quantum mechanics, as expressed in particular by statement (A′).

(G′) The quantal counterparts to various key mathematical constructs of classical statistical mechanics are given by these associations:

Construct	Classical representative	Quantal counterpart
I. System	Phase space	Hilbert space
II. State, or preparation, of system	Phase point (q, p)	Density operator ρ
III. Observable	Function of phase	Hermitian operator with complete orthonormal eigenvector set
IV. Ignorance of true state	Gibbsian coefficient of probability of phase	Subjective probability distribution defined over the density operators

5. THE MOST GENERAL LOGICAL SPECTRUM OF QUANTAL STATE PROPOSITIONS

Having corrected each of the quantal misunderstandings from which the standard logical spectrum has traditionally been derived, we may at last inquire as to whether that standard set of state propositions is in fact exhaustive and mutually exclusive.

That it is not exhaustive may be seen immediately from (A′) or (G′). The complete quantal list of possible state preparations includes cases for which ρ is not a projection operator and hence no $|\Psi\rangle$ exists; in other words, the list embraces not only all the pure states—one for each ray in Hilbert space—but also all the mixed states, and none of the latter can be adequately described by any single $|\Psi\rangle$. Thus a set of state propositions of the form, "$\mathscr{S}$ is prepared in the manner characterized by $\rho = |\psi_n\rangle\langle\psi_n|$," may have every element false even if the set $\{|\psi_n\rangle\}$ contains every ray in Hilbert space. If every element of a set of propositions may be false, that set is of course not exhaustive.

It is true that the propositions of the standard logical spectrum are mutually exclusive, but not for the reason usually given, viz., that (C) implies (D). The important idea is rather that the quantum state ρ is a construct whose empirical meaning is invested entirely by the statement (A′) together with the quantal trace formula for mean values: $\bar{A} = \mathrm{Tr}(\rho A)$. Thus two preparations ρ_1, ρ_2 are distinguishable if and only if

$$\mathrm{Tr}(\rho_1 A) \neq \mathrm{Tr}(\rho_2 A) \quad \text{for some observable } A \tag{14}$$

If they are distinguishable in this sense, they are certainly mutually exclusive. It cannot be simultaneously true that a preparation is characterized by ρ_1 and also by ρ_2; for if that preparation were repeated, generating an ensemble from which to extract by measurements a collective of A-data, the resultant mean value could not be both $\mathrm{Tr}(\rho_1 A)$ and $\mathrm{Tr}(\rho_2 A)$. The condition which asserts that two quantum states ρ_1, ρ_2 are *not* mutually exclusive is therefore

$$\mathrm{Tr}(\rho_1 A) = \mathrm{Tr}(\rho_2 A) \quad \text{for every observable } A \tag{15}$$

In the absence of superselection rules, (15) implies that ρ_1 and ρ_2 are the same operator. We conclude accordingly that two quantum states ρ_1, ρ_2 are mutually exclusive if and only if they are unequal, which is just the statement (D′) given earlier. [When there are superselection rules, (15) may hold even if ρ_1 and ρ_2 are unequal; but in that case (A') should be modified so that it associates with each preparation an equivalence class of density operators. Two state preparations would then be mutually exclusive if and only if they were characterized by two different equivalence classes of density operators.]

In view of (D′), it is naturally true that two orthogonal state vectors represent mutually exclusive quantum states, not because they are orthogonal but because they are not "parallel." The spurious argument that orthogonality is related to mutual exclusivity has already been identified as a by-product of misstatement (C).

We conclude that the standard logical spectrum is inconsistent with correct quantal principles in two ways: (1) It is not exhaustive, and hence is not even a valid logical spectrum; and (2) its elements are not only mutually exclusive of each other but also, contrary to what is commonly claimed, mutually exclusive of many other states as well. The most general logical spectrum of quantal state propositions is readily determined by (A′) and (D′) without reference to the other statements which are concerned with measurement theory and ensemble decomposition. It is simply the set of all propositions of this form: *System $\mathscr{S}$ has been prepared in a manner characterized by ρ.* For this set of propositions to be *exhaustive,* there must be one such proposition *for each different density operator ρ.* Since unequal density operators make distinguishable predictions, the set is also *mutually exclusive*, and hence it constitutes the true logical spectrum of quantal state propositions.

As long as the contemporary basic quantum theory with its irreducibly probabilistic interpretation continues to be accepted as the fundamental mechanics of nature, then this new logical spectrum should replace the standard one in serious developments of statistical quantum mechanics. A new mathematical framework for quantum statistics based on the correct logical spectrum will be constructed in a forthcoming series of papers.

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