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A General Method of Empirical State Determination in Quantum Physics: Part II

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Here, we offer concrete illustrations of the state determination method developed abstractly in Part I of this work. Quorums are found for finite-dimensional magnetic multipole problems as well as for the harmonic oscillator with an energy cutoff. There is, in addition, a discussion of general procedures for empirically distinguishing pure states from mixed states.

6.[1] MATRIX REPRESENTATION OF THE SPECIAL BASIS

To develop specific applications of the multipole expansions in operator space, it is necessary to have available matrix representations of the basic set $\{\tau_k \mid k = 0,..., 2J\}$. The Wigner–Eckart theorem immediately yields one such representation, known in angular momentum problems as the standard or *spherical* representation. Such matrices will of course be equally useful as a mathematical basis even if the index $M = +J,..., -J$, which labels rows and columns, is not interpreted as the magnetic quantum number.

We tabulate below the explicit matrices which represent the τ_{kq}'s for $\mathscr{H}_1$, $\mathscr{H}_2$, $\mathscr{H}_3$, and $\mathscr{H}_4$; the illustrations given below of our state determination method were

[1] The numbering of sections, equations, etc. in the present part of this work continues from where the numbering left off in Part I.[1]

developed using these tables. Calculation of the matrix elements given below is a straightforward arithmetical exercise using (42), (46), and a handbook[2] of 3-j symbols:

$\mathscr{H}_1, J = 0$

$$\{\mathsf{T}_0: \quad \tau_{00} = 1\}$$

$\mathscr{H}_2, J = \frac{1}{2}$

$$\mathsf{T}_0: \quad \left\{\tau_{00} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right\}$$

$$\mathsf{T}_1: \quad \left\{\tau_{1-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \tau_{10} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \tau_{11} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}\right\}$$

$\mathscr{H}_3, J = 1$

$$\mathsf{T}_0: \quad \left\{\tau_{00} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right\}$$

$$\mathsf{T}_1: \quad \left\{\tau_{1-1} = \sqrt{\tfrac{3}{2}}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \tau_{10} = \sqrt{\tfrac{3}{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tau_{11} = \sqrt{\tfrac{3}{2}}\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}\right\}$$

$$\mathsf{T}_2: \quad \left\{\tau_{2-2} = \sqrt{3}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \tau_{2-1} = \sqrt{\tfrac{3}{2}}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix},\right.$$

$$\left.\tau_{20} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tau_{21} = \sqrt{\tfrac{3}{2}}\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \tau_{22} = \sqrt{3}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right\}$$

$\mathscr{H}_4, J = \frac{3}{2}$

$$\mathsf{T}_0: \quad \left\{\tau_{00} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\right\}$$

$$\mathsf{T}_1: \quad \left\{\tau_{1-1} = \frac{2}{\sqrt{5}}\begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{\frac{3}{2}} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 \end{pmatrix}, \quad \tau_{10} = \frac{1}{\sqrt{5}}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix},\right.$$

$$\left.\tau_{11} = \frac{2}{\sqrt{5}}\begin{pmatrix} 0 & -\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & 0 & -\sqrt{2} & 0 \\ 0 & 0 & 0 & -\sqrt{\frac{3}{2}} \\ 0 & 0 & 0 & 0 \end{pmatrix}\right\}$$

$$\mathrm{T}_2: \left\{ \tau_{2-2} = \sqrt{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \tau_{2-1} = \sqrt{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix} \right.$$

$$\tau_{20} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \tau_{21} = \sqrt{2}\begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\left. \tau_{22} = \sqrt{2}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \right\}$$

$$\mathrm{T}_3: \left\{ \tau_{3-3} = 2\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \tau_{3-2} = \sqrt{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \right.$$

$$\tau_{3-1} = \frac{2}{\sqrt{5}}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & -\sqrt{3} & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \tau_{30} = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\tau_{31} = \frac{2}{\sqrt{5}}\begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \tau_{32} = \sqrt{2}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\left. \tau_{33} = 2\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \right\}$$

7. ILLUSTRATION: A *G*-QUORUM FOR A SPIN-1 MAGNETIC DIPOLE

A spin-1 magnetic dipole is characterized by a three-dimensional Hilbert space $\mathscr{H}_3$; among its observables is the magnetic dipole moment $\boldsymbol{\mu}$, an operator proportional to the angular momentum operator $\mathbf{J}$. The well-known matrix representations of $\mathbf{J}$ for $J = 1$ are easily expressed as multipole expansions in terms of our special basis (let $\hbar = 1$):

$$\left[\begin{aligned} J_x &= \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \frac{1}{\sqrt{3}}(\tau_{1-1} - \tau_{11}) \\ J_y &= \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} = \frac{i}{\sqrt{3}}(\tau_{1-1} + \tau_{11}) \\ J_z &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \sqrt{\tfrac{3}{2}}\,\tau_{10} \end{aligned}\right] \tag{61}$$

Since (61) involves only components of ITO τ_1, each one of J_x, J_y, J_z is a purely dipolar observable. The dipole component vectors[2] $\mathbf{J}_{x1}$, $\mathbf{J}_{y1}$, $\mathbf{J}_{z1}$ may be read immediately from (61); the triplets represented by these vectors are given below to within multiplicative constants which are unimportant in checking for linear independence:

$$\left\{\begin{array}{ll} \mathbf{J}_{x1}: & (1, 0, -1) \\ \mathbf{J}_{y1}: & (1, 0, 1) \\ \mathbf{J}_{z1}: & (0, 1, 0) \end{array}\right\} \tag{62}$$

(Throughout this paper, we shall use this system for displaying the relative directions of like multipole components of several observables.)

Obviously, these dipole component-vectors are mutually perpendicular. Hence, J_x, J_y, J_z may be taken as the dipole portion of a g-quorum.

Since $2J = 2$ in the present example, we must also find five quadrupolar-LI type 2 observables. Such observables may be constructed formally by considering Hermitian combinations of the components of the dyadic form $\mathbf{JJ}$. In particular, we have

$$\left\{\begin{array}{rl} J_x^2 &= \frac{2}{3}\tau_{00} + (1/2\sqrt{3})\,\tau_{2-2} - (1/3\sqrt{2})\,\tau_{20} + (1/2\sqrt{3})\,\tau_{22} \\ J_y^2 &= \frac{2}{3}\tau_{00} - (1/2\sqrt{3})\,\tau_{2-2} - (1/3\sqrt{2})\,\tau_{20} - (1/2\sqrt{3})\,\tau_{22} \\ J_xJ_y + J_yJ_x &= (i/\sqrt{3})(\tau_{2-2} - \tau_{22}) \\ J_yJ_z + J_zJ_y &= (i/\sqrt{3})(\tau_{2-1} + \tau_{21}) \\ J_zJ_x + J_xJ_z &= (1/\sqrt{3})(\tau_{2-1} - \tau_{21}) \end{array}\right\} \tag{63}$$

Note that J_x^2 and J_y^2 are of multipolar type 2, while the anticommutators, also of type 2, are purely quadrupolar. To ascertain whether these five operators are the quadrupole portion of a g-quorum, we need the directions of the quadrupolar components, which may be read off (63):

$$\left\{\begin{array}{rl} \mathbf{J}_{x2}^2: & (1, 0, -\sqrt{\tfrac{2}{3}}, 0, 1) \\ \mathbf{J}_{y2}^2: & (1, 0, \sqrt{\tfrac{2}{3}}, 0, 1) \\ (\mathbf{J}_x\mathbf{J}_y + \mathbf{J}_y\mathbf{J}_x)_2: & (1, 0, 0, 0, -1) \\ (\mathbf{J}_y\mathbf{J}_z + \mathbf{J}_z\mathbf{J}_y)_2: & (0, 1, 0, 1, 0) \\ (\mathbf{J}_z\mathbf{J}_x + \mathbf{J}_x\mathbf{J}_z)_2: & (0, 1, 0, -1, 0) \end{array}\right\} \tag{64}$$

It is easily checked that the determinant whose rows are the quintuplets of (63) does not vanish. Hence, J_x^2, J_y^2, and the three anticommutators constitute a set of quadrupolar-LI type 2 observables.

Hence, these eight observables constitute a g-quorum for $\mathscr{H}_3$:

$$\left\{\begin{array}{c} J_x, J_y, J_z \\ J_x^2, J_y^2, (J_xJ_y + J_yJ_x), (J_yJ_z + J_zJ_y), (J_zJ_x + J_xJ_z) \end{array}\right\} \tag{65}$$

To solve (60) for ρ, an ensemble of measurements of each of these eight observables must be performed and the corresponding mean values must be computed

[2] Cf. Definition 6 and Eq. (39) of Part I.

from the resultant data; the observable multipole components to be used in (60) are those displayed in (61) and (63). We have already physically identified J_x, J_y, J_z as angular momentum components. J_x^2 is just a function of J_x; so its mean value may be computed from J_x data. Similarly, it is clear how to find the mean value of J_y^2. The anticommutators are not, however, immediately recognizable as corresponding to any familiar observable.

To interpret the anticommutators, consider the interaction of the magnetic dipole moment $\boldsymbol{\mu}$ with a uniform external magnetic field $\mathbf{B}$. If $\mathbf{B}$ is switched on at the instant (call it $t = 0$) to which the unknown quantum state refers, then the unknown ρ becomes the initial condition for the temporal evolution of the quantum state generated by the Hamiltonian

$$H = -\boldsymbol{\mu} \cdot \mathbf{B} \tag{66a}$$

If $\mathbf{B}$ points in the z direction, then since $\boldsymbol{\mu}$ is proportional to $\mathbf{J}$, the operator structure of H is simply

$$H = gJ_z \tag{66b}$$

where g includes the proportionality constant between $\boldsymbol{\mu}$ and $\mathbf{J}$ as well as the field strength B_z. Similar forms of H describe the interaction of the dipole with fields in the y and z directions.

Suppose ensembles of J_x^2 measurements are performed at $t = 0$ and at short intervals thereafter until sufficient data are gathered to permit computation of

$$(d/dt)\langle J_x^2\rangle|_{t=0}^{z} \tag{67}$$

where the superscript z is a reminder that $\mathbf{B}$ is in the z direction.

But

$$\begin{aligned} d/dt\langle J_x^2\rangle &= \langle dJ_x^2/dt\rangle\langle(1/i)[J_x^2, H]\rangle = \langle(g/i)[J_x^2, J_z]\rangle \\ &= \langle(g/i)\{J_x[J_x, J_z] + [J_x, J_z]\, J_x\}\rangle \\ &= \langle -g(J_xJ_y + J_yJ_x)\rangle = -g\langle J_xJ_y + J_yJ_x\rangle \end{aligned} \tag{68}$$

Hence, measurement of the quantity (67) is tantamount to measurement of the mean value of one of the anticommutators in the g-quorum. Mean values for the remaining anticommutators are similarly calculable from J_y^2 and J_z^2 data yielded by experiments with the $\mathbf{B}$ field in the z and x directions, respectively.

8. GENERALIZATION: QUORUM DEVELOPMENT FOR HIGHER SPIN, HIGHER MAGNETIC MULTIPOLES

The illustration of Section 7 indicates that our strategy for quorum development depends in practice on the physical identification of observables encompassing the entire range of possible multipolar characteristics admissible in the operator space associated with the system of interest. Mathematically, it is always possible to solve higher-spin, higher-multipole problems by a simple extension of the steps given in Section 7 for the spin-1 magnetic dipole. However, due to difficulties in the physical identification of observables we find a different approach more amenable to generalization to any multipole with a 2^L-pole moment.

Imagine that is is in principle possible to measure the interaction energy between a multipole and an external magnetic field of known spherical harmonic structure. Specifically, let the scalar potential of the magnetic field have the form

$$\Phi(r) = R(r)\, Y_{lm}(\theta, \phi) \tag{69}$$

which is to be known in the neighborhood of the multipole. The multipole may be treated as a collection of magnetic poles of strength $+p$ and $-p$ arranged to have only 2^L-pole moment, generated by the coordinate displacement vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_L$. The energy of interaction between such a multipole and the magnetic field is then

$$W_L = [p(-1)^L/L!] \prod_{n=1}^{L} (\mathbf{a}_n \cdot \nabla)\, \Phi(\mathbf{r}) \tag{70}$$

where the gradient operators act only on the variable $\mathbf{r}$ in the function Φ. We may use the gradient formula[3] to write

$$\nabla R(r)\, Y_{lm}(\theta, \phi) = \sum_{\nu} G_{lm\nu} \xi_{\nu} \tag{71}$$

where ξ_ν are the unit vectors in coordinate space on the spherical representation, and

$$\begin{aligned} G_{lm\nu} = & -[(l+1)/(2l+1)]^{1/2} (dR/dr - R/r) \sum_{\nu} \langle l, 1, m-\nu, \nu \mid l+1, m\rangle\, Y_{l+1,m-\nu} \\ & + [l/(2l+1)]^{1/2} (dR/dr + (l+1)\, R/r) \sum_{\nu} \langle l, 1, m-\nu, \nu \mid l-1, m\rangle\, Y_{l-1,m-\nu} \end{aligned} \tag{72}$$

The displacement vectors $\{\mathbf{a}_n\}$ which characterize the multipole system have spherical expansions of the form

$$\mathbf{a}_n = \sum_{\mu} (-1)^{\mu}\, a_{1\mu}^{(n)} \xi_{-\mu} \tag{73}$$

where the a_1's transform like spherical harmonics. Thus, to obtain, for example, the interaction energy for a spin-3/2 octupole ($L = 3$), we need the sequence of operations indicated by

$$\mathbf{a}_1 \cdot \nabla\Phi = \sum_{\mu} (-1)^{\mu}\, a_{1\mu}^{(1)} G_{lm\nu} \xi_{-\mu} \cdot \xi_{\nu} = \sum_{\mu} (-1)^{\mu}\, a_{1\mu}^{(1)} G_{lm-\mu} \tag{74}$$

$$\begin{aligned} \mathbf{a}_2 \cdot \nabla \left(\sum_{\mu} (-1)^{\mu}\, a_{1\mu}^{(1)} G_{lm-\mu} \right) &= \sum_{\mu} (-1)^{\mu}\, a_{1\mu}^{(1)} \mathbf{a}_2 \cdot \nabla G_{lm-\mu} \\ &= \sum_{\mu\nu} (-1)^{\mu+\nu}\, a_{1\mu}^{(1)} a_{1\nu}^{(2)} G'_{lm,-\mu-\nu} \end{aligned} \tag{75}$$

where G' is to be derived from the gradient formula applied to G. The last step to the octupole expression yields

$$\mathbf{a}_3 \cdot \nabla \left(\sum (-1)^{\mu+\nu} a_{1\mu}^{(1)} a_{1\nu}^{(2)} G'_{lm,-\mu-\nu} \right) = \sum (-1)^{\mu+\nu+\sigma} a_{1\mu}^{(1)} a_{1\nu}^{(2)} a_{1\sigma}^{(3)} G''_{lm,-\mu-\nu-\sigma} \tag{76}$$

so that finally we have

$$W_3 = [p(-1)^3/3!] \sum (-1)^{\mu+\nu+\sigma} a_{1\mu}^{(1)} a_{1\nu}^{(2)} a_{1\sigma}^{(3)} G''_{lm,-\mu-\nu-\sigma} \tag{77}$$

Assuming that W_3 can be measured, and that the magnetic field can be manipulated at will so that only specified values of the indices l and m yield nonzero components of Φ, we can regard each $W_3(lm)$ as a distinct energy observable.

In the customary manner, we regard the classical derivation which led to Eq. (77) as adequate motivation to postulate that the quantum system properly called a spin-3/2 magnetic octupole is characterized by $\mathscr{H}_4$ (since $J = 3/2$) and, in an external magnetic field of the type (69), has an energy operator of the form (77) in which the spherical vector components $\{a_{1\mu}^{(n)}\}$ are now interpreted as rank one ITO's on the operator space associated with $\mathscr{H}_4$.

From Theorem 1 of Part I, we note that $a_1^{(n)}$ and τ_1 can differ only by a scalar multiplier. Hence, the energy operator for a spin-3/2 octupole in an external field like (69) has the form

$$W_3(lm) = \sum_{q_1 q_2 q_3} f_{q_1 q_2 q_3}(lm)\, \tau_{1q_1} \tau_{1q_2} \tau_{1q_3} \tag{78}$$

where the f's depend on numbers characterizing the multipole and on the *structure of the external magnetic field.*

Generalizing on this procedure, we conclude that a 2^L-pole quantum system in an external field like (69) has an energy operator of the form

$$W_L(lm) = \sum_{q_1 q_2 \cdots q_L} f_{q_1 q_2 \cdots q_L}(lm) \prod_{q=q_1}^{q_L} \tau_{1q} \tag{79}$$

By successive application of Theorem 10, the product of τ_{1q}'s may be expanded in the form (39) and thus $W_L(lm)$ may be classified according to its multipolar components. Since the f's in (79) are numbers that can be manipulated by altering the field environment (69), we can in principle generate a large class of energy observables having diverse multipole characteristics and from this class select a quorum of observables each of which has already been physically identified as an interaction energy in a known applied field. If fields like (69) should fail to offer sufficient flexibility in manipulating the f's in (70), more general external field structures constructed as series of terms like (69) could be used to obtain still more energy observables belonging to the system for which a quorum is sought.

9. EXTENSION OF THE METHOD TO INFINITE-DIMENSIONAL HILBERT SPACES WITH ONE CUTOFF OBSERVABLE

Let E denote an observable with eigenvalues $\{e_n\}$ and eigenvectors $\{| n\, d_n\rangle | d_n = 1,..., D_n\}$; i.e., $E | n\, d_n\rangle = e_n | n\, d_n\rangle$, and D_n is the degree of degeneracy of e_n.

Definition 12. If a physical system is so prepared that the probability for an E-measurement to yield any eigenvalue not included in some finite subset $\mathscr{C}$ of $\{e_n\}$ is zero, then E will be termed a cutoff observable for that system and preparation.

To avoid cumbersome notation, we assume below that each e_n is nondegenerate, i.e., each $D_n = 1$. This assumption does not affect the basic conclusion to be drawn concerning the structure of the density matrix in the presence of a cutoff observable. We assume further for notational convenience that the $\{e_n\}$ have been relabeled so that

$$\mathscr{C} = \{e_n \mid n = 1, 2,..., N\} \tag{80}$$

If the spectral expansion of the unknown density matrix is given by

$$\rho = \sum_k W_k \mid k\rangle\langle k \mid \tag{81}$$

then the probability that an E-measurement will yield the numerical result e_n is

$$Tr(\rho \mid n\rangle\langle n \mid) = \sum_k W_k \mid \langle n \mid k\rangle|^2 \tag{82}$$

But since E is a cutoff observable, (82) must vanish if e_n is not an element of $\mathscr{C}$; i.e.,

$$\sum_k W_k \mid \langle n \mid k\rangle|^2 = 0, \qquad n > N \tag{83}$$

Because ρ is positive semidefinite, each $W_k \geqslant 0$; hence, the vanishing sum in (83) has every term nonnegative. Thus, (83) can be satisfied if and only if for each k such that $W_k \neq 0$,

$$\langle n \mid k\rangle = 0, \qquad \text{for each} \quad n > N \tag{84}$$

It follows that the matrix elements of ρ in the representation diagonal in E have the property

$$\langle n \mid \rho \mid n'\rangle = \sum_k W_k\langle n \mid k\rangle\langle k \mid n'\rangle = 0 \tag{85}$$

if either e_n or $e_{n'}$ is not included in $\mathscr{C}$.

Thus, if a physical system is known to have a cutoff observable E, then the only part of the density matrix left to be determined is the square submatrix in the E-representation which has row and column indices n, n' satisfying

$$1 \leqslant n,\ n' \leqslant N \tag{86}$$

Geometrically, the situation may be described as follows. Let $\mathscr{H}(\mathscr{C})$ denote the subspace of Hilbert space spanned by $\{| n\rangle \mid n = 1,..., N\}$. The whole space $\mathscr{H}$ is the direct sum of $\mathscr{H}(\mathscr{C})$ and its complement $\mathscr{H}^{\perp}(\mathscr{C})$:

$$\mathscr{H} = \mathscr{H}(\mathscr{C}) \oplus \mathscr{H}^{\perp}(\mathscr{C}) \tag{87}$$

From (84), it follows that every $\mid k\rangle$ actually appearing (i.e., $W_k \neq 0$) in the expansion (81) is orthogonal to $\mathscr{H}^{\perp}(\mathscr{C})$. Hence, because of (87), every $\mid k\rangle$ in (81) is included in $\mathscr{H}(\mathscr{C})$. In short, the presence of a cutoff observable forces ρ to be a sum of projectors into the subspace $\mathscr{H}(\mathscr{C})$.

Let A be an arbitrary observable of a system with an infinite-dimensional Hilbert space and cutoff observable E. In a representation diagonal in E, we have

$$\langle A \rangle = \mathrm{Tr}(\rho A) = \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \langle n \mid \rho \mid n' \rangle \langle n' \mid A \mid n \rangle \tag{88}$$

But, since $\langle n \mid \rho \mid n' \rangle = 0$ if n or n' exceeds N, (88) becomes

$$\langle A \rangle = \sum_{n=1}^{N} \sum_{n'=1}^{N} \langle n \mid \rho \mid n' \rangle \langle n' \mid A \mid n \rangle \tag{89}$$

We summarize the main conclusions as follows:

Theorem 15. The density matrix in a representation diagonal in a cutoff observable E with $\mathscr{C} = \{e_n \mid n = 1, 2,..., N\}$ has nonvanishing elements only in the $N \times N$ submatrix with row and column indices n, n' satisfying $1 \leqslant n, n' \leqslant N$.

Theorem 16. In a representation diagonal in a cutoff observable E with $\mathscr{C} = \{e_n \mid n = 1, 2,..., N\}$, the only matrix elements of an observable A that contribute to the calculation of $\langle A \rangle$ are in the $N \times N$ submatrix A_c with row and column indices n, n' satisfying $1 \leqslant n, n' \leqslant N$.

Theorems 15 and 16 make it possible to treat the state determination problem for a physical system with an infinite-dimensional Hilbert space by using the g-quorum method for $\mathscr{H}_N$, provided the system has been prepared so that it has a cutoff observable. A physical illustration of this procedure is given below.

10. ILLUSTRATION: A *G*-QUORUM FOR A LINEAR HARMONIC OSCILLATOR WITH ENERGY CUTOFF

Consider a linear harmonic oscillator, characterized by the Hamiltonian

$$H = (p^2/2m) + \tfrac{1}{2}m\omega^2 x^2 \tag{90}$$

where position x and momentum p satisfy

$$[x, p] = i\hbar \tag{91}$$

Suppose energy data have revealed that the probability is zero for finding the oscillator with any energy other than one of the three lowest energy levels. Then, H is a cutoff observable with $\mathscr{C} = \{(n + \frac{1}{2})\hbar\omega \mid n = 0, 1, 2\}$. By Theorem 15, the only nonzero elements of the unknown density matrix are $\{\langle n \mid \rho \mid n' \rangle \mid 0 \leqslant n, n' \leqslant 2\}$, where the $\{\mid n \rangle\}$ are eigenvectors of H. Similarly, by Theorem 16, the only matrix elements of an oscillator observable A that will contribute to $\langle A\rangle$ are those in the submatrix A_c whose elements are $\{\langle n \mid A \mid n'\rangle \mid 0 \leqslant n, n' \leqslant 2\}$. Hence, the unknown elements of ρ may be determined if a g-quorum of Hermitian submatrices like A_c can be found.

However, to identify the physical meaning of such a submatrix, it is also necessary to know the whole matrix A of which A_c is a part. Accordingly, we attack the problem by first considering infinite-dimensional matrices whose operational definitions are known, and then extracting the submatrices relevant to the mathematical problem at hand.

In the energy representation, x and p have the following well-known matrices:

$$x = (\hbar/2m\omega)(a^\dagger + a), \qquad p = i(m\hbar\omega/2)(a^\dagger - a) \tag{92}$$

where

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & \\ 0 & 0 & 0 & \sqrt{3} & \\ 0 & 0 & 0 & 0 & \\ & & & & \ddots \end{pmatrix}, \qquad a^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & \sqrt{3} & 0 & \\ & & & & \ddots \end{pmatrix} \tag{93}$$

The submatrices x_c and p_c are easily found and expanded in terms of the special basis for the operator space associated with $\mathscr{H}_3$:

$$\begin{aligned} x_c &= \left(\frac{\hbar}{2m\omega}\right)^{1/2} \begin{pmatrix} 0 & \sqrt{1} & 0 \\ \sqrt{1} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left\{\frac{1+\sqrt{2}}{\sqrt{6}}\,\tau_{1-1} - \frac{1+\sqrt{2}}{\sqrt{6}}\,\tau_{11} + \frac{1-\sqrt{2}}{\sqrt{6}}\,\tau_{2-1} - \frac{1-\sqrt{2}}{\sqrt{6}}\,\tau_{21}\right\} \end{aligned} \tag{94}$$

$$\begin{aligned} p_c &= i\left(\frac{m\hbar\omega}{2}\right)^{1/2} \begin{pmatrix} 0 & -\sqrt{1} & 0 \\ \sqrt{1} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= i\left(\frac{m\hbar\omega}{2}\right)^{1/2} \left\{\frac{1+\sqrt{2}}{\sqrt{6}}\,\tau_{1-1} + \frac{1+\sqrt{2}}{\sqrt{6}}\,\tau_{11} + \frac{1-\sqrt{2}}{\sqrt{6}}\,\tau_{2-1} + \frac{1-\sqrt{2}}{\sqrt{6}}\,\tau_{21}\right\} \end{aligned} \tag{95}$$

Note that both x_c and p_c are of multipolar type 2; the directions of their quadrupolar components are given below in the manner introduced in Section 6:

$$\mathbf{x}_{c2}:\quad (0, 1, 0, -1, 0) \tag{96}$$

$$\mathbf{p}_{c2}:\quad (0, 1, 0, 1, 0) \tag{97}$$

We can similarly analyze other observables until a g-quorum has been constructed. The following observables round out the quadrupole portion of the quorum:

$$(x^2)_c = (\hbar/2m\omega)\begin{pmatrix} 1 & 0 & \sqrt{2} \\ 0 & 3 & 0 \\ \sqrt{2} & 0 & 5 \end{pmatrix}$$

$$= (\hbar/2m\omega)\{3\tau_{00} - 2\sqrt{\tfrac{2}{3}}\,\tau_{10} + \sqrt{\tfrac{2}{3}}\,\tau_{2-2} + \sqrt{\tfrac{2}{3}}\,\tau_{22}\} \tag{98}$$

$$(p^2)_c = (m\hbar\omega/2)\begin{pmatrix} 1 & 0 & -\sqrt{2} \\ 0 & 3 & 0 \\ -\sqrt{2} & 0 & 5 \end{pmatrix}$$

$$= (m\hbar\omega/2)\{3\tau_{00} - 2\sqrt{\tfrac{2}{3}}\,\tau_{10} - \sqrt{\tfrac{2}{3}}\,\tau_{2-2} - \sqrt{\tfrac{2}{3}}\,\tau_{2-2}\} \tag{99}$$

$$(\mathbf{x}^2)_{c2} \quad \text{or} \quad (\mathbf{p}^2)_{c2}: \quad (1, 0, 0, 0, 1) \tag{100}$$

$$(H^2)_c = (\hbar\omega/2)^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 9 & 0 \\ 0 & 0 & 25 \end{pmatrix}$$

$$= (\hbar\omega/2)^2\,(35/3)\,\tau_{00} - 12\sqrt{\tfrac{2}{3}}\,\tau_{10} + (8/3\,\sqrt{2})\,\tau_{20}\} \tag{101}$$

$$(\mathbf{H}^2)_{c2}: \quad (0, 0, 1, 0, 0) \tag{102}$$

$$(xp + px)_c = i\hbar\sqrt{2}\begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$= (i\hbar/m)\sqrt{\tfrac{2}{3}}\,\{\tau_{2-2} - \tau_{22}\} \tag{103}$$

$$(\mathbf{xp} + \mathbf{px})_{c2}: \quad (1, 0, 0, 0, -1) \tag{104}$$

To interpret the operator $xp + px$, we note that

$$i\hbar\frac{dx^2}{dt} = [x^2, H] = \frac{1}{2m}[x^2, p^2] = \frac{i\hbar}{m}(xp + px) \tag{105}$$

Hence,

$$(d/dt)\langle x^2\rangle = (1/m)\langle xp + px\rangle \tag{106}$$

Similarly, it can be demonstrated that

$$d\langle p^2\rangle/dt = -m\omega^2\langle xp + px\rangle \tag{107}$$

Thus, there exist two methods for empirically determining $\langle px + xp\rangle$.

Now, comparison of (96), (97), (100), (102), and (104) immediately shows that the set $\{x_c, p_c, (x^2)_c \text{ or } (p^2)_c, (H^2)_c, (xp + px)_c\}$ consists of five type-2 quadrupolar-Cartesian matrices; hence, we have found the quadrupole portion of a g-quorum.

To complete the quorum, we need three type-1 matrices, which may be chosen as follows. H itself provides one type-1 matrix:

$$H_c = \tfrac{1}{2}\hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$

$$= \tfrac{1}{2}\hbar\omega\{3\tau_{00} - 2\sqrt{\tfrac{2}{3}}\,\tau_{10}\} \tag{108}$$

$$\mathbf{H}_{c1}: \quad (0, 1, 0) \tag{109}$$

Two additional physically identifiable type-1 matrices may be constructed as functions of x and p, respectively. Consider x^3:

$$(x^3)_c = (\hbar/2m\omega)^{3/2} \begin{pmatrix} 0 & 3 & 0 \\ 3 & 0 & 6\sqrt{2} \\ 0 & 6\sqrt{2} & 0 \end{pmatrix}$$

$$= \sqrt{\tfrac{3}{2}}\,(\hbar/2m\omega)^{3/2}\{(1 + 2\sqrt{2})\,\tau_{1-1} - (1 + 2\sqrt{2})\,\tau_{11} + (1 + 2\sqrt{2})\,\tau_{2-1} - (1 - 2\sqrt{2})\,\tau_{21}\} \tag{110}$$

$$(\mathbf{x}^3)_{c1}: \quad (1, 0, -1) \tag{111}$$

$$(\mathbf{x}^3)_{c2}: \quad (0, 1, 0, -1, 0) \tag{112}$$

But from (94), (96), we have

$$\mathbf{x}_{c1}: \quad (1, 0, -1) \tag{113}$$

$$\mathbf{x}_{c2}: \quad (0, 1, 0, -1, 0) \tag{114}$$

Thus, we can find a linear combination $F(x)$ of x and x^3 such that $(F(x))_c$ has no quadrupole component and has dipole direction $(1, 0, -1)$. Such an $F(x)$ is defined by

$$F(x) \equiv (2m\omega/21\hbar)(3 - \sqrt{2})\,x^3 - x \tag{115}$$

$$(\mathbf{F}(\mathbf{x}))_{c1}: \quad (1, 0, -1) \tag{116}$$

Similarly, from

$$(p^3)_c = i(m\hbar\omega/2)^{3/2} \begin{pmatrix} 0 & -3 & 0 \\ 3 & 0 & -6\sqrt{2} \\ 0 & 6\sqrt{2} & 0 \end{pmatrix}$$

$$= i\sqrt{\tfrac{3}{2}}(m\hbar\omega/2)^{3/2}\{(1 + 2\sqrt{2})\,\tau_{1-1} + (1 + 2\sqrt{2})\,\tau_{11} + (1 - 2\sqrt{2})\,\tau_{2-1} + (1 - 2\sqrt{2})\,\tau_{21}\} \tag{117}$$

$$(\mathbf{p}^3)_{c1}: \quad (1, 0, 1) \tag{118}$$

$$(\mathbf{p}^3)_{c2}: \quad (0, 1, 0, 1, 0) \tag{119}$$

and (95), (97), we obtain a function $G(p)$ such that $(G(p))_c$ is type 1 with dipole direction (1, 0, 1):

$$G(p) \equiv (2/21m\hbar\omega)(3 - \sqrt{2})\,p^3 - p \tag{120}$$

$$(\mathbf{G}(\mathbf{p}))_{c1}:\quad (1, 0, 1) \tag{121}$$

Now, comparison of (109), (116), and (121) immediately shows that the set $\{H_c, (F(x))_c, (G(p))_c\}$ consists of three type-1 dipolar-Cartesian matrices; hence, we have the dipole portion of a g-quorum.

A complete g-quorum is therefore

$$\{H_c, F_c, G_c, (H^2)_c, x_c, p_c, (x^2)_c \text{ or } (p^2)_c, (dx^2/dt)_c \text{ or } (dp^2/dt)_c\} \tag{122}$$

where the coefficients to be used in Eq. (60) are displayed respectively in Eqs. (108), (115), (120), (101), (94), (95), (98) or (99), and (103) with (106) or (107).

Speaking in terms of observables instead of submatrices, we may summarize by stating that for a linear harmonic oscillator with energy cutoff at $n = 2$, the following set provides one example of a quorum of observables:

$$\{H, H^2, x, x^2, x^3, p, dx^2/dt, p^2\} \tag{123}$$

Since some elements of (123) are functionally related, it is actually necessary to obtain measurement collectives of data only for $\{H, x, p\}$ at the instant of interest (say $t = 0$) and for x during a time interval in the neighborhood of $t = 0$. Statistical analysis would then provide the eight mean values needed.

11. TRANSFORMATION TO A HERMITIAN BASIS FOR OPERATOR SPACE

The special basis $\{\boldsymbol{\tau}_k\}$ consists of Hermitian tensor operators in the sense of Definition 2, but individual τ_{kq}'s other than τ_{k0}'s are not Hermitian operators. It is, however, possible to form in a systematic fashion $(2k + 1)$ Hermitian operators which span the same subspace as the components of any $\boldsymbol{\tau}_k$.

For example, if we define

$$\begin{pmatrix} \sigma_x \propto (\tau_{1-1} - \tau_{11}) \\ \sigma_y \propto i(\tau_{1-1} + \tau_{11}) \\ \sigma_z \propto \tau_{10} \end{pmatrix} \tag{124}$$

the three operators $\boldsymbol{\sigma}$ are each Hermitian and orthogonal in operator space. Once real proportionality constants are selected for (124), the dipole term in the multipole expansion of an observable A may be written as

$$\begin{aligned} \sum_{q=-1}^{1} A_{1q}\tau_{1q} &= A_x\sigma_x + A_y\sigma_y + A_z\sigma_z \\ &\equiv \mathbf{A} \cdot \boldsymbol{\sigma} \end{aligned} \tag{125}$$

(The 3-vector **A** should not be confused with ($N^2 - 1$)-dimensional complex vector **A** of Section 4.)

Since $\boldsymbol{\sigma}$ has Hermitian components and A is Hermitian, then **A** must be a real vector. If $J = \frac{1}{2}$, the components of $\boldsymbol{\sigma}$ can be chosen to be the Pauli spin matrices, a convention adopted in a previous publication which dealt with state determination for two-dimensional Hilbert spaces.

It is not difficult to continue the "Hermitization" procedure indicated by (113) to higher-rank multipoles; similarly, higher-rank generalizations of (114) generate real coefficients that can be subscripted like rectangular components of higher-rank tensors:

$$\begin{gathered}\sigma_{xx} \propto \tau_{2,-2} + \tau_{2,2}\,, \qquad \sigma_{xy} \propto i(\tau_{2,-2} - \tau_{2,2}), \qquad \sigma_{yz} \propto i(\tau_{2,-1} + \tau_{2,1}), \\ \sigma_{zx} \propto \tau_{2,-1} - \tau_{2,1}\,, \qquad \sigma_{zz} \propto \tau_{2,0}\end{gathered} \tag{126}$$

The following explicit Hermitian basis for $J = 1$ will be used in Section 12 to illustrate the multipolar properties of pure quantum states:

$$1: \quad \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}$$

$$\sigma_\alpha : \quad \left\{ \begin{aligned} &\sigma_x = (1/\sqrt{2}) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \sigma_y = (1/\sqrt{2}) \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \\ &\sigma_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \end{aligned} \right\}$$

$$\sigma_{\alpha\beta} : \quad \left\{ \begin{aligned} &\sigma_{xx} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \sigma_{xy} = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \\ &\sigma_{yz} = (1/\sqrt{2}) \begin{pmatrix} 0 & -i & 0 \\ i & 0 & i \\ 0 & -i & 0 \end{pmatrix}, \quad \sigma_{zx} = (1/\sqrt{2}) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \\ &\sigma_{zz} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{aligned} \right\}$$

In terms of this basis, the density matrix has the form

$$\rho = \tfrac{1}{3}1 + \sum_{\alpha} \rho_\alpha \sigma_\alpha + \sum_{\alpha\beta} \rho_{\alpha\beta} \sigma_{\alpha\beta} \tag{127}$$

where α, β run over x, y, z.

It will also prove useful to associate with ρ two second-rank tensors defined as follows:

$$\boldsymbol{\rho\rho} \equiv \begin{pmatrix} \rho_x^2 & \rho_x\rho_y & \rho_x\rho_z \\ \rho_y\rho_x & \rho_y^2 & \rho_y\rho_z \\ \rho_z\rho_x & \rho_z\rho_y & \rho_z^2 \end{pmatrix} \tag{128}$$

$$\mathsf{S} \equiv \begin{pmatrix} \rho_{xx} - \rho_{zz} & \rho_{xy} & \rho_{zx} \\ \rho_{xy} & -\rho_{xx} - \rho_{zz} & \rho_{yz} \\ \rho_{zx} & \rho_{yz} & 2\rho_{zz} \end{pmatrix} \tag{129}$$

Important properties of $\boldsymbol{\rho\rho}$ and S are given by

$$\mathrm{Tr}\, \boldsymbol{\rho\rho} = \boldsymbol{\rho} \cdot \boldsymbol{\rho} \equiv \rho_x^2 + \rho_y^2 + \rho_z^2 \tag{130}$$

$$\mathrm{Tr}\, \mathsf{S} = 0 \tag{131}$$

and

$$\mathrm{Tr}\, \mathsf{S}^2 = 2[3\rho_{zz}^2 + \rho_{xx}^2 + \rho_{xy}^2 + \rho_{yz}^2 + \rho_{zx}^2] \tag{132}$$

Finally, the specific transformation, induced by the relation between σ's and τ's, from rectangular to spherical multipole components of ρ for $J = 1$ is easily worked out:

$$\left\{\begin{array}{lll} \rho_{1-1} = (1/\sqrt{3})(\rho_x + i\rho_y), & \rho_{10} = \sqrt{\tfrac{2}{3}}\, \rho_z\,, & \rho_{11} = -(1/\sqrt{3})(\rho_x - i\rho_y) \\ \rho_{2-2} = (1/\sqrt{3})(\rho_{xx} + i\rho_{xy}), & \rho_{2-1} = (1/\sqrt{3})(\rho_{zx} + i\rho_{yz}) & \\ \rho_{20} = \sqrt{2}\, \rho_{zz}\,, & \rho_{21} = -(1/\sqrt{3})(\rho_{zx} - i\rho_{yz}), & \rho_{22} = (1/\sqrt{3})(\rho_{xx} - i\rho_{xy}) \end{array}\right\} \tag{133}$$

12. MULTIPOLAR CHARACTERISTICS OF PURE STATES

Once a density matrix has been determined, it may be of interest to know whether the state it represents describes a pure or mixed ensemble. A criterion, involving multipole components of ρ, for testing the statistical purity of the density matrix is given by the following theorem.

Theorem 17. If ρ is the density matrix describing the preparation of a physical system with Hilbert space $\mathscr{H}_N$, then ρ is a pure state if and only if

$$\sum_{k=1}^{2J} \boldsymbol{\rho}_k^* \cdot \boldsymbol{\rho}_k = \frac{2J}{(2J+1)^2}, \quad N = 2J + 1 \tag{134}$$

where

$$\rho = \frac{1}{(2J+1)}\, \boldsymbol{\tau}_0 + \sum_{k=1}^{2J} \boldsymbol{\rho}_k \cdot \boldsymbol{\tau}_k \tag{135}$$

Proof. From (40) or (123), we have

$$\rho = \sum_{k=0}^{2J} \boldsymbol{\rho}_k \cdot \boldsymbol{\tau}_k \tag{136}$$

Hence,

$$\rho^2 = \Big(\sum_k \boldsymbol{\rho}_k \cdot \boldsymbol{\tau}_k\Big)\Big(\sum_l \boldsymbol{\rho}_l \cdot \boldsymbol{\tau}_l\Big)$$

$$= \sum_{k=0}^{2J} \sum_{l=0}^{2J} \sum_{q=-k}^{k} \sum_{r=-l}^{l} \rho_{kq}\rho_{lr}\tau_{kq}\tau_{lr} \tag{137}$$

By a familiar theorem in quantum mechanics, ρ is a pure state if and only if

$$\operatorname{Tr} \rho^2 = 1 \tag{138}$$

(For a mixture, $\operatorname{Tr} \rho^2 < 1$.)

Substituting (137) into (138) and using (30), we get

$$\operatorname{Tr} \rho^2 = \sum_{klqr} \rho_{kq}\rho_{lr} \operatorname{Tr}(\tau_{kq}\tau_{lr}) = \sum_{klqr} \rho_{kq}\rho_{lr}(-1)^q (\tau_{k-q} \mid \tau_{lr})$$

$$= \sum_{klqr} \rho_{kq}\rho_{lr}(-1)^q \delta_{kl}\, \delta_{q,-r}(2J+1) = (2J+1) \sum_{k=0}^{2J} \sum_{q=-k}^{k} \rho_{kq}^{*}\rho_{kq} = 1 \tag{139}$$

Thus, ρ is pure if and only if

$$\sum_{k=0}^{2J} \boldsymbol{\rho}_k{}^* \cdot \boldsymbol{\rho}_k = 1/(2J+1) \tag{140}$$

But by Theorem 8b, $\boldsymbol{\rho}_0 = 1/(2J+1)$; so (140) becomes

$$\frac{1}{2J+1}\,\frac{1}{2J+1} + \sum_{k=1}^{2J} \boldsymbol{\rho}_k{}^* \cdot \boldsymbol{\rho}_k = \frac{1}{2J+1}$$

or

$$\sum_{k=1}^{2J} \boldsymbol{\rho}_k{}^* \cdot \boldsymbol{\rho}_k = \frac{2J}{(2J+1)^2}$$

which completes the proof.

In addition to Hermiticity and normalization, a further property required of the density matrix is positive-semidefiniteness (nonnegative eigenvalues). To see how this constraint is expressed in terms of the multipole components of ρ, consider a representation in which ρ is a diagonal matrix with eigenvalues

$$\{W_M \mid M = 2J, 2J-1, \ldots, -2J\}.$$

From (42) and Theorem 9, we have

$$\langle JM \mid \tau_{kq} \mid JM' \rangle = [(2J+1)(2k+1)]^{1/2} (-1)^{-J+k-M} \begin{pmatrix} J & k & J \\ M' & q & -M \end{pmatrix} \tag{141}$$

To expand the diagonal ρ, we need only those τ's with some diagonal elements

$\langle JM \mid \tau_{kq} | JM \rangle \neq 0$. If $M = M'$, the 3-j symbol in (141) vanishes unless $q = 0$. Thus, for a diagonal ρ, we have

$$\rho = \sum_{k=1}^{2J} \rho_{k0} \tau_{k0} \tag{142}$$

Now,

$$W_M = \mathrm{Tr}(\rho \mid JM \rangle\langle JM \mid) = \sum_{k=0}^{2J} \rho_{k0} \langle JM \mid \tau_{k0} \mid JM \rangle$$

Substituting (141), we obtain

$$W_M = (2J+1)^{1/2} (-1)^{J+M} \sum_{k=0}^{2J} (-1)^k (2k+1)^{1/2} \rho_{k0} \begin{pmatrix} k & J & J \\ 0 & -M & M \end{pmatrix} \tag{143}$$

There are $(2J+1)$ linear equations like (143) which uniquely determine the $(2J+1)$ numbers $\{\rho_{k0}\}$; i.e., each ρ_{k0} is a function of the $\{W_M\}$.

Consider $\boldsymbol{\rho}_k{}^* \cdot \boldsymbol{\rho}_k$ in the present representation:

$$\boldsymbol{\rho}_k{}^* \cdot \boldsymbol{\rho}_k = \rho_{k0}^2 = [\rho_{k0}(\{W_M\})]^2 \tag{144}$$

The positive-definiteness and normalization of ρ require that

$$0 \leqslant W_M \leqslant 1 \tag{145}$$

In light of (145), we conclude that $[\rho_{k0}(\{W_M\})]^2$ must have an absolute maximum B_k and absolute minimum b_k; hence, the positive-definiteness of ρ will generally be expressed by constraints of the form

$$b_k \leqslant \boldsymbol{\rho}_k{}^* \cdot \boldsymbol{\rho}_k \leqslant B_k \tag{146}$$

(It can be shown that (146) is independent of the representation chosen for ρ since all representations are related unitarily.)

To illustrate (134), consider again the case $J = 1$. The condition (134) for ρ to be pure is then

$$\boldsymbol{\rho}_1{}^* \cdot \boldsymbol{\rho}_1 + \boldsymbol{\rho}_2{}^* \cdot \boldsymbol{\rho}_2 = \tfrac{2}{9} \tag{147}$$

Using (133), we transform (147) to rectangular form to obtain

$$\tfrac{2}{3}(\rho_x{}^2 + \rho_y{}^2 + \rho_z{}^2) + \tfrac{1}{3}[2(3\rho_{zz}^2 + \rho_{xx}^2 + \rho_{xy}^2 + \rho_{yz}^2 + \rho_{zx}^2)] = \tfrac{2}{9} \tag{148}$$

In terms of the 3×3 tensors $\boldsymbol{\rho\rho}$ and S defined in (128) and (129), (148) becomes, after using (130) and (132),

$$\tfrac{2}{3}\,\mathrm{Tr}\,\boldsymbol{\rho\rho} + \tfrac{1}{3}\,\mathrm{Tr}\,\mathsf{S}^2 = \tfrac{2}{9}$$

or

$$2\,\mathrm{Tr}\,\boldsymbol{\rho\rho} + \mathrm{Tr}\,\mathsf{S}^2 = \tfrac{2}{3} \tag{149}$$

To illustrate (146) for this same example, consider a representation in which $\boldsymbol{\rho}$ is diagonal with eigenvalues $\{W_n \mid n = 1, 2, 3\}$, where each W_n satisfies $0 \leqslant W_n \leqslant 1$.

Using the matrix representations of the $\{\tau_k\}$ given in Section 6, we readily find that

$$\rho = \begin{pmatrix} W_1 & 0 & 0 \\ 0 & W_2 & 0 \\ 0 & 0 & W_3 \end{pmatrix} = \tfrac{1}{3}\tau_{00} + (1/\sqrt{6})(W_1 - W_3)\,\tau_{10} + (1/\sqrt{2})(\tfrac{1}{3} - W_2)\,\tau_{20} \quad (150)$$

Hence,

$$\boldsymbol{\rho}_1{}^* \cdot \boldsymbol{\rho}_1 = \rho_{10}^2 = \tfrac{1}{6}(W_1 - W_3)^2 \quad (151)$$

Since $0 \leqslant W_n \leqslant 1$, it follows that

$$0 \leqslant \boldsymbol{\rho}_1{}^* \cdot \boldsymbol{\rho}_1 \leqslant \tfrac{1}{6} \quad (152)$$

Similarly, from (150), we find that

$$\boldsymbol{\rho}_2{}^* \cdot \boldsymbol{\rho}_2 = \tfrac{1}{2}(\tfrac{1}{3} - W_2)^2 \quad (153)$$

Thus,

$$0 \leqslant \boldsymbol{\rho}_2 \cdot \boldsymbol{\rho}_2 \leqslant \tfrac{2}{9} \quad (154)$$

Transforming (152) and (154) to rectangular form, we get

$$0 \leqslant \mathrm{Tr}\, \boldsymbol{\rho}\boldsymbol{\rho} \leqslant \tfrac{1}{4} \quad (155)$$

$$0 \leqslant \mathrm{Tr}\, \mathsf{S}^2 \leqslant \tfrac{2}{3} \quad (156)$$

Finally, the condition (149) for pure states together with inequalities (155) and (156) imply the following interesting restriction on the tensor S when ρ is pure:

$$\tfrac{1}{6} \leqslant \mathrm{Tr}\, \mathsf{S}^2 \leqslant \tfrac{2}{3} \quad (157)$$

Similar rectangular forms of the general test for pure states given by Theorem 17 could be developed for higher values of J.

13. SUMMARY

In Part I, we have developed the multipole algebra for classifying observables in such a way as to facilitate the search for a quorum of observables needed to determine the density matrix characterizing an ensemble prepared in some specified manner.

In Part II, we described several examples in which the quorum of observables can be stated explicitly, and in addition, discussed general criteria for empirically distinguishing pure and mixed ensembles. However, there is a sense in which our theory of empirical state determination is still incomplete. We have regarded quorum observables as "physically identified" whenever they could be related to such familiar, classically motivated quantal concepts as position or energy. Yet, in actuality, such constructs are, in the quantum physics of microsystems, quite remote from direct experience, the connection being only through complex operational definitions which are notably indirect.

Thus, in Section 7, if the spin-1 magnetic dipole were an atomic object, the direct measurement of the angular momentum would not in fact be possible. And in Section 10, if the harmonic oscillator were an atomic system, the direct measurement of position, or of momentum, at any given time, would be a purely "gedanken" operation, not an actual laboratory procedure.

We believe that it should be possible to carry out our program for atomic objects where measurements must be made via suitable probing devices—in particular the interaction with radiation. Perhaps a hint of this can be seen in our discussion of the spin-$\frac{3}{2}$ magnetic octupole in Section 8, but the full development of this idea is reserved for a future paper.

REFERENCES

1. James L. Park and William Band, *Found. Phys.* **1** (3), 211 (1971).
2. M. Rotenberg, R. Bivins, N. Metropolis, and J. K. Wooten, Jr., *The 3-j and 6-J Symbols* (The Technology Press, Massachusetts Institute of Technology, Cambridge, 1959).
3. M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, New York, 1957), p. 124.