Quantum state determination: Quorum for a particle in one dimension

William Band and James L. Park
Department of Physics, Washington State University, Pullman, Washington 99164
(Received 7 June 1977; accepted 16 October 1977)

In this paper we wish to illuminate the axiom that the quantal state describes a statistical ensemble of similar systems identically prepared, and is not to be identified with any single system. The mathematical representative of the general quantum state is the density matrix or statistical operator in Hilbert space. We demonstrate how this operator may be determined empirically by calculations involving only the measured mean values of a set of observables we call a "quorum." As an example of this approach a state determination procedure is described for a spinless particle moving in one dimension; the corresponding quorum turns out to involve only position data associated with various instants subsequent to the act of preparation.

I. HISTORICAL REMARKS

Until perhaps the middle 1960's the quantum state was quite generally identified with a vector in Hilbert space. In graduate courses one learned that when the precise state was not known, the density matrix could be used to make statistical judgments. However, to paraphrase a quote from ter Haar's text on statistical mechanics[1] (1954), one was always careful to distinguish between the statistical aspects inherent in quantum mechanics—the uncertainty principle—and the statistical aspects introduced by ensembles and the density matrix. This feeling that the uncertainty principle had a much "deeper meaning" than the deviations or fluctuations observed in the results of ensemble measurements, was implicit in the Copenhagen Interpretation, and persisted in the literature for many years in spite of repeated disclaimers (Margenau *et al.*).[2] Over the past ten years it has become more widely recognized that the probabilistic elements of quantum mechanics are essentially identical with the statistical nature of all physical measurement. No true measurement exists, even in classical physics, that does not involve an ensemble of repeated observations of identically prepared individual systems. The assignment of a Hilbert space vector to describe the state of a single individual system is an inadequate mathematical scheme to take care of this broader understanding. Yet graduate texts on quantum mechanics of the past decade have persisted in basing the theory on this assignment, and restricting the discussion of the density matrix to exotic exceptional cases, or even relegating the topic to an appendix.

According to the newer philosophy the "state" of a system is regarded as referring not to the individual system, but to the mode of preparation of the system prior to measurement; repeated identical preparations result in an ensemble which is describable by the density matrix, or more properly the statistical operator, ρ in Hilbert space. The special cases where ρ is a projection operator in the Hilbert space $\mathcal{H}$ are, of course, equivalent to the old standard state vectors. We do not now regard ρ as merely a device for handling states that are not precisely known: if ρ is determined, then the state is known completely.

We have for some years been responsible for an unstructured weekly graduate seminar with the broad mandate to discuss the foundations of quantum mechanics, and one of us has for the past ten years taught a graduate course on quantum mechanics based on the unified statistical philosophy. There has been no text available that covers the subject *ab initio* from this point of view, which, perhaps facetiously, has been dubbed by our students as "The Palouse Interpretation."[3] In standard courses, problems are usually posed in the form: given a system in such-and-such a state, what are the observable values and how will they evolve in time? From the new point of view a basic question comes naturally to mind; how does one determine the state of a system that has been prepared in some specified manner? In standard treatments this question is seldom asked and rarely answered satisfactorily. Until this question can be asked and properly answered, quantum mechanics can hardly claim to be a completely logical theory.

Illustrations of unknown states are usually presented in terms of spin, a system without classical analog. In this paper we address a purely classical problem—a single particle without spin in a one-dimensional domain. We do this repeatedly with the same gun and equivalent domain, thus preparing an ensemble upon which we can make measurements. How do we determine the quantum statistical operator that describes this preparation?

The answer to this question demands that we identify a set of observables we call the quorum, the measurement of which permits the precise determination of ρ. Aside from this identification—which has not been made before for the one-particle problem—a significant conclusion of this work is the following: while it is easy enough to say, for example, "let a particle be in a pure momentum state," it is by no means a trivial matter to make sure that in practice any given preparation scheme actually results in some desired state. Even if the system has in fact been prepared in a pure momentum state, that fact is not really known unless in principle the entire quorum of observables has been measured, and that turns out to be a denumerably infinite set!

II. QUORUM CONCEPT

According to the most general form of quantum mechanics, every reproducible state preparation scheme Π is characterized by a statistical operator ρ in the sense that

 0002-9505/79/020188-04$00.50

$$\langle A \rangle = Tr(\rho A), \quad (1)$$

where A is the Hermitian operator corresponding to some observable and $\langle A \rangle$ denotes the arithmetic mean of data obtained for that observable from measurements upon an ensemble of systems each prepared in the prescribed manner Π. Contemplation of this axiom leads immediately to the following basic problem: given a reproducible operational procedure Π and the empirical means to gather enough data for computation of the mean of any observable, find a set of observables $\{A\}$ whose associated mean values $\{\langle A \rangle\}$ constitute sufficient information to determine the unknown ρ. In earlier work we have termed such a set $\{A\}$ a *quorum* of observables. In this paper we are particularly concerned with the mathematical identification and physical interpretation of a quorum suitable for a spinless quantal particle in one dimension with Hamiltonian of the form

$$H = (1/2)P^2 + V(Q), \quad (2)$$

where

$$[Q,P] = i. \quad (3)$$

In previous articles[4-6] we have developed systematic procedures for the construction of quorums for physical systems with N-dimensional Hilbert spaces and, under certain restrictions, for systems with infinite-dimensional Hilbert spaces. Other authors who have considered the problem of quantum state determination include Feenberg,[7] Kemble,[8] and Gale, Guth, and Trammell.[9]

III. MATHEMATICAL FORMULATION OF THE QUORUM PROBLEM FOR THE PARTICLE IN ONE DIMENSION

For an N-dimensional space, a quorum can be found mathematically by choosing N^2-1 observables $\{A\}$ such that the N^2-1 corresponding relations (1) turn out to be a system of linear algebraic equations possessing a unique solution set for the N^2-1 real unknowns required to define the Hermitian, unit trace $N \times N$ density matrix representing statistical operator ρ.

In the problem posed above, however, the Hilbert space is infinite dimensional; and an alternative approach proves superior. We base the development on an old form suggested by Weyl[10] for operators associated with spinless quantum particles:

$$\rho = \int d\gamma \int d\lambda\, \omega(\gamma,\lambda) e^{i(\gamma Q+\lambda P)}. \quad (4)$$

This operator version of Fourier transform theory has been studied rigorously by Pool[11]; there are no physically significant restrictions on its application in the present context. Equation (4) may be inverted by elementary manipulations to obtain

$$\omega(\gamma,\lambda) = (1/2\pi) Tr\{\rho e^{-i(\gamma Q+\lambda P)}\}. \quad (5)$$

Using a well-known (Baker-Hausdorff) identity and the commutation relations (3), we have

$$\begin{aligned} e^{i(\gamma Q+\lambda P)} &= e^{i\gamma Q} e^{i\lambda P} e^{i\lambda\gamma/2} \\ e^{-i(\lambda P+\gamma Q)} &= e^{-i\lambda P} e^{-i\gamma Q} e^{-i\lambda\gamma/2}. \end{aligned} \quad (6)$$

Thus (4) and (5) may be combined to yield

$$\rho = \frac{1}{2\pi} \int d\lambda \int d\gamma\, Tr\{\rho\, e^{-i\lambda P} e^{-i\gamma Q}\} e^{i\gamma Q} e^{i\lambda P}. \quad (7)$$

Next we derive from (7) a typical matrix element of ρ in the q representation; observing that $e^{i\lambda P}$ is a space displacement operator, we find immediately that

$$\langle q-\lambda | \rho | q \rangle = \frac{1}{2\pi} \int d\gamma\, Tr\{\rho e^{-i\lambda P} e^{-i\lambda Q}\}\, e^{i\gamma(q-\lambda)}. \quad (8)$$

The kernel of this integral may be expanded as

$$\sum_{m,n} \left\{\frac{(-i\lambda)^n}{n!}\right\} (-i\gamma)^m\, Tr \left\{\frac{\rho P^n Q^m}{m!}\right\}, \quad (9)$$

and we shall write

$$P^n Q^m/m! = (1/2)(B_{mn} + iA_{mn}), \quad (10)$$

where A_{mn} and B_{mn} are the Hermitian operators

$$\begin{aligned} A_{mn} &\equiv i(Q^m P^n - P^n Q^m)/m! \equiv (i/m!)[Q^m,P^n] \\ B_{mn} &\equiv (Q^m P^n + P^n Q^m)/m! \equiv (1/m!\ [Q^m,P^n]_+. \end{aligned} \quad (11)$$

Then $Tr\,\{\rho P^n Q^m/m!\}$ is to be interpreted as the ensemble mean of the (complex valued) operator written down in (10). If the ensemble mean values $\langle A_{mn} \rangle$ and $\langle B_{mn} \rangle$ can be experimentally measured, then the state ρ of the system can be determined from (8); to be explicit

$$\begin{aligned} \langle q-\lambda | \rho | q \rangle &= \frac{1}{2} \frac{1}{2\pi} \sum_{m,n} \frac{(-i\lambda)^n}{n!}\Big\} \\ &\times \{\langle B_{mn} \rangle + i \langle A_{mn} \rangle\} \int d\gamma\, (-i\gamma)^m e^{i\gamma(q-\lambda)}. \end{aligned} \quad (12)$$

IV. THEOREM CONCERNING COMMUTATORS AND ANTICOMMUTATORS

It may appear from the above remarks that the set of operators defined in (11) could be regarded as a quorum of observables for the determination of the state ρ. Mathematically speaking, this is correct. However, the search for a physically meaningful quorum is a bit more involved; for there is no known physical apparatus that measures the rather esoteric operators in question. Moreover, even the mathematical prescription is unduly cumbersome, since the commutators are in fact expressible in terms of the anticommutators. To see this, let us write

$$Q_m \equiv Q^m/m!. \quad (13)$$

Then it is not difficult to prove by induction that

$$\begin{aligned} -iA_{mn} &= \sum_{\substack{m\le n,\, k=n-m \\ m\ge n,\, k=0}}^{n-1} (i)^{n-k} \binom{n}{k} P^k Q_{m-n+k} \\ &= - \sum_{\substack{k=n-m \\ k=0}}^{n-1} (-i)^{n-k} \binom{n}{k} Q_{m-n+k} P^k \end{aligned} \quad (14)$$

$$\begin{aligned} &= \frac{1}{2} \sum_{\substack{k=n-m \\ k=0}}^{n-1} \Big\{ (i)^{n-k} \binom{n}{k} P^k Q_{m-n+k} \\ &\qquad - (-i)^{n-k} \binom{n}{k} Q_{m-n+k} P^k \Big\}. \end{aligned} \quad (15)$$

The lower limit of the sum is $n - m$ unless $n < m$ in which case the lower limit is zero. When n is even we have, therefore,

$$-iA_{mn} = \frac{1}{2}\sum_{k\ \mathrm{odd}}^{n-1} (i)^{n-k}\binom{n}{k}B_{m-n+k,k} + \frac{1}{2}i\sum_{k\ \mathrm{even}}^{n-2}(i)^{n-k}\binom{n}{k}A_{m-n+k,k} \quad (16)$$

and when n is odd

$$-iA_{mn} = \frac{1}{2}\sum_{k\ \mathrm{even}}^{n-1} (i)^{n-k}\binom{n}{k}B_{m-n+k,k} + \frac{1}{2}i\sum_{k\ \mathrm{odd}}^{n-2}(i)^{n-k}\binom{n}{k}A_{m-n+k,k}. \quad (17)$$

To each of the commutators A_{mn} on the right side of either (16) or (17) we can apply the same equation and proceed successively to reduce the power index of P in the commutators by two at each step. If n is even the index drops eventually to zero, so no commutators remain on the right side; while if n is odd the lowest index is unity: but we know that

$$A_{m1} = i[Q_m,P] = -Q_{m-1}, \quad (18)$$

so again there are no commutators remaining on the right. We have, therefore, proved the theorem that any commutator of the form $[Q_m,P^n]$ can be expressed entirely in terms of anticommutators, together with perhaps Q_m or the identity operator. This theorem means that in seeking a physical quorum we need only to find a set of empirical quantities from which one may compute the mean values of the anticommutator B_{mn}.

V. PHYSICAL QUORUM FOR A PARTICLE IN ONE DIMENSION

We adopt now the hypothesis that there do exist empirical procedures for directly measuring position and all of its nth time derivatives and seek to prove now that such a set constitutes a physical quorum for the particle in one dimension. Let

$$Q_{s,n} \equiv \left(\frac{d}{dt}\right)^n Q_{s+n}, \quad (19)$$

where s and n are any integers, positive or zero.

Using (2) we obtain first the well-known relation

$$\frac{dQ}{dt} = -i[Q,H] = P, \quad (20)$$

which with (19) makes the identification

$$P = Q_{0,1}. \quad (21)$$

We can then prove easily that

$$Q_{s,1} = \frac{d}{dt}Q_{s+1} = Q_sP - (1/2)iQ_{s-1}. \quad (22)$$

For the special case of a free particle [V(Q) = 0], by induction it now follows generally that:

$$Q_{s,n} = \sum_{k=0}^{\min(s,n)} (-i)^k \left(\frac{1}{2}\right)^k \binom{k}{n} Q_{s-k}P^{n-k}. \quad (23)$$

Alternatively we can also show that

$$Q_{s,1} = \frac{d}{dt}Q_{s+1} = PQ_s + (1/2)iQ_{s-1} \quad (24)$$

and again in the free-particle case by induction

$$Q_{s,n} = \sum_{k=0}^{\min(s,n)} (-i)^k \left(-\frac{1}{2}\right)^k \binom{n}{k} P^{n-k}Q_{s-k}. \quad (25)$$

(The upper limit on k is in each case the lesser of s or n.) Combining (23) and (25) we have

$$Q_{s,n} = \sum_{k\ \mathrm{even}}^{\min(s,n)} \left(\frac{1}{2}\right)^{k+1}(-1)^{k/2}\binom{n}{k}B_{s-k,n-k} + \sum_{k\ \mathrm{odd}}^{\min(s,n)} \left(\frac{1}{2}\right)^{k+1}(-1)^{(k+1)/2}\binom{n}{k}A_{s-k,n-k}. \quad (26)$$

We select any value of s and write down from (26) the expressions for the first few values of n in increasing order:

$$Q_{s,0} = (1/2)B_{s0} = Q^s/s!, \quad (27a)$$

$$Q_{s,1} = (1/2)B_{s1}, \quad (27b)$$

$$Q_{s,2} = (1/2)B_{s2} - (1/8)B_{s-2,0} - (1/2)A_{s-1,1}, \quad (27c)$$

$$Q_{s,3} = (1/2)B_{s3} - (3/8)B_{s-2,1} - (3/4)A_{s-1,2}. \quad (27d)$$

The left sides of these equations are all directly measurable. We learn at once that the anticommutators B_{s0} and B_{s1} are therefore measurable. But in (27c) $A_{s-1,1} = i[Q_{s-1},P] = -Q_{s-2}$ which is measurable, so that (27c) indirectly permits B_{s2} to be calculated. Also in (27d), $A_{s-1,2} = i[Q_{s-1},P^2] = 2(d/dt)Q_{s-1} = -2Q_{s-1,1}$ and is therefore measurable. Therefore from (27d) B_{s3} can be calculated from measurements. Quite generally we can compare $Q_{s,n+2}$ with $Q_{s,n}$, and note that the only terms contained in $Q_{s,n+2}$ that are not contained in $Q_{s,n}$ are $B_{s,n+2}$ and $A_{s-1,n+1}$. But (16) and (17) show that $A_{s-1,n+1}$ can be expressed entirely in terms of the B_{mn} already taken care of in $Q_{s,n}$. Thus each successive $Q_{s,n+2}$ can be used to calculate $B_{s,n+2}$ from directly measurable observables by going through the sequence started in (27). We therefore regard this set $\{Q_{s,n}\}$ as a physical quorum for the free particle in one dimension.

It is not difficult to prove that this same physical quorum $Q_{s,n}$ is also sufficient when the Hamiltonian has the more general form (2) in which $V(Q) \neq 0$. Because in this case P does not commute with H, the expressions replacing (26) contain terms involving the space derivatives of V. Provided only that $V(Q)$ is an analytic function, the proof is not essentially different from the free-particle case. In general it can be asserted again that any product of the noncommuting operators can be expressed as a sum of commutator and anticommutator; the commutators can all be reduced to lower-order anticommutators and commutators, and eventually to a sum of anticommutators alone, of successively lower order in P. Every $Q_{s,n}$ can, therefore, be expressed as a linear combination of anticommutators whose highest order in P is n, and hence by measuring all the means $\{\langle Q_{s,n}\rangle\}$ one can determine the means of the anticommutators. The theorem of Sec. III is independent of the Hamiltonian, so that again, through (12), the density matrix can be determined.

Incidentally it is now easy to prove also that the statistical state of a spinless particle in three-dimensional space can in principle be determined by measuring the following quorum of observables:

$$\{Q^\alpha_{s_\alpha,n_\alpha}\} \equiv \left\{\frac{(d/dt)^{n_\alpha}Q_\alpha{}^{s_\alpha+n_\alpha}}{(s_\alpha+n_\alpha)!}\right\}, \alpha = 1,2,3 \quad (28)$$

where the Q_α are components of the position operator **Q**.

VI. EMPIRICAL DETERMINATION OF ρ

The notion of direct measurement of the quorum of observables $\{Q_{s,n}\}$ may be understood in the following way. The particle is prepared in some prescribed fashion Π described theoretically by the unknown statistical operator ρ. At some specified time t following the completion of Π a measuring device $\mathcal{M}$ is caused to interact with the system, $\mathcal{M}$ being designed to record the position $q(t)$ of the particle at time t.

Because the interaction with $\mathcal{M}$ is expected to disturb the particle either the latter must be reprepared in the manner Π or a duplicate system must be subjected to Π before the $\mathcal{M}$ interaction is used again to record the position, again at time t following the completion of Π. From the ensemble of results $\{q(t)\}$ obtained by many such repeated measurement interactions it is then possible to calculate the value of $\langle Q\rangle$ at time t. In order to measure the quorum set $\{Q_{s,n}\}$ an ensemble of measurement results $q(t)$ must be recorded for each of a series of t values, say $0, \tau, 2\tau, 3\tau, \ldots, n\tau, \ldots$. Then, for example, a reading of $Q_{s,2}$ is given by the computation of

$$Q_{s,2} \equiv \left(\frac{d}{dt}\right)^2 Q_{s+2} = \lim_{\tau\to 0} \frac{1}{\tau^2}\{q_{s+2}(2\tau) - 2q_{s+2}(\tau) + q_{s+2}(0)\}, \quad (29)$$

where

$$q_{s+2}(t) \equiv q(t)^{s+2}/(s+2)! \quad (30)$$

and the $q(t)$ values are samples taken from the recorded ensemble. The ensemble average $\langle Q_{s,2}\rangle$ which is one of the quorum means required for the determination of ρ is then simply

$$\langle Q_{s,2}\rangle \equiv \left\langle \left(\frac{d}{dt}\right)^2 Q_{s+2} \right\rangle = \lim_{\tau\to 0} \frac{1}{\tau^2}\{\langle q_{s+2}(2\tau)\rangle - 2\langle q_{s+2}(\tau)\rangle + \langle q_{s+2}(0)\rangle\}. \quad (31)$$

In general we have

$$\langle Q_{s,n}\rangle \equiv \left\langle \left(\frac{d}{dt}\right)^n Q_{s+n} \right\rangle = \lim_{\tau\to 0} \left(\frac{1}{\tau^n}\right) \sum_{k=0}^{n} \binom{n}{k} (-1)^k \langle q_{s+n}[(n-k)\tau]\rangle. \quad (32)$$

In Sec. IV we proved that from $Q_{s,n}$ we can compute the anticommutators B_{sn}, and in Sec. III that the commutators A_{mn} can be expressed in terms of the B_{mn}. Hence from $\{\langle Q_{s,n}\rangle\}$ we have the information required to derive, using (12), the q-representation density matrix for ρ. We conclude therefore that the statistical operator ρ characterizing a reproducible preparation Π may in principle be determined empirically by analyzing position data associated with various instants subsequent to the act of preparation. The relationship between this procedure and the somewhat analogous method of determining classical densities in phase by measuring ensemble averages of moments $\{q^m p^n\}$ will be explored in another paper.

[1]D. ter Haar, Elements of Statistical Mechanics (Rinehart, New York, 1954), Chap. VII.

[2]H. Margenau, Philos. Sci. **4**, 337 (1937); **25**, 23 (1958); **30**, 1 (1963); **30**, 138 (1963).

[3]Our Palouse country has been described by John Gunther, in *Inside USA*, (Harper, New York, 1947), Chap. 9 as part of probably the most prolific (wheat) region in the world!

[4]W. Band and J. L. Park, Found. Phys. **1**, 133 (1970).

[5]J. L. Park and W. Band, Found. Phys. **1**, 211 (1971).

[6]W. Band and J. L. Park, Found. Phys. **1**, 339 (1971).

[7]E. Feenberg, thesis, Harvard University (1933) (unpublished).

[8]E. C. Kemble, *Fundamental Principles of Quantum Mechanics* (McGraw-Hill, New York, 1937), p. 71.

[9]W. Gale, C. Guth, and G. T. Trammell, Phys. Rev. **165**, 1434 (1968).

[10]H. Weyl, *The Theory of Groups and Quantum Mechanics* (Dutton, New York, 1931), p. 275.

[11]J. C. T. Pool, J. Math. Phys. **7**, 66 (1966).