Relations among elements of the density matrix. I. Definiteness inequalities

William Band and James L. Park*

Washington State University, Pullman, Washington 99163
(Received 6 June 1972; revised manuscript received 16 November 1972)

The statistical operator of quantum theory may be determined empirically by computations based upon the measured mean values of a set of observables we have called a quorum. The requirement that a statistical operator be positive semidefinite is then used to generate a family of inequalities connecting these quorum means. Like the simpler uncertainty relations, these inequalities are universal, valid for all quantum states. In the special case of pure states, the method yields a family of equalities.

1. THE QUORUM CONCEPT

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

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

where A is the Hermitian operator for an observable of interest and $\langle A \rangle$ denotes the arithmetic mean of data for that observable gathered from an ensemble of systems each prepared in the manner Π. Recently we have explored[1,2,3] the problem of empirical state determination, formulated as follows: given Π and the means to measure any A, how much data is needed in order to determine the unknown ρ? This problem has been attacked in the past by several authors, including Feenberg,[4] Kemble,[5] and Gale, Guth, and Trammell.[6]

For an N-dimensional Hilbert space, any matrix representation of relation (1) contains $N^2 - 1$ independent real unknowns in the statistical matrix ρ (also commonly called the density matrix). This is a consequence of the Hermiticity of ρ and of its unit trace. The unknowns occur linearly; hence, if $N^2 - 1$ observables $\{A\}$ are chosen so that the associated $N^2 - 1$ linear algebraic equations like (1) possess a unique solution set, then the elements of the ρ matrix may be determined in terms of the $N^2 - 1$ mean values $\{\langle A \rangle\}$ by standard methods for solving linear systems of equations.

We have elsewhere called a set of observables $\{A\}$ whose mean values $\{\langle A \rangle\}$ constitute sufficient information to deduce the statistical operator ρ a *quorum* of observables.

In the present paper it is sufficient to acknowledge simply that such quorums exist, that the statistical operator ρ may be expressed as a function of quorum means $\{\langle A \rangle\}$. It will be demonstrated below that such representations of ρ, when considered in the light of an old theorem in matrix algebra, permit us to generate families of quantal inequalities reminiscent of, but more elaborate than, the uncertainty relations. In the sequel (Paper II) we shall investigate a new class of conserved quantities which are revealed by the study of quorums.

The present authors have developed systematic procedures for the construction of quorums for physical systems with N-dimensional Hilbert spaces and, under certain circumstances, for systems with infinite-dimensional Hilbert spaces.

Directly verifiable illustrations of density matrices as functions of quorum means will be given below; the reader interested in the philosophical and mathematical origins of the quorum theory is referred to the literature cited earlier.

2. DEFINITENESS OF THE STATISTICAL MATRIX

Three independent defining properties are customarily attributed to the statistical operator:

(i) hermiticity,

(ii) unit trace,

(iii) positive semidefiniteness.

Characteristics (i) and (ii) have already been incorporated into the quorum theory; every matrix representation of ρ which satisfies (1) and whose elements are functions of quorum means will automatically be Hermitian, and of trace unity.

Property (iii) may be derived[7] from the consistency condition that a dichotomic observable, represented by a projector $|\phi\rangle\langle\phi|$ onto a Hilbert vector ϕ, must have a nonnegative mean value since the eigenvalues of the projector are 0 and 1. Thus,

$$\mathrm{Tr}(\rho\,|\phi\rangle\langle\phi|) = \langle\phi|\rho|\phi\rangle \geq 0. \tag{2}$$

But ϕ is arbitrary; hence by definition ρ is positive semidefinite, or nonnegative definite.

It follows that the quorum means of which statistical-matrix elements are functions must be interrelated in such a manner that the statistical matrix will be nonnegative definite. Such a connection among the quorum observables is established by application of the old algebraic theorem[8] which states that all principal minor determinants of a nonnegative definite matrix must be nonnegative.

To be explicit, consider an $N \times N$ statistical matrix ρ with (k, l) element ρ_{kl}. An n-dimensional principal minor matrix is obtained by striking out $N - n$ rows and their *corresponding* columns; thus, the common element of each struck row-column pair will be in the principal diagonal of ρ. The standard proof that the determinants of these minor matrices are all nonnegative is based on the Hermiticity of the quadratic form (2) and on the invariance of determinants under similarity transformations.

Since each ρ_{kl} is a function of quorum means $\{\langle A \rangle\}$, the nonnegativity of principal minor determinants is ultimately expressible as a family of inequalities involving the quorum means. Like the celebrated uncertainty relations, these *definiteness inequalities* are valid for all preparations of state.

The family of definiteness inequalities becomes a family of equalities for $n > 1$ whenever the preparation is pure. For a pure state, ρ is a projector $|\psi\rangle\langle\psi|$; in terms of matrix elements,

$$\rho_{kl} = \psi_k \psi_l^*. \tag{3}$$

A typical minor determinant of a pure statistical matrix will therefore have the form

$$e^{b_1 b_2 \cdots b_n} (\psi_{a_1}\psi_{b_1}^*)(\psi_{a_2}\psi_{b_2}^*) \cdots (\psi_{a_n}\psi_{b_n}^*) = (\psi_{a_1}\psi_{a_2} \ldots \psi_{a_n})\, e^{b_1 b_2 \cdots b_n}\, \psi_{b_1}^* \psi_{b_2}^* \cdots \psi_{b_n}^*. \tag{4}$$

Since the e-system is totally skew-symmetric and $\psi_{b_1}^*\psi_{b_2}^* \cdots \psi_{b_n}^*$ is completely symmetric, the minor determinant vanishes, provided $n > 1$. Hence for a pure statistical matrix all principal minor determinants with $n > 1$ vanish; we can therefore generate a family of definiteness *equalities* relating the various quorum means in any *pure* state.

3. ILLUSTRATIONS

Several expressions are given below for matrix elements of the statistical operator expressed as functions of quorum means. As noted above, the procedures[9] used to discover quorum observables will not be reproduced here, nor will the straightforward but sometimes lengthy algebra by which the matrix elements are obtained from systems of linear equations. There is, however, no need for the reader to accept the matrix elements on faith; their validity may be checked directly by using (1).

A. Spin-½ system

Quorum: $\sigma_x, \sigma_y, \sigma_z$ (standard Pauli matrices).

Statistical matrix:

$$(\rho) = \tfrac{1}{2}\begin{pmatrix} 1 + \langle\sigma_z\rangle & \langle\sigma_x\rangle - i\langle\sigma_y\rangle \\ \langle\sigma_x\rangle + i\langle\sigma_y\rangle & 1 - \langle\sigma_z\rangle \end{pmatrix}. \tag{5}$$

Definiteness inequalities:

(1) One-dimensional minors:

$$1 + \langle\sigma_z\rangle \geq 0, \qquad 1 - \langle\sigma_z\rangle \geq 0. \tag{6}$$

The relations (6), involving only one component of the polarization vector $\langle\boldsymbol{\sigma}\rangle$, are uninteresting since they convey no information not already obvious from the spectrum $\{-1, +1\}$ of σ_z.

(2) Two-dimensional minor (detρ):

$$\tfrac{1}{4}(1 - \langle\sigma_z\rangle^2 - \langle\sigma_x\rangle^2 - \langle\sigma_y\rangle^2) \geq 0 \quad \text{or} \quad \langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 \leq 1. \tag{7}$$

Pure state definiteness equality:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1. \tag{8}$$

By subtracting (8) from the familiar equation

$$\langle\sigma_x^2\rangle + \langle\sigma_y^2\rangle + \langle\sigma_z^2\rangle = 3, \tag{9}$$

we obtain the following relation among uncertainties for any pure spin-$\frac{1}{2}$ state:

$$(\Delta\sigma_x)^2 + (\Delta\sigma_y)^2 + (\Delta\sigma_z)^2 = 2. \tag{10}$$

B. Spin-½ system (alternative quorum)

Quorum: P_x, P_y, P_z, where P_k denotes the projector onto the σ_k-eigenvector belonging to eigenvalue + 1, etc. $\langle P_k\rangle$ is the probability that a σ_k-measurement will yield + 1.

Statistical matrix:

$$(\rho) = \begin{pmatrix} \langle P_z\rangle & (\langle P_x\rangle - \frac{1}{2}) - i(\langle P_y\rangle - \frac{1}{2}) \\ (\langle P_x\rangle - \frac{1}{2}) + i(\langle P_y\rangle - \frac{1}{2}) & 1 - \langle P_z\rangle \end{pmatrix}. \tag{11}$$

Definiteness inequalities:

(1) One-dimensional minors:

$$0 \leq \langle P_z\rangle \leq 1. \tag{12}$$

(2) Two-dimensional minor (detρ):

$$(\langle P_x\rangle + \langle P_y\rangle + \langle P_z\rangle) - (\langle P_x\rangle^2 + \langle P_y\rangle^2 + \langle P_z\rangle^2 \geq \tfrac{1}{2}. \tag{13}$$

C. Harmonic oscillator with 2-level energy cutoff

Quorum theory is readily applicable to systems with infinite-dimensional Hilbert spaces whenever it is known that the state preparation Π has this property: there is an observable C (the cutoff observable[10]) whose probability distribution vanishes except for a finite number n of C-eigenvalues. Thus in a representation diagonal in C the (infinite) statistical matrix will have only n nonzero diagonal elements. From the inequality[11]

$$|\rho_{kl}| \leq (\rho_{kk}\rho_{ll})^{1/2} \tag{14}$$

valid for any positive semidefinite ρ, it then follows that all elements of the statistical matrix vanish except for an $n \times n$ submatrix.

In the present example, the cutoff observable is energy H and $n = 2$; specifically, only the two lowest energy levels have nonzero probability.

Quorum: x (position), p (momentum),

$$H = (p^2/2m) + (m\omega^2/2)x^2.$$

Statistical matrix:

Let ρ_c denote the 2×2 nonzero submatrix of ρ. Then

$$\rho_c = \tfrac{1}{2}\begin{pmatrix} 3 - \langle K\rangle & \langle X\rangle - i\langle P\rangle \\ \langle X\rangle + i\langle P\rangle & -1 + \langle K\rangle \end{pmatrix}, \tag{15}$$

where

$$K \equiv (2/\hbar\omega)H, \qquad X \equiv (2m\omega/\hbar)^{1/2}x, \qquad P \equiv (2/m\hbar\omega)^{1/2}p. \tag{16}$$

Definiteness inequalities:

(1) One-dimensional minors:

$$1 \leq \langle K\rangle \leq 3 \quad \text{or} \quad \hbar\omega/2 \leq \langle H\rangle \leq 3\hbar\omega/2. \tag{17}$$

Relation (17) is expected for a harmonic oscillator certain to yield upon energy measurement one of its two lowest eigenvalues.

(2) Two-dimensional minor:

$$\mathcal{E}(\langle x\rangle, \langle p\rangle) \leq 2\langle H\rangle - (\hbar\omega)^{-1}\langle H\rangle^2 - (3/4)\hbar\omega \tag{18}$$

where

$$\mathcal{E}(\langle x\rangle, \langle p\rangle) \equiv (\langle p\rangle^2/2m) + (m\omega^2/2)\langle x\rangle^2.$$

The expression (18) is of interest in connection with the classical limit problem since $\mathcal{E}$ is the classical energy function with quantal means $\langle x\rangle$ and $\langle p\rangle$ as arguments; thus, (18) reflects a basic disparity between classical and quantal energy concepts. We intend to investigate the quorum theory approach to the classical limit problem in another publication.

The foregoing illustrations in a two-dimensional Hilbert space yielded several inequalities derivable also from the well known relation

$$\mathrm{Tr}\rho^2 \leq 1. \qquad (19)$$

However, in higher dimensional spaces a matrix of unit trace may satisfy this inequality and yet fail to be nonnegative definite. Thus our approach will in general produce additional inequalities which are not derivable from (19).

D. Spin-1 system

Quorum: J_x, J_y, J_z (angular momentum components), J_x^2, J_y^2, J_{xy}, J_{zx}, where $J_{ab} \equiv J_a J_b + J_b J_a$. A discussion concerning measurement of quorum members J_{ab} is given in Ref. 3.

Statistical matrix (representation diagonal in J_z; $\hbar = 1$):

$$(\rho) = \begin{pmatrix} 1 + \frac{1}{2}(\langle J_z\rangle - \langle J_x^2\rangle - \langle J_y^2\rangle) & (1/2\sqrt{2})[\langle J_x\rangle + \langle J_{zx}\rangle - i(\langle J_y\rangle + \langle J_{yz}\rangle)] & \frac{1}{2}(\langle J_x^2\rangle - \langle J_y^2\rangle - i\langle J_{xy}\rangle) \\ (1/2\sqrt{2})[\langle J_x\rangle + \langle J_{zx}\rangle + i(\langle J_y\rangle + \langle J_{yz}\rangle)] & -1 + \langle J_x^2\rangle + \langle J_y^2\rangle & (1/2\sqrt{2})[\langle J_x\rangle - \langle J_{zx}\rangle - i(\langle J_y\rangle - \langle J_{yz}\rangle)] \\ \frac{1}{2}(\langle J_x^2\rangle - \langle J_y^2\rangle + i\langle J_{xy}\rangle) & (1/2\sqrt{2})[\langle J_x\rangle - \langle J_{zx}\rangle + i(\langle J_y\rangle - \langle J_{yz}\rangle)] & 1 - \frac{1}{2}(\langle J_z\rangle + \langle J_y^2\rangle + \langle J_x^2\rangle) \end{pmatrix}. \qquad (20)$$

Definiteness inequalities:

(1) One-dimensional minors: Consider for instance the (2, 2) element, which yields

$$\langle J_x^2\rangle + \langle J_y^2\rangle \geq 1. \qquad (21)$$

This is expected, since for spin-1 we know that

$$\langle J_x^2\rangle + \langle J_y^2\rangle + \langle J_z^2\rangle = 2 \qquad (22)$$

and

$$\langle J_z^2\rangle \leq 1 \qquad (23)$$

(2) Two-dimensional minors: At this level the method begins to reveal complicated new relationships among the quorum observables that are not anticipated intuitively. As an example, we compute the upper left minor determinant of (20).

$$[1 + \tfrac{1}{2}(\langle J_z\rangle - \langle J_x^2\rangle - \langle J_y^2\rangle)][-1 + \langle J_x^2\rangle + \langle J_y^2\rangle] - \tfrac{1}{8}[(\langle J_x\rangle + \langle J_{zx}\rangle)^2 + (\langle J_y\rangle + \langle J_{yz}\rangle)^2] \geq 0. \qquad (24)$$

The first term in (24) may be simplified by applying (22) to obtain

$$\tfrac{1}{2}(\langle J_z\rangle + \langle J_z^2\rangle)(1 - \langle J_z^2\rangle) - \tfrac{1}{8}[(\langle J_x\rangle + \langle J_{zx}\rangle)^2 + (\langle J_y\rangle + \langle J_{yz}\rangle)^2] \geq 0. \qquad (25)$$

The expression (25) typifies the complex interconnections among the means of quantal observables that may be discovered by generating definiteness inequalities. Moreover, the equality case of (25) is illustrative of the definiteness equalities which link quorum means for systems prepared in pure quantum states.

*Work supported by Research Corporation.

[1]W. Band and J. L. Park, Found. Phys. 1, 133 (1970).
[2]J. L. Park and W. Band, Found. Phys. 1, 211 (1971).
[3]W. Band and J. L. Park, Found. Phys. 1, 339 (1971).
[4]E. Feenberg [thesis (Harvard University, 1933)] considered one-dimensional wave mechanics only and assumed in effect that ρ was known in advance to be a projector onto a ray ψ (wavefunction), the problem being to determine ψ.
[5]E. C. Kemble in *Fundamental Principles of Quantum Mechanics* (McGraw-Hill, New York, 1937), p. 71, attempted to extend Feenberg's work (Ref. 4) to multidimensional wave mechanics.
[6]W. Gale, E. Guth, and G. T. Trammell in Phys. Rev. 165, 1434 (1968) corrected an error in Kemble (Ref. 5) and developed an approach extensible to general density matrices.
[7]J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, transl. by R. T. Beyer (Princeton U. P., Princeton, N.J., 1955), p. 317.
[8]F. Hohn, *Elementary Matrix Algebra* (Macmillan, New York, 1964), 2nd ed., p. 353.
[9]Refs. 2, 3.
[10]Ref. 3.
[11]Ref. 7, p. 101.