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A General Theory of Empirical State Determination in Quantum Physics: Part I

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This paper develops a method for extracting from data the quantum theoretical state representation belonging to any reproducible empirical scheme for preparing a physical system, provided only that at least one observable has its possible values limited to a finite set. In Part I, we formulate a general systematic procedure, based on the concept of irreducible tensor operators, for the selection of sets of observables sufficiently large to permit the unambiguous determination of an unknown quantum state.

1. INTRODUCTION

Since in quantum physics the epistemic connection between the state concept and the datal experience to which it refers is inherently probabilistic, the problem of assigning the proper quantum theoretical state representation to a given empirical state preparation is not so transparent as the analogous problem in classical physics. In a previous publication,[1] we illustrated this problem of empirical state determination by discussing a quantum system whose Hilbert space had only two dimensions, i.e., the observables were restricted to having each only two eigenvalues.

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Simple criteria were given by means of which the quantum state could be deduced from empirical data on such "spin-$\frac{1}{2}$ type" observables. Here, we shall generalize the discussion to cover quantum systems with observables having any number of eigenvalues, the Hilbert spaces being expanded appropriately.

2. THE MULTIPOLE APPROACH TO STATE DETERMINATION

The following quantum mechanical propositions are adopted as axioms:

*A*1: To every physical *system* there corresponds a Hilbert space $\mathscr{H}$.

*A*2: Hermitian operators on $\mathscr{H}$ represent physical *observables* associated with the physical system.

*A*3: To every reproducible empirical scheme for the *preparation* of the physical system, there corresponds a density operator on $\mathscr{H}$, namely ρ, such that, given any observable A on $\mathscr{H}$, the arithmetical mean value of a statistical collective of A-measurements obtained from an ensemble of systems all prepared identically in the manner symbolized by ρ, is equal to

$$\langle A \rangle = \mathrm{tr}(\rho A) \tag{1}$$

In our discussion, the term quantum state refers to the ensemble, not to any individual system[1]; the state determination is synonymous with the determination of the density operator ρ. Mathematically, therefore, the problem of state determination may now be concisely expressed as follows:

Given an $\mathscr{H}$, find a set of A's such that the system of corresponding equations (1) can be solved uniquely for ρ.

Consider an N-dimensional Hilbert space $\mathscr{H}_N$. The representation of a Hermitian operator in this space will be an $N \times N$ matrix of complex numbers; Hermiticity of this matrix restricts the number of independent coefficients to N^2. It follows that to determine any such operator on $\mathscr{H}_N$ requires N^2 real numbers. In particular, the density operator, conventionally constrained to have a unit trace, requires for its determination $N^2 - 1$ real numbers. Thus, we need a system of $N^2 - 1$ observables to generate $N^2 - 1$ equations like (1) for a determination of the quantum state of our ensemble. The problem is to determine what sets of observables will in fact yield $N^2 - 1$ *independent* equations for this purpose. In our earlier paper,[1] where $N = 2$, a very simple solution to this problem emerged. For $N = 3$, we need to find a minimum of eight independent observables, and it is already clear that an acceptable set of observables may be far from self-evident. For larger values of N, it is obvious that some systematic procedures are absolutely necessary to ensure a successful search for the required minimum set of $N^2 - 1$ observables.

The procedure we have adopted arises from the fact that the number N^2 is related to the number of independent elements in a sequence of tensors defined in

[1] An ensemble may be generated, however, by taking a single system alternately prepared, measured, identically reprepared, etc.

terms of angular momentum operators, and referred to elsewhere in physics as multipoles. Thus, a multipole tensor operator of rank k, T_{kq}, usually called a 2^k-pole tensor operator, has $2k + 1$ independent component operators, $q = -k, \ldots, k$, and because

$$\sum_{k=0}^{N-1} (2k + 1) = N^2 \tag{2}$$

we shall speculate that any observable in $\mathscr{H}_N$ can be expressed as a linear combination of the N^2 operators included in the set of all tensor operator components $\{T_{kq}\}$, $k = 0, 1, \ldots, N - 1$. In effect, these N^2 operators constitute the basis for an N^2-dimensional Hilbert space, referred to below as operator space, in which every observable of interest is a vector.

In our earlier paper,[1] we had $N = 2$, $N^2 = 4$, and the multipole operators were the 2×2 spin tensors (three components of a dipole operator) and the identity (a monopole) operator. To prove the generality of this procedure, we shall show that the T_{kq} in fact constitute a complete orthogonal set in operator space, and we shall also show how to determine their $N \times N$ representations. Since we are interested in the trace of a product of two operators—Eq. (1)—we also need a theorem concerning the trace of a product of two T's. These purely mathematical considerations are developed in Sections 4 and 5.

The virtue of this scheme is of course that we are able to characterize intuitively a sequence of observables as a "monopole," a triplet of "dipoles," five "quadrupoles," ..., $2k + 1$ "2^k-poles," and so on, and to proceed systematically along this sequence until we have a sufficient number of independent observables to determine the quantum state of the ensemble. Hopefully, this will provide a general mathematical procedure that can be applied to any ensemble.

3. OPERATOR SPACE: MULTIPOLE EXPANSIONS OF OBSERVABLES AND DENSITY MATRICES

Our first definition is as follows.

Definition 1. A *multipole operator*, or more explicitly, an *irreducible tensor operator* (ITO) of rank k is a $(2k + 1)$-plet of operators $\{T_{kq} \mid q = -k, \ldots, k\}$ defined to satisfy the equations

$$[J_z, T_{kq}] = qT_{kq} \tag{3}$$

$$[J_\pm, T_{kq}] = [k(k + 1) - q(q \pm 1)]^{1/2}\, T_{kq\pm1} \tag{4}$$

where J_z and $J_\pm$ are the familiar angular momentum operators for three-dimensional space:

$$J_\pm = J_x \pm iJ_y, \qquad \mathbf{J} \times \mathbf{J} = i\mathbf{J} \tag{5}$$

(k is always understood to be a nonnegative integer.)

For any system whose Hilbert space is $\mathscr{H}_N$, we anticipate needing a sequence of ITO's with ranks $k = 0, 1, \ldots, N-1$, to obtain a basis for the operator space mentioned above.

The observables for such a system have N eigenvalues, and may be represented by $N \times N$ matrices; hence, it will be useful to have an $N \times N$ representation of all these ITO's. We can obtain this by adopting a notation based on the standard angular momentum eigenkets $\{| J, M\rangle | M = -J, \ldots, J\}$, with $N = 2J + 1$.

Since an isomorphism exists between any two Hilbert spaces of the same dimensionality, mathematical procedures in the quantum theory of angular momentum that are used in connection with N-dimensional spaces invariant and irreducible under the rotation group will be formally transferrable to any $\mathscr{H}_N$. Hence, the standard angular momentum eigenkets $\{| J, M\rangle | M = -J, \ldots, J\}$ may be regarded as spanning any $\mathscr{H}_N$, provided $N = 2J + 1$, even if the $\mathscr{H}_N$ occurs in connection with a physical system for which "angular momentum" is undefined. Accordingly, in what follows, it should be understood that the standard angular momentum operator and quantum number notation does not necessarily have its usual physical interpretation. (Note: since J may be any nonnegative integer or half-integer, there is a J for every admissible N value.)

We begin with a brief survey of those rudiments of irreducible tensor operator theory which are germane to our present purpose. Only proofs of theorems not readily available in the literature[2] will be given.

Theorem 1. (Wigner–Eckart, special case). The matrix elements of an ITO T_k with components $\{T_{kq}\}$ on a $(2J + 1)$-dimensional $\mathscr{H}$ are given by

$$\langle JM \mid T_{kq} \mid JM' \rangle = (2J+1)^{-1/2} \langle J \| \mathsf{T}_k \| J \rangle \langle JkM'q \mid JM \rangle \tag{6}$$

where $\langle JkM'q \mid JM\rangle$ is a Clebsch–Gordan coefficient and $\langle J \| \mathsf{T}_k \| J\rangle$ is a quantity (so-called reduced matrix element) independent of M, M', q.

We shall need in particular the reduced matrix element for the identity:

$$\langle J \| 1 \| J \rangle = (2J+1)^{1/2} \tag{7}$$

Theorem 2. If T_{k_1} and U_{k_2} are ITO's, then

$$V_{kq}^{k_1 k_2} \equiv \sum_{q_1 q_2} \langle kq \mid k_1 k_2 q_1 q_2 \rangle \, T_{k_1 q_1} U_{k_2 q_2}, \qquad q = -k, \ldots, k \tag{8}$$

are components of an ITO ($\langle kq \mid k_1 k_2 q_1 q_2\rangle$ are Clebsch–Gordan coefficients).

The expression (8) may be inverted, using Clebsch–Gordan orthogonality relations, to yield

$$T_{k_1 q_1} U_{k_2 q_2} = \sum_{kq} \langle k_1 k_2 q_1 q_2 \mid kq \rangle \, V_{kq}^{k_1 k_2} \tag{9}$$

Theorem 3. If T_k is an ITO on a $(2J + 1)$-dimensional space, then

$$\operatorname{tr} T_{kq} = \delta_{k0} (2J+1)^{1/2} \langle J \| \mathsf{T}_0 \| J \rangle \tag{10}$$

In particular, if we apply (10) to (8), there results

$$\operatorname{tr} V_{kq}^{k_1k_2} = \delta_{k0}(2J+1)^{1/2} \langle J \| \mathsf{V}_0^{k_1k_2} \| J \rangle \tag{11}$$

Now, it is possible to take the trace of (9) to obtain

$$\begin{aligned} \operatorname{tr}(T_{k_1q_1}U_{k_2q_2}) &= \sum_{kq} \langle k_1k_2q_1q_2 \mid kq \rangle\, \delta_{k0}(2J+1)^{1/2} \langle J \| \mathsf{V}_0^{k_1k_2} \| J \rangle \\ &= (2J+1)^{1/2} \langle k_1k_2q_1q_2 \mid 00 \rangle \langle J \| \mathsf{V}_0^{k_1k_2} \| J \rangle \end{aligned} \tag{12}$$

But from tables, we find that

$$\begin{aligned} \langle k_1k_2q_1q_2 \mid 00 \rangle &= \delta_{k_1k_2}\, \delta_{q_1-q_2} \langle k_1k_1q_1 - q_1 \mid 00 \rangle \\ &= \delta_{k_1k_2}\, \delta_{q_1-q_2}\, (-1)^{k_1+q_1}/(2k_1+1)^{1/2} \end{aligned} \tag{13}$$

Substituting (13) into (12), we get

$$\operatorname{tr}(T_{k_1q_1}U_{k_2q_2}) = (2J+1)^{1/2} \frac{\delta_{k_1k_2}\, \delta_{q_1-q_2}\, (-1)^{k_1+q_1}}{(2k_1+1)^{1/2}} \langle J \| \mathsf{V}_0^{k_1k_2} \| J \rangle \tag{14}$$

i.e., the only nonzero traces of products of ITO components have this form:

$$\operatorname{tr}(T_{kq}U_{k-q}) = [(2J+1)/(2k+1)]^{1/2} (-1)^{k+q} \langle J \| \mathsf{V}_0^{kk} \| J \rangle \tag{15}$$

where

$$V_{00}^{kk} = \sum_{q_1q_2} \langle 00 \mid kk\; q_1q_2 \rangle\, T_{k_1q_1}U_{k_2q_2} \tag{16}$$

Combining (13) and (16), we have

$$\begin{aligned} V_{00}^{kk} &= \sum_{q_1q_2} \frac{\delta_{q_1q_2} (-1)^{k+q_1}}{(2k+1)^{1/2}}\, T_{kq_1}U_{kq_2} \\ &= \frac{(-1)^k}{(2k+1)^{1/2}} \sum_{q=-k}^{k} (-1)^q\, T_{kq}U_{k-q} \end{aligned} \tag{17}$$

Now, from (5), we see that any rank-zero ITO, like V_{00}^{kk}, must satisfy

$$[J_z, V_{00}^{kk}] = [J_\pm, V_{00}^{kk}] = 0 \tag{18}$$

i.e., V_{00}^{kk} commutes with the generators of the rotation group; thus, by Schur's lemma,

$$V_{00}^{kk} = C_k 1 \tag{19}$$

where C_k is a complex number depending only on T_k, U_k.

Combining (7) and (19), we get

$$\langle J \| V_{00}^{kk} \| J \rangle = C_k(2J+1)^{1/2} \tag{20}$$

By substituting (20) into (15), and combining (17) and (19), we obtain the following theorem.

Theorem 4. If T_{k_1} and U_{k_2} are ITO's,

$$\begin{aligned} &\text{(a)} \quad \mathrm{tr}(T_{k_1q_1}U_{k_2q_2}) = 0 \qquad \text{unless} \quad k_1 = k_2\,, \quad q_1 = -q_2 \\ &\text{(b)} \quad \mathrm{tr}(T_{kq}U_{k-q}) = (2J+1)(-1)^{k+q}\,(2k+1)^{-1/2}\,C_k \end{aligned} \tag{21a}$$

where

$$C_k 1 = \frac{(-1)^k}{(2k+1)^{1/2}} \sum_{q=-k}^{k} (-1)^q\, T_{kq}U_{k-q} \tag{21b}$$

We shall require only the special case of Theorem 4 where $\mathsf{T}_k = \mathsf{U}_k$, which we shall formulate as the following theorem.

Theorem 5. If T_k is an ITO, then

$$\begin{aligned} &\text{(a)} \quad \mathrm{tr}(T_{kq}T_{k'q'}) = 0, \qquad k \neq k'; \\ &\text{(b)} \quad \mathrm{tr}(T_{kq}T_{k-q}) = [(-1)^q/(2k+1)]\, g_k(2J+1), \end{aligned} \tag{22a}$$

where

$$g_k 1 = \sum_{q=-k}^{k} (-1)^q\, T_{kq}T_{k-q} \tag{22b}$$

Definition 2. An ITO T_k is said to be Hermitian if and only if

$$\mathsf{T}_k{}^{\dagger} = \mathsf{T}_k \tag{23}$$

where

$$(\mathsf{T}_k{}^{\dagger})_q \equiv (-1)^q\,(\mathsf{T}_k)_{-q}^{\dagger} = (-1)^q\, T_{k-q}^{\dagger} \tag{24}$$

(The dagger on the right side of (24) is just the ordinary Hermitian conjugate of a single operator.)

Thus, for a Hermitian T_k,

$$T_{k-q} = (-1)^q\, T_{kq}^{\dagger} \tag{25}$$

If T_k is Hermitian in the sense of Definition 2, Eq. (22) may be expressed in terms of $\{T_{kq}\}$ and $\{T_{kq}^{\dagger}\}$ as follows:

$$\mathrm{tr}(T_{kq}T_{kq}^{\dagger}) = [(2J+1)/(2k+1)]\, g_k \tag{26a}$$

where

$$g_k 1 = \sum_{q=-k}^{k} T_{kq}T_{kq}^{\dagger} \tag{26b}$$

Note that g_k is in this case real.

To adapt the ITO formalism to the problem of state determination, we shall construct an auxiliary vector space, to be called *operator space*, whose elements are the linear operators on $\mathscr{H}_N$. Operator space is defined by specifying a basis:

Definition 3. Any sequence of ITO's of the form $\{\mathrm{T}_k \mid k = 0, 1,..., 2J\}$ will be called a *basis* for the N^2-dimensional operator space auxiliary to $\mathscr{H}_N$, where $N = 2J + 1$. The elements of operator space are all the linear combinations of the basis components.

For convenience, we adopt a basis consisting of *Hermitian* ITO's with a specified normalization:

Definition 4. In the *special basis* $\{\tau_k \mid k = 0, 1,..., 2J\}$ for the operator space auxiliary to $\mathscr{H}_N$, $N = 2J + 1$, (a) each τ_k is Hermitian in the sense of Definition 2, and (b) we have the following:

$$\sum_{q=-k}^{k} \tau_{kq}\tau_{kq}^{\dagger} = (2k + 1)\, 1, \qquad k = 0,..., 2J \tag{27}$$

Henceforth, we shall use the special basis exclusively; any element A of operator space is then a linear combination of the form

$$A = \sum_{k=0}^{2J} \sum_{q=-k}^{k} A_{kq}\tau_{kq} \tag{28}$$

where the $\{A_{kq}\}$ are in general complex numbers.

Definition 5. The *scalar product* of two elements A, B of operator space is defined by

$$(A \mid B) \equiv \mathrm{tr}(A^{\dagger}B) \tag{29}$$

From Theorem 5, (26), and (27), we then have in particular

$$(\tau_{k_1q_1} \mid \tau_{k_2q_2}) = \delta_{k_1k_2}\, \delta_{q_1q_2}\, (2J + 1) \tag{30}$$

Now, (30) implies that the elements of the special basis are mutually orthogonal in the sense of the scalar product in Definition 5. As we shall see in detail in Section 4, Theorem 1 may be used to construct $(2J + 1)$-dimensional matrix representations of the $\{\tau_{kq}\}$; thus, (28) may be regarded as an expression for an $N \times N$ matrix A in terms of $N \times N$ matrices $\{\tau_{kq}\}$, where $N = 2J + 1$. Thus, the question of completeness arises: Given an arbitrary $N \times N$ matrix A, can a set $\{A_{kq}\}$ be found such that A may be expressed in the form (28)?

To verify that the set $\{\tau_{kq}\}$ is in fact complete in this sense, it suffices to note that the total number of orthogonal $\{\tau_{kq}\}$ is

$$\sum_{k=0}^{2J=N-1} (2k + 1) = N^2 \tag{31}$$

which is of course the number of elements in the arbitrary matrix A. Hence, given A, the components $\{A_{kq}\}$ for the expansion (28) may be ascertained as follows.

Multiply (28) by τ_{lm} and take the scalar product:

$$(\tau_{lm} \mid A) = \sum_{kq} A_{kq}(\tau_{lm} \mid \tau_{kq}) \tag{32}$$

Using (30), we then obtain

$$\begin{aligned}(\tau_{lm} \mid A) &= \sum_{kq} A_{kq}\delta_{lk}\delta_{mq}(2J + 1)\\ &= A_{lm}(2J + 1)\end{aligned}$$

Hence

$$A_{kq} = (\tau_{kq} \mid A)/(2J + 1) \tag{33}$$

We summarize the considerations leading to (33) as the following theorem.

Theorem 6. The operator space spanned by the special basis of Definition 4 is complete for all linear operators on $\mathscr{H}_N$, $N = 2J + 1$.

It follows as a corollary that any observable (Hermitian operator) associated with a physical system whose Hilbert space is $\mathscr{H}_N$ will be an element of the operator space and expressible in the form (28).

Theorem 7. If A is Hermitian and

$$A = \sum_{k=0}^{2J} \sum_{q=-k}^{k} A_{kq}\tau_{kq}$$

then

$$A_{k-q} = (-1)^q A_{kq}^* \tag{34}$$

The Hermiticity condition (34) is an immediate consequence of (25). From (34), it follows that in the expansion (28) of any Hermitian A, the $(2k + 1)$ complex A_{kq} associated with each value of k will involve only $(2k + 1)$ independent real numbers. In light of the discussion of the multipole concept given in Section 2, it seems appropriate therefore to adopt the following terminology:

Definition 6. If A is an observable in the operator space auxiliary to $\mathscr{H}_N$, $N = 2J + 1$, so that

$$A = \sum_{k=0}^{2J} \sum_{q=-k}^{k} A_{kq}\tau_{kq}$$

then the $(2k + 1)$-plet $\{A_{kq}\}$ will be called the 2^k-pole component of A. Similarly, for a density matrix

$$\rho = \sum_{k=0}^{2J} \sum_{q=-k}^{k} \rho_{kq}\tau_{kq} \tag{35}$$

the $(2k + 1)$-plet $\{\rho_{kq}\}$ will be called the 2^k-pole component of ρ.

Theorem 8a. The monopole component of an observable A associated with a physical system with Hilbert space $\mathscr{H}_N$ is $1/N$ times the sum of the eigenvalues of A.

To prove this proposition, consider the monopole ($k = 0$) case of (33):

$$A_{00} = \frac{(\tau_{00} \mid A)}{2J + 1} = \frac{1}{N} \operatorname{tr}(\tau_{00}^{\dagger} A) \tag{36}$$

By the same reasoning that led to (19), plus the normalization requirement (27), we find that

$$\tau_{00} = 1 \tag{37}$$

Hence, $A_{00} = (1/N) \operatorname{tr} A$ and Theorem 8a is demonstrated.

Since a density matrix has trace unity, we have also the following theorem.

Theorem 8b. The monopole component of the density matrix for a physical system with Hilbert space $\mathscr{H}_N$ is $1/N = 1/(2J + 1)$.

Hence,

$$\rho = \frac{1}{2J + 1} 1 + \sum_{k=1}^{2J} \sum_{q=-k}^{k} \rho_{kq} \tau_{kq} \tag{38}$$

Later, we shall find it convenient to write down these multipole expansions of observables and density matrices in the following, more compact form: Let $\mathbf{A}_k$ denote a $(2k + 1)$-vector whose components are $\{A_{kq}\}$. Then,

$$A = \sum_{k=0}^{2J} \mathbf{A}_k \cdot \boldsymbol{\tau}_k \equiv \sum_{k=0}^{2J} \sum_{q=-k}^{k} A_{kq} \tau_{kq} \tag{39}$$

Similarly,

$$\rho = \frac{1}{2J + 1} \boldsymbol{\tau}_0 + \sum_{k=1}^{2J} \boldsymbol{\rho}_k \cdot \boldsymbol{\tau}_k \tag{40}$$

Thus, for example, the dipole component of A is a 3-vector $\mathbf{A}_1$; the quadrupole component, a 5-vector $\mathbf{A}_2$; the octupole component, a 7-vector $\mathbf{A}_3$; etc.

4. THE ALGEBRA OF OPERATOR SPACE

In this section, we derive several useful relations involving the special basis $\{\boldsymbol{\tau}_k\}$. Theorem 1 (Wigner–Eckart) plays a significant role in these developments; however, we shall henceforth express it in terms of 3-j symbols instead of Clebsch–Gordan coefficients.

Since the 3-j symbol is defined by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-1)^{j_1 - j_2 - m_3}}{(2j_3 + 1)^{1/2}} \langle j_1 j_2 m_1 m_2 \mid j_3 - m_3 \rangle \tag{41}$$

(6) may be expressed with $T_{kq} = \tau_{kq}$ as follows:

$$\langle JM \mid \tau_{kq} \mid JM' \rangle = \langle J \| \tau_k \| J \rangle (-1)^{-J+k-M} \begin{pmatrix} J & k & J \\ M' & q & -M \end{pmatrix} \tag{42}$$

Theorem 9. $\langle J \| \tau_k \| J \rangle = [(2J+1)(2k+1)]^{1/2}$.

Proof. Combining (26) and (27), we find

$$\operatorname{tr}(\tau_{kq}^{\dagger} \tau_{kq}) = 2J + 1. \tag{43}$$

An application of (42) then yields

$$\begin{aligned} \operatorname{tr}(\tau_{kq}^{\dagger} \tau_{kq}) &= \sum_{MM'} \langle JM' \mid \tau_{kq}^{\dagger} \mid JM \rangle \langle JM \mid \tau_{kq} \mid JM' \rangle \\ &= \sum_{MM'} \langle J \| \tau_k \| J \rangle^2 (-1)^{-2J+2k-2M} \begin{pmatrix} J & k & J \\ M' & q & -M \end{pmatrix}^2 \\ &= \langle J \| \tau_k \| J \rangle^2 \sum_{MM'}^{2} \begin{pmatrix} J & k & J \\ M' & q & -M \end{pmatrix}^2 = 2J + 1 \end{aligned}$$

Hence,

$$\langle J \| \tau_k \| J \rangle = \left[(2J+1) \Big/ \sum_{MM'} \begin{pmatrix} J & k & J \\ M' & q & -M \end{pmatrix}^2 \right]^{1/2} \tag{44}$$

The denominator in (44) is evaluated using the following identity involving 3-j symbols:

$$\sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{\delta_{j_3 j_3'} \, \delta_{m_3 m_3'}}{2j_3 + 1} \tag{45}$$

Thus, we obtain the desired result:

$$\langle J \| \tau_k \| J \rangle = \left[\frac{2J+1}{(2k+1)^{-1}} \right]^{1/2} = [(2J+1)(2k+1)]^{1/2} \tag{46}$$

Theorem 10.

$$\tau_{k_1 q_1} \tau_{k_2 q_2} = \sum_{k=0}^{2J} \sum_{q=-k}^{k} E_J(k_1 q_1 k_2 q_2 k q) \, \tau_{kq} \tag{47a}$$

where

$$\begin{aligned} E_J \equiv {} & \delta_{q, q_1+q_2} [(2J+1)(2k+1)(2k_1+1)(2k_2+1)]^{1/2} \\ & \times \sum_{M=-J}^{J} \begin{pmatrix} k & J & J \\ q_1+q_2 & M-(q_1+q_2) & -M \end{pmatrix} (-1)^{J+M+q_1} \\ & \times \begin{pmatrix} k_1 & J & J \\ q_1 & M-q_1 & -M \end{pmatrix} \begin{pmatrix} k_2 & J & J \\ q_2 & M-(q_1+q_2) & -M+q_1 \end{pmatrix} \end{aligned} \tag{47b}$$

Proof. Using (33), we obtain an expression for the kq-component in the multipole expansion of $\tau_{k_1q_1}\tau_{k_2q_2}$:

$$(\tau_{k_1q_1}\tau_{k_2q_2})_{kq} = (\tau_{kq} \mid \tau_{k_1q_1}\tau_{k_2q_2})/(2J+1)$$

i.e.,

$$(2J+1)(\tau_{k_1q_1}\tau_{k_2q_2})_{kq} = \mathrm{tr}(\tau_{kq}^{\dagger}\tau_{k_1q_1}\tau_{k_2q_2}) \tag{48}$$

The trace in (48) may be evaluated using (42); to simplify the expressions, let

$$R_k \equiv \langle J \| \tau_k \| J\rangle = [(2J+1)(2k+1)]^{1/2}$$

and (49)

$$\langle M \mid \tau_{kq} \mid M'\rangle \equiv \langle JM \mid \tau_{kq} \mid JM'\rangle$$

Then, (48) becomes

$$\begin{aligned}
&\sum_{MM'M''} \langle M' \mid \tau_{kq}^{\dagger} \mid M\rangle\langle M \mid \tau_{k_1q_1} \mid M''\rangle\langle M'' \mid \tau_{k_2q_2} \mid M'\rangle \\
&= \sum_{MM'} \langle M' \mid \tau_{kq}^{\dagger} \mid M\rangle \sum_{M''} R_{k_1}(-1)^{-J+k_1-M} \begin{pmatrix} J & k_1 & J \\ M'' & q_1 & -M\end{pmatrix} \\
&\quad \times R_{k_2}(-1)^{-J+k_2-M''} \begin{pmatrix} J & k_2 & J \\ M' & q_2 & -M''\end{pmatrix}
\end{aligned} \tag{50}$$

But a 3-j symbol

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{pmatrix}$$

vanishes unless $m_1 + m_2 + m_3 = 0$. Hence, (50) may be written as follows:

$$\begin{aligned}
\mathrm{tr}(\tau_{kq}^{\dagger}\tau_{k_1q_1}\tau_{k_2q_2}) &= \sum_{MM'} \langle M' \mid \tau_{kq}^{\dagger} \mid M\rangle\, R_{k_1}R_{k_2}(-1)^{k_1+k_2-M} \\
&\quad \times \sum_{M''} (-1)^{-M''} \begin{pmatrix} J & k_1 & J \\ M'' & q_1 & -M\end{pmatrix}\begin{pmatrix} J & k_2 & J \\ M' & q_2 & -M''\end{pmatrix} \\
&= \sum_{MM'} \langle M' \mid \tau_{kq}^{\dagger} \mid M\rangle\, R_{k_1}R_{k_2}(-1)^{k_1+k_2+q_1} \\
&\quad \times \begin{pmatrix} J & k_1 & J \\ -q_1+M & q_1 & -M\end{pmatrix}\begin{pmatrix} J & k_2 & J \\ M' & q_2 & -q_2-M'\end{pmatrix} \\
&\quad \times \delta_{q_2+M',-q_1+M}
\end{aligned} \tag{51}$$

The remaining $\tau_{kq}^{\dagger}$ matrix element in (51) may be expressed in terms of a 3-j symbol using (42). The presence of the Kronecker delta makes possible summing over M'. In addition, the following property of 3-j symbols helps eliminate some of the exponents of (-1):

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3\end{pmatrix}$$

Finally, we obtain

$$(\tau_{k_1q_1}\tau_{k_2q_2})_{kq} = E_J(k_1q_1k_2q_2kq) \tag{52}$$

where E_J is defined as in (47b); thus, the theorem is proved. Using Theorem 10, it is possible to derive expressions for commutators and anticommutators in terms of their multipole expansions. Moreover, Theorem 10 is useful in the process (to be exemplified in Part II) of analyzing the multipolar character of operators formed by multiplication of other operators whose multipole components are already known.

5. STATE DETERMINATION: THE QUORUM OF OBSERVABLES

The fundamental mean value equation (1) may be expanded in terms of the multipole components of an observable A and density matrix ρ:

$$\begin{aligned}\langle A\rangle &= \mathrm{tr}(\rho A)\\ &= \sum_{k'q'}\sum_{kq} \rho_{k'q'}A_{kq}\,\mathrm{tr}(\tau_{k'q'}\tau_{kq})\\ &= \sum_{k'q'}\sum_{kq} \rho_{k'q'}A_{kq}(-1)^q\,(2J+1)\,\delta_{k'k}\,\delta_{q,-q'}\\ &= (2J+1)\sum_{kq}\rho_{kq}A_{kq}^{*}\end{aligned} \tag{53}$$

where the relations (25) and (30) have been used.

We next express $\langle A\rangle$ in terms of the $(2k+1)$-vectors introduced in (39), (40), and apply Theorem 8 to obtain

$$\begin{aligned}\langle A\rangle &= (2J+1)\sum_{k=0}^{2J} \boldsymbol{\rho}_k\cdot\mathbf{A}_k{}^{*}\\ &= A_{00} + (2J+1)\sum_{k=1}^{2J} \boldsymbol{\rho}_k\cdot\mathbf{A}_k{}^{*}\end{aligned} \tag{54}$$

Recall that A_{00} is the average of all the eigenvalues of A (Theorem 8a), so that, having decided upon the operator A, A_{00} is known. Thus, the experimental data which give $\langle A\rangle$ also yield the value of $\delta A \equiv \langle A\rangle - A_{00}$; and Eq. (54) can be written

$$\sum_{k=1}^{2J} \boldsymbol{\rho}_k\cdot\mathbf{A}_k{}^{*} = \frac{\delta A}{2J+1} \tag{55}$$

Equation (55) is linear with $N^2 - 1$ unknowns $\{\boldsymbol{\rho}_k \mid k = 1,..., 2J\}$, where $N = 2J + 1$. Thus, a system of $N^2 - 1$ equations like (55) is required in general to determine ρ uniquely. Accordingly, the problem of state determination for a physical system with Hilbert space $\mathscr{H}_N$ is essentially a search for $N^2 - 1$ observables such that the corresponding system of $N^2 - 1$ equations like (55) will be determinate.

Definition 7. A set of $N^2 - 1$ observables $\{A^n \mid n = 1,..., N^2 - 1\}$ whose multipole components $\{\mathbf{A}_k{}^n\}$ are such that the system of linear equations

$$\left\{\sum_{k=1}^{2J} \boldsymbol{\rho}_k \cdot \mathbf{A}_k^{n*} = \frac{\delta A^n}{2J+1} \,\middle|\, n = 1,..., N^2 - 1\right\} \tag{56}$$

possesses a unique solution set $\{\boldsymbol{\rho}_k\}$ will be termed a *quorum* of observables. (Note that n is a label, not an exponent.)

In a previous paper[1] which dealt exclusively with the $J = \frac{1}{2}$ case, we suggested the phrase *minimal set of noncommuting observables* to describe the quorum concept. In that context, the phrase seemed appropriate for contrast with the notion of *complete set of commuting observables* which is sometimes erroneously linked to the problem of state determination. Moreover, in the $J = \frac{1}{2}$ case, noncommutability of $\{A^n\}$ is alone sufficient (and necessary) for determinateness of the system (56), because the determinant of the coefficients in (56) vanishes if any two of the $\{A^n\}$ commute. However, this simple connection between that determinant and the commutability of the $\{A_n\}$ does not generalize to $J > \frac{1}{2}$, because of the complicated 3-j symbols in the expressions for commutators that may be derived using Theorem 10.

The determinant of the coefficients for equations (56) has rows which are $(N^2 - 1)$-plets expressible in terms of the multipole components of A^n; the nth row is

$$\mathbf{A}^n \equiv (\mathbf{A}_1{}^n, \mathbf{A}_2{}^n,..., \mathbf{A}_{2J}^n) \tag{57}$$

i.e., $\mathbf{A}^n$ denotes the $(N^2 - 1)$-plet in (57) and $\boldsymbol{\rho}$ the analog for the unknown density matrix.

The system of equations (56) then becomes

$$\left\{\boldsymbol{\rho} \cdot \mathbf{A}^{n*} = \frac{\delta A^n}{2J+1} \,\middle|\, n = 1,..., N^2 - 1\right\} \tag{58}$$

Now, the determinant of the coefficients for (58) will be nonzero and hence the state ρ may be determined if and only if the set $\{\mathbf{A}^n\}$ is linearly independent (LI). Thus, the problem of state determination—the search for a quorum—centers on the formulation of physically useful criteria enabling selection of an observable set $\{A^n\}$ such that the associated set of $(N^2 - 1)$-dimensional vectors $\{\mathbf{A}^n\}$ is LI.

To develop a systematic procedure, we return to the multipole expansions.

Definition 8. A *purely* 2^l-polar observable is one having only a 2^l-pole component. For example, a purely octupolar observable O would have the form

$$O = \mathbf{O}_3 \cdot \boldsymbol{\tau}_3$$

Theorem 11. If L is a purely 2^l-polar observable, then

$$\boldsymbol{\rho}_l \cdot \mathbf{L}^* = \delta L/(2J + 1) \tag{59}$$

The proof follows immediately from (55) and Definition 8. Moreover, from (57) and Definition 8, we obtain the following theorem.

Theorem 12. If L and M are purely 2^l- and 2^m-polar observables, respectively, then **L** and **M** are perpendicular, provided $l \neq m$.

From Theorem 11, we see that the 2^l-pole component of ρ may be determined from measurements of purely 2^l-polar observables. Specifically, to determine $\boldsymbol{\rho}_l$, we need $(2l + 1)$ purely 2^l-polar observables $\{L^n\}$ such that the associated vectors $\{\mathbf{L}_l{}^n\}$ are LI. Thus, one procedure for constructing a quorum of observables would be to choose three purely dipolar observables $\{D^n\}$ with LI $\{\mathbf{D}_1{}^n\}$, five purely quadrupolar observables $\{Q^n\}$ with LI $\{\mathbf{Q}_2{}^n\}$,..., and $2(2J) + 1$ purely 2^{2J}-polar observables $\{Z^n\}$ with LI $\{\mathbf{Z}_{2J}^n\}$. Recalling that $N = 2J + 1$, this is consistent with our introductory remarks about Eq. (2). Theorem 12 affirms the consistency of this procedure with the remarks following (58). We shall call a quorum consisting entirely of purely 2^l-polar observables a *natural quorum* or *n-quorum*.

A somewhat more flexible procedure for generating a quorum of observables may be developed in terms of a class of observables defined as follows.

Definition 9. An observable G is of *multipolar type l* if and only if

$$G = \sum_{k=0}^{l} \mathbf{G}_k \cdot \boldsymbol{\tau}_k$$

i.e., all multipole components $\mathbf{G}_k = 0$ for $k > l$. (Note that the purely 2^l-polar observable of Definition 8 is a special case of the type l observable of Definition 9.)

A quorum for determining ρ may be formed by choosing three type-1 observables $\{D^n\}$ with LI $\{\mathbf{D}_1{}^n\}$, five type-2 observables $\{Q^n\}$ with LI $\{\mathbf{Q}_2{}^n\}$,..., $(2l + 1)$ type-l observables with LI 2^l-pole components,..., and $2(2J) + 1$ type-$(2J)$ observables $\{Z^n\}$ with LI $\{\mathbf{Z}_{2J}^n\}$. To see in detail why such a set constitutes a quorum, consider the following sequence of operations.

If the quorum just proposed is substituted into (56), we obtain

$$\left\{ \boldsymbol{\rho}_1 \cdot \mathbf{D}_1^{n*} = \frac{\delta D^n}{2J + 1} \,\middle|\, n = 1, 2, 3 \right\} \tag{60a}$$

$$\left\{ \boldsymbol{\rho}_2 \cdot \mathbf{Q}_2^{n*} = \frac{\delta Q^n}{2J + 1} - \boldsymbol{\rho}_1 \cdot \mathbf{Q}_1{}^n \,\middle|\, n = 1,..., 5 \right\} \tag{60b}$$

$$\cdots$$

$$\left\{ \boldsymbol{\rho}_{2J} \cdot \mathbf{Z}_{2J}^{n*} = \frac{\delta Z^n}{2J + 1} - \sum_{k=1}^{2J-1} \boldsymbol{\rho}_k \cdot \mathbf{Z}_k{}^n \,\middle|\, n = 1,..., 2(2J) + 1 \right\} \tag{60c}$$

The system (60a) may be solved for $\boldsymbol{\rho}_1$ since $\{\mathbf{D}_1{}^n\}$ is LI. The right-hand side of (60b) is then known; hence, (60b) may be solved for $\boldsymbol{\rho}_2$. By continuing this pattern, we could find all the $\{\boldsymbol{\rho}_k\}$, hence determine the state ρ.

The foregoing method for state determination may be formally expressed as follows.

Definition 10. A set of observables $\{I^n\}$ is 2^l*-polar-LI* if and only if the 2^l-pole components $\{\mathbf{I}_l{}^n\}$ constitute a linearly independent set.

Theorem 13. Let $\{I^n\}_l$ denote a set of $(2l + 1)$ 2^l-polar-LI type-l observables. Then, the set of such sets

$$\{\{I^n\}_l \mid l = 1,..., 2J\}$$

constitutes a quorum of observables for determining the state ρ of a physical system with Hilbert space $\mathscr{H}_N$, $N = 2J + 1$.

Let $\det\{\{\mathbf{I}^n\}_l\}$ signify the determinant whose rows are the vectors of the kind defined in (57) which are associated with the quorum defined in Theorem 13; similarly, let $\det\{\mathbf{I}_l{}^n\}_l$ denote the subdeterminant whose rows are 2^l-pole components of the $\{I^n\}_l$. Then, from Definitions 9 and 10, it is tedious but straightforward to verify the following theorem, which only validates in another way the quorum of Theorem 13.

Theorem 14. The following holds:

$$\det\{\{\mathbf{I}^n\}_l\} = \prod_{k=1}^{2J} \det\{\mathbf{I}_k{}^n\}_k \neq 0$$

Perhaps the simplest way to assure that $(2l + 1)$ type-l observables are 2^l-polar-LI is to choose type-l observables $\{C^n\}$ such that the $(2l + 1)$ vectors $\{\mathbf{C}_l{}^n\}$ are mutually perpendicular.

Definition 11. A set of observables $\{C^n\}$ is *2^l-polar-Cartesian* if and only if the 2^l-pole components $\{\mathbf{C}^n\}$ constitute a mutually perpendicular set.

Since 2^l-polar-Cartesian is a special case of 2^l-polar-LI, Theorems 12 and 13 apply.

Other quorums could be discovered by seeking decompositions of the determinant of the coefficients different from that given by Theorem 14. We shall henceforth refer to the quorum described in Theorem 13 as a *graduated quorum* or simply g-quorum. Note the n-quorum is a special case of the g-quorum.

Using the concept of 2^l-polar-LI observables, we summarize now our simple method for generating a quorum of observables, and thence determining the quantum state.

(1) Choose three dipolar-LI type-1 observables $\{D^n\}$, obtain $\{\delta D^n\}$ by analyzing data gathered from an ensemble of measurements of the $\{D^n\}$, and solve (60a) for $\boldsymbol{\rho}_1$.

(2) Choose five quadrupolar-LI type-2 observables $\{Q_n\}$, obtain $\{\delta Q^n\}$ from data, and solve (60b) for $\boldsymbol{\rho}_2$.

(3) Continue the procedure until all multipole components of ρ are determined.

The pragmatic value of this state determination procedure depends of course on whether actual empirical measurement procedures can be identified that constitute operational definitions for the 2^l-polar-LI type-l observables constructed abstractly. Specific physical examples which suggest that the g-quorum method here proposed is indeed reasonably efficacious will be presented in the sequel to this paper.

REFERENCES

1. W. Band and J. L. Park, *Found. Phys.* **1**, 133 (1970).
2. U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press, New York, 1959).