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The Empirical Determination of Quantum States

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A common approach to quantum physics is enshrouded in a jargon which treats state vectors as attributes of physical systems and the concept of state preparation as a filtration scheme wherein a process involving measurement selects from a primordial assembly of systems those bearing some prescribed vector of interest. By contrast, the empirical experiences with which quantum theory is actually concerned relate measurement and preparation in quite an opposite manner. Reproducible preparation schemes are logically and temporally anterior to measurement acts. Measurement extracts numbers from systems prepared in a specified manner; these data are then regularized by the theory by means of a state concept which is in turn used to characterize succinctly the given mode of preparation. The present paper offers, in a simple spin model, a method for determining the quantum state that represents any reproducible preparation.

1. TWO MODELS FOR QUANTAL MEASUREMENT PROCEDURES

It is commonplace to read in the literature of quantum physics that the state vector concisely summarizes the "maximum possible information" about a physical system. The concept of mixed state, representable only by a density matrix, is then introduced as an artifice for describing systems about which less is known than might in principle be known. Yet, critical analysis of the physical meaning of pure states and mixtures,

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i.e., of the epistemic rules actually employed in the practice of physics to link these theoretical constructs to data, reveals that in *both* the pure and mixed cases ensembles of identically prepared systems are required to validate the physical predictions inherent in the state vector or density matrix. Thus, the physical referent even of a pure state is already an ensemble; for every state vector entails probabilistic information, testable only by comparison with relative frequencies obtained from statistical collectives of data. To regard a mixed state as indicative of ignorance—less than "maximum possible information"—leads therefore to the use of such meaningless clauses as "the probability that the mean value of observable E is $\langle e_n \mid E \mid e_n \rangle$ is w_n," or "the probability that a system in the ensemble has state vector $\mid e_n \rangle$ is w_n." This phraseology assumes that every physical system possesses some state vector $\mid e_n \rangle$ as an attribute which might be known or unknown, and thereby ignores the paramount physical fact that state vectors refer not to single systems but to ensembles of identically prepared systems.

Against this background, the philosophical underpinnings and consequences of which are elaborated more fully elsewhere,(1) the present work attempts to provide a method for the empirical determination of quantum states which is consonant with the actual format of experimental science, and which does not presuppose that pure states are objective properties of systems while mixed states are subjective measures of human ignorance.

The problem of empirical determination of quantum states is frequently confused in the literature with the mathematical problem of providing enough labels (quantum numbers) for the unambiguous specification of Hilbert vectors. The latter problem is solved by finding maximal Abelian sets of Hermitian operators (Dirac's complete sets of commuting observables). Unfortunately, this purely formal procedure is often described in terms of an old, untenable theory of measurement based upon the famous notion of wave-packet reduction. The verbal result, frequently couched in the jargon of *filtration* gedankenexperiments, superficially gives the appearance of an empirical method for state determination.

This filtration model for quantal measurement procedures ignores the fundamental distinction between preparation and measurement, the two physical acts that mark the beginning and end, respectively, of each run in a typical experiment. Instead, it is imagined that a quantum system can be prepared in a particular eigenstate $\mid e_1 \rangle$ of observable E merely by "measuring" E, and retaining the system if the numerical result is e_1 but rejecting it if another result is obtained. Such "selective" measurements are to be performed using ideal devices called filters. If E is by itself a maximal Abelian set, the procedure is described as having measured, selected, or prepared the system in state $\mid e_1 \rangle$; if not, E must be supplemented by enough additional observables and corresponding filters to make up a maximal set. In this model, mixtures are introduced subjectively as representing ignorance as to which vector $\mid e \rangle$ the system really possesses, a state of affairs presumably traceable to the use of a low-quality filter. Now, it is our belief that the filtration model does not adequately cope with the actual experimental situations that quantum theory is called upon to analyze. In particular, the following shortcomings of filtration should be noted:

1. The idea that a measurement of an observable E that yields the datum e_1 is equivalent to finding or preparing the system in state $| e_1\rangle$ is erroneous. There is a finite probability for the eigenvalue e_1 to result from an E-measurement on a system in almost any state whatever—pure or mixed; hence, a single E-measurement yielding e_1 cannot be interpreted as revealing a preexisting state $| e_1\rangle$. However, an ensemble of many measurements *all* resulting in e_1 is a necessary condition for the verdict $| e_1\rangle$ *after the event*. Neither can such a measurement or series of measurements be regarded as *preparing* $| e_1\rangle$; such preparation coincident with measurement is not impossible, but in view of the catastrophic effects of detectors upon microsystems, it is certainly rare.

2. The filtration model focuses attention on the terminal phase of an experiment —the measurement act—and by treating measurement as equivalent to preparation for a later experiment inverts the fundamental physical question that experiments seek to answer. That is, instead of asking what measurements must be made to determine the state of a system that has been subjected to a given preparation, the filtration model attempts unsuccessfully to effect preparations by the performance of measurements.

3. Since ensembles are equally necessary for the operational definition of pure states as well as mixed states, and for other reasons⁽²⁾ too complex to review here, it is improper to pretend that each individual system possesses some vector $| e_n\rangle$, perhaps "unknown." Hence, the problem of empirical determination of the quantum state associated with a given preparation should not be predicated on any assumption that each system has a state vector waiting to be discovered. If a preparation scheme does in fact produce a pure ensemble, that information must emerge from an analysis of the data, not from an *a priori* conviction. Similarly, no other assumption should be made in advance concerning the spectral structure of the density matrix. For example, if a preparation gives a mixture of $| e_1\rangle$ and $| e_2\rangle$, that information must emerge from the data; subjective *a priori* statements that assume that each system in an ensemble has either $| e_1\rangle$ or $| e_2\rangle$ are unreasonable, since the correct density matrix may not admit of the proposed decomposition.

Instead of the filtration model, we espouse instead what may be termed the *preparation–measurement model*⁽³,⁴⁾ for experiments in quantum physics. Its essential framework has already been discussed above in connection with the foregoing critique of the filtration picture. In the following sections, we derive for a simple spin system a method for determining the density matrix that characterizes any given preparation. It turns out that measurement of a maximal Abelian set is in general insufficient to determine the state, even if the state is known in advance to be pure. Indeed, what must be measured is not a complete set of commuting observables, but what we shall call a *minimal set of noncommuting observables.*

2. MINIMAL SETS OF NONCOMMUTING OBSERVABLES

We assume that some reproducible preparation scheme Π is given and that a measurement is to be performed following each preparation for the purpose of determining the density matrix that characterizes the given preparation. By repeating Π and a measurement of some observable E many times, we gather a collective of numerical data from which may be inferred statistical quantities like $\langle E \rangle$ (the arithmetic mean of the E-data), ΔE (the standard deviation of E-data), and $\langle F(E) \rangle$ (the arithmetic mean of some prescribed function F of the E-data). Our project is to find sufficient statistical data to determine the unknown ρ.

For simplicity, we consider a quantum system whose Hilbert space has only two dimensions. The density matrix ρ and matrix representatives of observables are of second rank. Hermiticity of ρ and of the observables implies that four real numbers suffice to determine the matrices unambiguously; in the case of ρ, the auxiliary normalization condition $\operatorname{Tr} \rho = 1$ reduces the number of independent real numbers occurring in the (complex) elements of the density matrix to three.

Any Hermitian matrix on this Hilbert space may be expressed in the following manner, which displays explicitly the real numbers that determine the matrix:

$$E = \sum_{k=0}^{3} E_k \sigma_k = E_0 \sigma_0 + \mathbf{E} \cdot \boldsymbol{\sigma} \tag{1}$$

where σ_0 is the identity and the components of $\boldsymbol{\sigma}$ are the three standard Pauli spin matrices; Hermiticity implies that the E_k are all real.

Let e_1, e_2 denote the eigenvalues of E; the trace of E is then $(e_1 + e_2)$; therefore, since $\operatorname{Tr} \sigma_0 = 2$, $\operatorname{Tr} \boldsymbol{\sigma} = 0$, we obtain

$$E_0 = \tfrac{1}{2}(e_1 + e_2) \tag{2}$$

Similarly, for a density matrix ρ, we have

$$\rho = \tfrac{1}{2}\sigma_0 + \boldsymbol{\rho} \cdot \boldsymbol{\sigma} \tag{3}$$

since $\operatorname{Tr} \rho = 1$.

The arithmetic mean of E-data is related to the unknown ρ through the fundamental trace equation

$$\operatorname{Tr}(\rho E) = \langle E \rangle \tag{4}$$

The trace may be expanded as follows using (1) and (3):

$$\operatorname{Tr}(\rho E) = \sum_{\substack{k=0 \\ l=0}}^{3} \rho_k E_l \operatorname{Tr}(\sigma_k \sigma_l) = 2 \sum_{k} \rho_k E_k = E_0 + 2\boldsymbol{\rho} \cdot \mathbf{E} \tag{5}$$

Combining (4) and (5), we obtain

$$2\boldsymbol{\rho} \cdot \mathbf{E} = \langle E \rangle - E_0 \equiv \delta E \tag{6}$$

Note that E_0 is the mean value for E-data that would be predicted on the basis of equal *a priori* probability for each possible value; δE is a measure of the departure of the actual preparation from one that yields random E-data.

Equation (6) is linear and has three unknowns—the components of $\boldsymbol{\rho}$. If two additional linear equations like (6) can be found, then $\boldsymbol{\rho}$ will be determined. This program is easily achieved by performing measurements of observables A and B upon ensembles prepared in the manner Π. When the data are analyzed to obtain δA and δB, we shall have three real linear equations in three unknowns,

$$\begin{aligned} 2\boldsymbol{\rho} \cdot \mathbf{E} &= \delta E \\ 2\boldsymbol{\rho} \cdot \mathbf{A} &= \delta A \\ 2\boldsymbol{\rho} \cdot \mathbf{B} &= \delta B \end{aligned} \tag{7}$$

which may be solved to obtain

$$2\boldsymbol{\rho} = \frac{\delta E(\mathbf{A} \times \mathbf{B}) + \delta A(\mathbf{B} \times \mathbf{E}) + \delta B(\mathbf{E} \times \mathbf{A})}{\mathbf{E} \cdot \mathbf{A} \times \mathbf{B}} \tag{8}$$

Note that, if $\delta E = \delta A = \delta B = 0$, ρ is given by $\rho = \frac{1}{2}\sigma_0$, the density matrix that assigns probability $\frac{1}{2}$ to each eigenvalue of every observable.

Equation (8) determines $\boldsymbol{\rho}$ and hence ρ if and only if the scalar triple product in the denominator does not vanish. Therefore, the observables E, A, and B will be adequate to determine ρ if and only if

$$\mathbf{E} \cdot \mathbf{A} \times \mathbf{B} \neq 0 \tag{9}$$

The condition expressed in (9) is not, however, in the form readily accessible to normal quantum-theoretical modes of thought. We shall therefore demonstrate that the content of (9) may be stated in terms of commutation relations.

The commutator of two observables A, B expanded in the form (1) is calculated as follows:

$$[A, B] = \sum_{\substack{k=0 \\ j=0}}^{3} A_k B_j [\sigma_k\,, \sigma_j] = \sum_{\substack{k=1 \\ j=1}}^{3} A_k B_j\, 2i \sum_{p=1}^{3} \epsilon_{kjp} \sigma_p \tag{10}$$

since σ_0 commutes with $\boldsymbol{\sigma}$.

Rearranging, we obtain

$$[A, B] = 2i \sum_{p=1}^{3} \left\{ \sum_{\substack{k=1 \\ j=1}}^{3} \epsilon_{pkj} A_k B_j \right\} \sigma_p = 2i(\mathbf{A} \times \mathbf{B}) \cdot \boldsymbol{\sigma} \tag{11}$$

i.e.,

$$(\text{vector component of } [A, B]) = 2i(\mathbf{A} \times \mathbf{B}) \tag{12}$$

Now, $\mathbf{E} \cdot \mathbf{A} \times \mathbf{B} \neq 0$ if and only if

$$\mathbf{E} \times \mathbf{A} \neq 0, \qquad \mathbf{A} \times \mathbf{B} \neq 0, \qquad \mathbf{B} \times \mathbf{E} \neq 0 \tag{13}$$

But, by (11), (13) is equivalent to the statement that E, A, and B are noncommuting observables.

Hence, the condition (9) *for the adequacy of E, A, and B to determine ρ can be fulfilled if and only if E, A, and B do not commute.*

We shall call such a set of observables that yield the data δE, etc. sufficient to determine ρ via equations like (7) a *minimal set of noncommuting observables.* (In the present example involving a two-dimensional Hilbert space, the minimal set has only three elements.)

Note that three distinct types of measurement apparatus must be employed; i.e., several statistical quantities like $\langle E\rangle$, $\langle E^3\rangle$, $\langle \sin E\rangle$ drawn from the same collective E-data are insufficient to determine ρ, since all functions of E are mutually commutable.

3. UNCERTAINTY AND CERTAINTY

The uncertainty theorem of quantum mechanics,

$$\Delta A\, \Delta B \geqslant \tfrac{1}{2}\, |\langle \psi \mid [A, B] \mid \psi\rangle|, \qquad \psi \ \text{ arbitrary} \tag{14}$$

is easily extended to mixed states via a triangular inequality. Let the spectral expansion of ρ be

$$\rho = r_1 \mid r_1\rangle\langle r_1 \mid + r_2 \mid r_2\rangle\langle r_2 \mid, \qquad r_1 + r_2 = 1 \tag{15}$$

If

$$c_1 \equiv \langle r_1 \mid \tfrac{1}{2}[A, B] \mid r_1\rangle, \qquad c_2 \equiv \langle r_2 \mid \tfrac{1}{2}[A, B] \mid r_2\rangle \tag{16}$$

and $| c_1 | \geqslant | c_2 |$, then

$$\begin{aligned} \Delta A\, \Delta B &\geqslant | c_1 | = (r_1 + r_2) | c_1 | \geqslant r_1 | c_1 | + r_2 | c_2 | \geqslant | r_1 c_1 + r_2 c_2 | \\ &= | \operatorname{Tr} \rho\{\tfrac{1}{2}[A, B]\}| = \tfrac{1}{2}\, |\langle [A, B]\rangle| \end{aligned} \tag{17}$$

From (3), (11), we find

$$|\langle [A, B]\rangle| = 4\boldsymbol{\rho} \cdot \mathbf{A} \times \mathbf{B}$$

Then (17) implies

$$\Delta A\, \Delta B \geqslant 2 \mid \boldsymbol{\rho} \cdot \mathbf{A} \times \mathbf{B} \mid \tag{18}$$

Now, it might be supposed that a deviation ΔA could be obtained experimentally as an item of information independent of the mean value $\langle A\rangle$. However, in the present simple Hilbert space, such is not the case. Using, for example, the A-representation we have

$$\langle A\rangle = \operatorname{Tr}(\rho A) = a_1\rho_{11} + a_2\rho_{22} \tag{19}$$

$$\langle A^2\rangle = \operatorname{Tr}(\rho A^2) = a_1^2\rho_{11} + a_2^2\rho_{22} \tag{20}$$

which pair can be solved for ρ_{11} and ρ_{22} :

$$\rho_{11} = (\langle A^2\rangle - a_2\langle A\rangle)/a_1(a_1 - a_2)$$

$$\rho_{22} = (\langle A^2\rangle - a_1\langle A\rangle)/a_2(a_2 - a_1)$$

and, because identically $\rho_{11} + \rho_{22} = 1$, we have

$$\langle A^2 \rangle = (a_1 + a_2)\langle A \rangle - a_1 a_2 \tag{21}$$

which is of course an invariant relation independent of the representation used in the deduction. Thus, $\langle A^2 \rangle$ is not an independent bit of information beyond $\langle A \rangle$. From (21), we further have

$$(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2 = (a_1 - \langle A \rangle)(\langle A \rangle - a_2)$$

and similarly

$$(\Delta B)^2 = (b_1 - \langle B \rangle)(\langle B \rangle - b_2) \tag{22}$$

The left side of the uncertainty relation (18) is thus in fact

$$\Delta A\, \Delta B = [(a_1 - \langle A \rangle)(\langle A \rangle - a_2)(b_1 - \langle B \rangle)(\langle B \rangle - b_2)]^{1/2} \tag{23}$$

Combining (8), (18), and (23), we have the following relationship connecting $\langle A \rangle$, $\langle B \rangle$, and $\langle E \rangle$ as a consequence of the uncertainty theorem:

$$\begin{aligned} &[(a_1 - \langle A \rangle)(\langle A \rangle - a_2)(b_1 - \langle B \rangle)(\langle B \rangle - b_2)]^{1/2} \\ &\quad \geqslant \left| \frac{\delta E(\mathbf{A} \times \mathbf{B}) \cdot (\mathbf{A} \times \mathbf{B}) + \delta A(\mathbf{B} \times \mathbf{E}) \cdot (\mathbf{A} \times \mathbf{B}) + \delta B(\mathbf{E} \times \mathbf{A}) \cdot (\mathbf{A} \times \mathbf{B})}{\mathbf{E} \cdot \mathbf{A} \times \mathbf{B}} \right| \end{aligned} \tag{24}$$

Suppose Π were such that $\langle A \rangle = a_1$; then, $\Delta A = 0$ and $\delta A = \frac{1}{2}(a_1 - a_2)$. The right side of (24) must therefore vanish; hence, δB and δE are no longer independent.

Actually, the observation $\langle A \rangle = a_1$ alone suffices to fix $\rho = | a_1 \rangle \langle a_1 |$, as is easily proved. It might therefore be conjectured, perhaps in defense of the filtration idea, that only one observable, rather than the minimal set, is adequate to determine a pure density matrix. This reasoning is fallacious, however, since (i) there is in general no way to know *a priori* that a state is pure, and (ii) finding that specific observable A for the given Π such that $\langle A \rangle = a_1$ would require a *search* through an infinity of observables. By contrast, our method involving a minimal set of noncommuting observables is a definite procedure for determining the ρ belonging to any Π whatever.

4. CARTESIAN MINIMAL SETS

From equations like (8) and (24), it is obvious that our results would be greatly simplified if the three vectors **A**, **B**, and **E** were mutually perpendicular. We shall call a minimal set of noncommuting observables E, A, B for which **E**, **A**, **B** are mutually perpendicular a Cartesian minimal set. In a representation diagonal in E, a Cartesian minimal set may be expressed as follows:

$$\begin{aligned} E &= \tfrac{1}{2}(e_1 + e_2)\,\sigma_0 + \tfrac{1}{2}(e_1 - e_2)\,\sigma_3 \\ A &= \tfrac{1}{2}(a_1 + a_2)\,\sigma_0 + \tfrac{1}{2}(a_1 - a_2)\,\sigma_1 \\ B &= \tfrac{1}{2}(b_1 + b_2)\,\sigma_0 + \tfrac{1}{2}(b_1 - b_2)\,\sigma_2 \end{aligned} \tag{25}$$

Within this set, we have the following:

$$\begin{gathered}\mathbf{E}\cdot\mathbf{A}\times\mathbf{B}=\tfrac{1}{8}(a_1-a_2)(b_1-b_2)(e_1-e_2)\\ \mathbf{A}\cdot\mathbf{B}=\mathbf{B}\cdot\mathbf{E}=\mathbf{A}\cdot\mathbf{E}=0\end{gathered}\tag{26}$$

and

$$\mathbf{A}\times\mathbf{B}=\frac{\mathbf{E}(a_1-a_2)(b_1-b_2)}{2(e_1-e_2)}\tag{27}$$

and two similar relations. Since **E** has only the one component, $E_3=\frac{1}{2}(e_1-e_2)$, $\mathbf{A}\times\mathbf{B}$ also has only the one component, $[\mathbf{A}\times\mathbf{B}]_3=\frac{1}{4}(a_1-a_2)(b_1-b_2)$, and the components of $\boldsymbol{\rho}$ in (8) become

$$\left(\frac{\delta A}{a_1-a_2},\frac{\delta B}{b_1-b_2},\frac{\delta E}{e_1-e_2}\right)\tag{28}$$

so that the density matrix is

$$\rho=\frac{1}{2}\sigma_0+\frac{\delta A}{(a_1-a_2)}\sigma_1+\frac{\delta B}{(b_1-b_2)}\sigma_2+\frac{\delta E}{(e_1-e_2)}\sigma_3\tag{29}$$

Using (27) and (29) in (18) yields the following set of uncertainty relations:

$$\begin{aligned}\Delta A\,\Delta B&\geqslant\tfrac{1}{2}\,\delta E(a_1-a_2)(b_1-b_2)/(e_1-e_2)\\ \Delta B\,\Delta E&\geqslant\tfrac{1}{2}\,\delta A(b_1-b_2)(e_1-e_2)/(a_1-a_2)\\ \Delta E\,\Delta A&\geqslant\tfrac{1}{2}\,\delta B(e_1-e_2)(a_1-a_2)/(b_1-b_2)\end{aligned}\tag{30}$$

Note that (30) implies that, to obtain a precise value of, say, the observable E, $\Delta E=0$, both δA and δB must vanish.

When a Cartesian minimal set is used, it becomes possible to derive a rather simple formula for the density matrix in terms of the relative frequencies of measurement results. Let f_{e_n} denote the relative frequence with which E-measurements yield e_n; then, since $\langle E\rangle=f_{e_1}e_1+f_{e_2}e_2$ and $f_{e_1}+f_{e_2}=1$, we have

$$f_{e_1}=(\langle E\rangle-e_2)/(e_1-e_2)\tag{31}$$

The relative frequency f_{e_1} is just the mean value of the function $P_1(E)$ defined by the spectral expansion

$$P_1(E)=\sum_{n=1}^{2}P_1(e_n)\mid e_n\rangle\langle e_n\mid\tag{32}$$

where $P_1(e_n)=\delta_{1n}$; i.e.,

$$P_1(E)=\mid e_1\rangle\langle e_1\mid\equiv P_{e_1}\tag{33}$$

$$\langle P_{e_1}\rangle=f_{e_1}\tag{34}$$

From (6) and the fact that $P_1(E)$ is a projector with trace unity, we now obtain

$$\delta P_{e_1} = f_{e_1} - \tfrac{1}{2} \tag{35}$$

Combining (31) and (35), we obtain

$$\delta P_{e_1} = \frac{\langle E\rangle - e_2}{e_1 - e_2} - \frac{1}{2} \tag{36}$$

But since, by (6), $\langle E\rangle = \delta E + \tfrac{1}{2}(e_1 + e_2)$, we get

$$\delta P_{e_1} = \delta E/(e_1 - e_2) \tag{37}$$

Comparison with (29) then yields the following simple expression for the density matrix:

$$\rho = \tfrac{1}{2}\sigma_0 + \delta P_{a_1}\sigma_1 + \delta P_{b_1}\sigma_2 + \delta P_{e_1}\sigma_3 \tag{38}$$

where $\delta P_{a_1} = f_{a_1} - \tfrac{1}{2}$, etc.

Note that, if E, A, B had been chosen as projectors at the outset, Eq. (29) would have taken the form (38) automatically, since the eigenvalues of any projector are 0 and 1. Since, in quantum theory, projectors represent observables variously known as dichotomic variables, propositions, or questions, we shall use the term *Cartesian questions* to designate a Cartesian minimal set of projection operators. Equation (38) now suggests a simple reformulation of our procedure for determining the density matrix corresponding to a given Π: Select three kinds of measurement apparatus capable of giving "yes" or "no" answers to three Cartesian questions P_e, P_a, P_b; if f_a, f_b, f_e are the measured relative frequencies of "yes" answers, then the density matrix characterizing the preparation under investigation will be, in a representation diagonal in P_e,

$$\rho = \tfrac{1}{2}\sigma_0 + (f_a - \tfrac{1}{2})\,\sigma_1 + (f_b - \tfrac{1}{2})\,\sigma_2 + (f_e - \tfrac{1}{2})\,\sigma_3 \tag{39}$$

5. EMPIRICAL SIGNIFICANCE OF PURE AND MIXED STATES

In Section 1, we argued that an operational definition of the density matrix cannot reasonably presuppose any particular spectral structure for the matrix; for, until data become available, it cannot be known that a system prepared in the manner Π has a state vector at all, nor can it be known that the system has some "probability w_n of having a prescribed state $|e_n\rangle$." Accordingly, we have developed the method of minimal noncommuting sets for determining the density matrix without making *a priori* assumptions about its mathematical form; it has been demanded neither that $\rho = |e\rangle\langle e|$, with $|e\rangle$ to be determined, nor that $\rho = \sum_n w_n |e_n\rangle\langle e_n|$, with the "possibilities" $|e_n\rangle$ known and the w_n to be determined.

However, now that we have a procedure for constructing the density matrix from an examination of data, it is possible of course to discover by further analysis whether systems prepared in the manner Π are in pure states or mixed states. (More accurately, whether an ensemble of systems prepared in the manner Π is pure or mixed.)

The condition for the pure state is

$$\rho^2 = \rho \tag{40}$$

which may be written as follows by using the expansion (3):

$$\left(\sum_{j=0}^{3} \rho_j \sigma_j\right)\left(\sum_{k=0}^{3} \rho_k \sigma_k\right) = \sum_{m=0}^{3} \rho_m \sigma_m \tag{41}$$

or

$$\rho_0{}^2\sigma_0 + 2\rho_0 \sum_{j=1}^{3} \rho_j \sigma_j + \sum_{j=1}^{3} \rho_j{}^2 \sigma_0 + \sum_{j \neq k \neq 0}^{3} \rho_j \rho_k \sigma_j \sigma_k = \sum_{m=0}^{3} \rho_m \sigma_m \tag{42}$$

Because $\sigma_j \sigma_k = -\sigma_k \sigma_j$, the last term on the left vanishes, and, from $\rho_0 = \frac{1}{2}$, we find (42) yields $\frac{1}{4} + \sum_{j=1} \rho_j{}^2 = \frac{1}{2}$ or

$$\text{Pure state:} \qquad \boldsymbol{\rho} \cdot \boldsymbol{\rho} = \tfrac{1}{4} \tag{43}$$

A trivial example of a pure state would be to take $\rho_3 = \frac{1}{2}$, $\rho_1 = \rho_2 = 0$, when $\rho = \begin{pmatrix} 10 \\ 00 \end{pmatrix}$. Another: $\rho_2 = \frac{1}{2}$, $\rho_1 = \rho_3 = 0$: $\rho = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$, which can be diagonalized to $\begin{pmatrix} 10 \\ 00 \end{pmatrix}$. On the other hand, any density matrix can be diagonalized to the form $\begin{pmatrix} \rho_{11} & 0 \\ 0 & \rho_{22} \end{pmatrix}$, with two nonzero elements if it is not a pure case. In the diagonal form, it can be written as $\rho_0 \sigma_0 + \rho_3 \sigma_3$, where $\rho_0 = \frac{1}{2}$ and $\rho_3 = \frac{1}{2}(\rho_{11} - \rho_{22})$. In this case, we have

$$\boldsymbol{\rho} \cdot \boldsymbol{\rho} = \rho_3{}^2 = \tfrac{1}{4}[\rho_{11}^2 + (1 - \rho_{11})^2 - 2\rho_{11}(1 - \rho_{11})] = \tfrac{1}{4} + \rho_{11}^2 - \rho_{11} \tag{44}$$

Since $\rho_{11} < 1$, (44) implies that, for a mixture,

$$\text{Mixed state:} \qquad \boldsymbol{\rho} \cdot \boldsymbol{\rho} < \tfrac{1}{4} \tag{45}$$

By combining (8), (43), and (45), we may write the conditions for pure (or mixed) states in terms of experimental data:

$$|\, \delta A \mathbf{A}^* + \delta B \mathbf{B}^* + \delta E \mathbf{E}^* \,|^2 \leqslant 1 \tag{46}$$

where we have written $\mathbf{A}^*$ for the vector $(\mathbf{B} \times \mathbf{E})/(\mathbf{E} \cdot \mathbf{A} \times \mathbf{B})$ reciprocal to $\mathbf{A}$, etc.

For a Cartesian minimal set E, A, B, the criterion for a pure state expressed by the equality in (46) becomes

$$\left(\frac{\delta A}{|\,\mathbf{A}\,|}\right)^2 + \left(\frac{\delta B}{|\,\mathbf{B}\,|}\right)^2 + \left(\frac{\delta E}{|\,\mathbf{E}\,|}\right)^2 = 1 \tag{47}$$

since $\mathbf{A}^* = (1/|\,\mathbf{A}\,|)\,\mathbf{A}/|\,\mathbf{A}\,|$, etc., for mutually perpendicular $\mathbf{A}$, $\mathbf{B}$, $\mathbf{E}$.

For a minimal set of Cartesian questions P_e, P_a, P_b, (47) reduces to

$$(\delta P_a)^2 + (\delta P_b)^2 + (\delta P_e)^2 = \tfrac{1}{4} \tag{48}$$

since $|\,\mathbf{P}_a\,| = |\,\mathbf{P}_b\,| = |\,\mathbf{P}_e\,| = \tfrac{1}{2}$. In terms of relative frequencies of "yes" answers, (48) may be expressed as

$$(f_a - \tfrac{1}{2})^2 + (f_b - \tfrac{1}{2})^2 + (f_e - \tfrac{1}{2})^2 = \tfrac{1}{4} \tag{49}$$

This suggests the following simple empirical test for ascertaining whether or not a given preparation Π is producing a pure state: Select three Cartesian questions, "ask" the questions of systems prepared in the manner Π (i.e., measure the observables represented by the projectors), compute the relative frequencies of "yes" answers. If these relative frequencies satisfy (49), Π is a pure-state preparation scheme; if (49) is not satisfied, Π produces a mixed state.

If the state prepared in the manner Π is pure, then any one of the relative frequencies is determined by the other two through (49). This represents the fact that only two independent real numbers are required to specify a state vector in the present Hilbert space. Any state vector $|\,\psi\rangle$ may be expanded in terms of the eigenvectors of E as follows:

$$|\,\psi\rangle = r\,|\,e_1\rangle + c\,|\,e_2\rangle \tag{50}$$

where r may be assumed real and positive due to the arbitrary overall phase of $|\,\psi\rangle$. Moreover, r is determined by the modulus of c through the normalization requirement: $r = +(1 - |\,c\,|^2)^{1/2}$. Hence, only the modulus and phase of c—two real numbers—are needed to find $|\,\psi\rangle$, provided it is known that a $|\,\psi\rangle$ exists (an assumption made implicitly in Feenberg's method[5] for determining nonrelativistic wave functions). However, to know whether a $|\,\psi\rangle$ does exist for a given Π, it is necessary to "ask" *all* the questions in a minimal set and successfully apply the criterion (49). If (49) is satisfied, it is then a simple algebraic procedure to determine the coefficients in (50) from the elements of ρ.

Similarly, if it could be known in advance that a mixture is present and can be subdivided into pure states $|\,e_1\rangle$ and $|\,e_2\rangle$, then only one real number would be required to specify the density matrix in the present Hilbert space; i.e., if

$$\rho = w_1\,|\,e_1\rangle\langle e_1\,| + w_2\,|\,e_2\rangle\langle e_2\,| \tag{51}$$

where $w_2 = 1 - w_1$, then the real number w_1 determines ρ. Thus, measurements of P_e alone would determine ρ. But, of course, to learn whether the density matrix for a given Π admits of the particular expansion (50), it is first necessary to "ask" *all* the questions in a minimal set.

The reader is free to interpret the formalism used above in terms of the spin observables of a fermion, when, of course, $e_1 = a_1 = b_1 = \tfrac{1}{2}$, $e_2 = a_2 = b_2 = -\tfrac{1}{2}$. We have, however, deliberately refrained from this throughout the work because the accidental simplification of various formulae that occurs for spin components does little more than obscure the statistical significance of the formalism.

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