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Geometrical description of quantal state determination

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Abstract. Under the assumption that every quantal measurement may give data about the post-measurement state of the inspected ensemble, the problem of the state determination is reconsidered. It is shown that orthogonal decomposition of the set of complex, $n\times n$, Hermitian matrices into the commutative subsets allows operators to be found such that post-measurement information on these observables allows a partial (in some cases total) determination of the pre-measurement state to be effected.

1. Introduction

In the ordinary formalism of quantum mechanics the state of a quantum ensemble is described by a statistical operator W. In complex n-dimensional space C^n, W is a complex $n\times n$ Hermitian matrix characterised by $W\geqslant 0$ and $\mathrm{Tr}(W)=1$. The mean value of some observable A is given by $\langle A\rangle=\mathrm{Tr}(AW)$.

If W is some unknown state, it may be determined using n^2 mean values $\langle A^{(k)}\rangle$ obtained from measurements, if the set $\{A^{(k)}\}$ is a basis in the space of all complex Hermitian $n\times n$ matrices, $V_{\mathrm{h}}(C^n)$. The case of the complete determination was solved by Fano (1957) and later by Park and Band (1971). The case of incomplete determination was solved by Wichmann (1963).

In this note we shall consider the case that occurs when measurement of an observable $A=\Sigma\, a_kP_k$, besides the mean value $\langle A\rangle=\Sigma\, w_ka_k$, gives the probability distribution $\{w_k\}$ or, equivalently, if it gives $\langle A\rangle, \langle A^2\rangle, \ldots, \langle A^{n-1}\rangle$ in the case that A is a non-degenerate observable. This means that $n-1$ observables A^k are measured by the same measurement procedure. A necessary condition is that the number of elements in the ensemble must be very large. The spin measurement by means of a Stern–Gerlach type procedure belongs to this class.

Accepting this possibility, every complete measurement (measurement of an observable with non-degenerate spectrum) will give n mean values $\langle P_k\rangle=\mathrm{Tr}(WP_k)=w_k$, $k=1,\ldots,n$, where P_k are eigen-projectors of the measured observable.

The set $\{P_k\}$ is a complete, orthogonal set of one-dimensional projectors (CPS). It will be shown that different CPS $\{P_k\}, \{Q_j\}, \ldots$ can be found that possess the property

$$\mathrm{Tr}(P_kQ_j)=1/n.$$

When these CPS are associated with observables subject to measurement as described above, we shall demonstrate the possibility of partially (in some cases totally) reconstructing the pre-measurement state from the measurement data. The assumption that every Hermitian operator corresponds to some observable (Swift and Wright 1980) is adopted in this note.

2. States and measurements

Following the usual description (Wichmann 1963, Bloore 1976, Harriman 1978), the set of all W, $W(C^n)$, is a subset of $V_h(C^n)$. Over the field of real numbers $V_h(C^n)$ is an n^2-dimensional real Euclidean space with scalar product $(A, B) = \mathrm{Tr}(AB)$, for $A, B \in V_h(C^n)$, and norm $\|A\| = (\mathrm{Tr}\, A^2)^{1/2}$. $W(C^n)$ is a convex set, having one-dimensional projectors as the extremal points and boundary points W with $\det W = 0$.

The non-selective, complete measurement of the observable $A = \Sigma_{k=1}^{n} a_k P_k^{(A)}$ will change the pre-measurement state $W = \Sigma_k w_k P_k^{(W)}$ into

$$W^{(A)} = \boldsymbol{M}(A)\,W = \boldsymbol{M}(\{P_k^{(A)}\})\,W = \sum_{k=1}^{n} P_k^{(A)} W P_k^{(A)} = \sum_{k=1}^{n} w_k^{(A)} P_k^{(A)}, \tag{1}$$

where $\boldsymbol{M}(P_k)A = P_k A P_k$ is a projector in $V_h(C^n)$ (projecting on P_k) and $\boldsymbol{M}(\{P_k\}) = \Sigma\, \boldsymbol{M}(P_k)$ is a projector into the subspace $V(\{P_k\}) \in V_h(C^n)$. In the case of (1) $W^{(A)} \in V(\{P_k^{(A)}\})$ and $V(\{P_k^{(A)}\})$ is a subspace spanned by $\{P_k^{(A)}\}$. $\dim[V(\{P_k^{(A)}\})] = n$ because $\{P_k^{(A)}\}$ is CPS. In $V_h(C^n)$, (1) is the orthogonal projection of W into the $V(\{P_k^{(A)}\})$, determined by n projections $\langle P_k^{(A)} \rangle = w_k^{(A)}$ of which $n-1$ are independent $(\Sigma_k w_k^{(A)} = 1)$.

It may occur that the ensemble that should be described by $W^{(A)}$, i.e. the post-measurement ensemble, was in fact destroyed by the act of measurement, but this point is unimportant. A more important fact is that if one concentrates on a single element of the ensemble, e.g. that described by $P_i^{(W)}$, the measurement process will change it into some $P_k^{(A)}$ with probability $w_{ki} = \mathrm{Tr}(P_i^{(W)} P_k^{(A)})$, and in $V_h(C^n)$ this change $P_i^{(W)} \to P_k^{(A)}$ is a rotation, not a projection. However, for an ensemble of elements described by $P_i^{(W)}$ the measurement process will project it into $V(\{P_k^{(A)}\})$.

If $\{w_k\}$ and $\{w_k^{(A)}\}$ are non-increasingly ordered sequences of eigenvalues of W and $W^{(A)}$,

$$\sum_{k=1}^{r} w_k \geqslant \sum_{k=1}^{r} w_k^{(A)} \tag{2}$$

for $r = 1, 2, \ldots, n$, then

$$\|W\| = \Big(\sum_k w_k^2\Big)^{1/2} \geqslant \|W^{(A)}\|$$

and

$$S(W) = -\sum_k w_k \ln w_k \leqslant S(W^{(A)})$$

(Ruch and Mead 1976).

If $P(W) = \Sigma_k P_k^{(W)}$ and $P(W^{(A)}) = \Sigma_k P_k^{(A)}$, where k numbers only non-zero eigenvalues of W and $W^{(A)}$,

$$P(W) \leqslant P(W^{(A)}). \tag{3}$$

3. Determination of W

The set $W_X^{(A)}$ of all pre-measurement states associated with a particular post-measurement state via equation (1) is a convex subset of $W(C^n)$, and every $W \in W_X^{(A)}$ must satisfy (2) and (3).

Pure, extremal points of $W_X^{(A)}$ are projectors on vectors

$$\sum_k (w_k^{(A)})^{1/2} \exp(\mathrm{i}\varphi_k)|a_k\rangle \tag{4}$$

where $P_k^{(A)} = |a_k\rangle\langle a_k|$ and φ_k are free parameters. A boundary point may be obtained as a convex combination of extremals, or in the following way: if $W^{(A)} = aW_1 + (1-a)W_2$, $0 \leq a \leq 1$, $W_1, W_2, W^{(A)} \in V(\{P_k^{(A)}\})$, and if Q_1 and Q_2 are pure states such that $\boldsymbol{M}(A)Q_1 = W_1$ and $\boldsymbol{M}(A)Q_2 = W_2$, then $W' = aQ_1 + (1-a)Q_2 \in W_X^{(A)}$, etc. Geometrically, $W_X^{(A)}$ is the intersection of n, (n^2-1)-dimensional hyperplanes $h_k = \{H \in V_{\mathrm{h}}(C^n) | \operatorname{Tr}(HP_k^{(A)}) = w_k^{(A)}\}$ and $W(C^n)$.

If m complete measurements of observables

$$A^{(r)} = \sum_{k=1}^{n} a_k^{(r)} P_k^{(r)}$$

are performed and m post-measurement states

$$W^{(r)} = \boldsymbol{M}^{(r)} W_x = \sum_{k=1}^{n} w_k^{(r)} P_k^{(r)} \tag{5}$$

obtained, for $r = 1, 2, \ldots, m$, the pre-measurement state W_x may be any state from the intersection

$$W_X^{(1)} \cap W_X^{(2)} \cap \ldots \cap W_X^{(m)} = W_X^{\Sigma m}. \tag{6}$$

When the set of states, (6), contains only one state the determination is completed, and in the general case $m \geq n+1$. The equality is achieved when $n+1$ measured observables $A^{(r)}$ have such CPS that n^2 projectors

$$\{P_k^{(1)}\}_{k=1}^{n}, \{P_k^{(2)}\}_{k=1}^{n-1}, \ldots, \{P_k^{(n+1)}\}_{k=1}^{n-1}$$

are linearly independent. In $V_{\mathrm{h}}(C^n)$ this set will be some non-orthogonal normed basis.

Two non-commuting projectors P and Q cannot be orthogonal but their projections in the hyperplane $\bar{V}_{\mathrm{h}}(C^n)$, $\bar{V}_{\mathrm{h}}(C^n) = \{H \in V_{\mathrm{h}}(C^n) | \operatorname{Tr} HW_0 = 1/n\}$, $\bar{P} = P - W_0$ and $\bar{Q} = Q - W_0$, where $W_0 = (1/n)1$, are orthogonal if $\operatorname{Tr}(PQ) = 1/n$. Furthermore, two CPS, e.g. $\{P_k\}$ and $\{Q_j\}$, are orthogonal in $\bar{V}_{\mathrm{h}}(C^n)$ if

$$\operatorname{Tr}(P_k Q_j) = 1/n \tag{7}$$

for $k, j = 1, 2, \ldots, n$. This property was used by Schwinger (1960) for similar purposes, and in particular, if (7) is satisfied

$$\boldsymbol{M}(\{Q_k\})(\Sigma\, a_j P_j) = \boldsymbol{M}(\{P_j\})(\Sigma\, b_k Q_k) = W_0, \tag{8}$$

for any real combination $\Sigma\, a_j = \Sigma\, b_j = 1$.

The convenience of CPS orthogonal in $\bar{V}_{\mathrm{h}}(C^n)$ is more visible from the following. If m post-measurement states, (5), are known so that for $s, r = 1, 2, \ldots, m$ and $j, k = 1, 2, \ldots, n$

$$\operatorname{Tr}(P_j^{(s)} P_k^{(r)}) = (1/n)(1 - \delta_{sr} + n\delta_{sr}\delta_{jk}) \tag{9}$$

then

$$W_{0x} = \sum_{r=1}^{m} W^{(r)} - (m-1) W_0 \in W_X^{\Sigma m} \tag{10}$$

if $W_{0x} \geq 0$, and

$$\|W_{0x}\| \leq \|W'_x\|, \qquad W'_x \in W_X^{\Sigma m}. \tag{11}$$

Applying (8) and having in mind that $M^{(r)} W^{(r)} = W^{(r)}$, $M^{(r)} W_{0x} = W^{(r)}$ for $r = 1, 2, \ldots, m$ and $W_{0x} \in W_X^m$. The proof of (11) is as follows. If $W'_x = W_{0x} + A$, $\mathrm{Tr}\, A = 0$. $M^{(r)} W'_x = W^{(r)}$ and $M^{(r)} A = 0$ so that $\mathrm{Tr}(W^{(r)} A) = 0$ for $r = 1, \ldots, m$. $\|W'_x\| = (\mathrm{Tr}(W_{0x} + A)^2)^{1/2} = (\mathrm{Tr}\, W_{0x}^2 + \mathrm{Tr}\, A^2)^{1/2} \geq \|W_{0x}\|$.

The significance of (11) stems from the fact that incomplete determination asks for some side criterion in order to point out a certain characteristic state from $W_X^{\Sigma m}$. (10) is of minimal norm which is, for simple systems, quite similar to the maximal entropy (Wichmann 1963) and (11) is the consequence of the fact that W_{0x} is a linear combination of orthogonal, mutually 'orthogonal', projections.

The special case of (11) is when $m = n + 1$, and then

$$W = \sum_{r=1}^{n+1} W^{(r)} - 1 \tag{12}$$

is the unique reconstruction of the pre-measurement state.

4. Example of orthogonal decomposition of $\bar{V}_h(C^n)$

In order to find $n + 1$ CPS orthogonal in $\bar{V}_h(C^n)$, satisfying (9), one should solve the set of equalities

$$|\langle a_j^s | a_k^r \rangle| = n^{-1/2} (1 - \delta_{sr} + n^{1/2} \delta_{sr} \delta_{jk}) \tag{13}$$

where $P_k^{(r)} = |a_k^r\rangle\langle a_k^r|$. One may arrange $n + 1$ unitary operators whose rows are vectors from (13). When n is a prime number, the corresponding unitary operators are

$$\begin{aligned}
&[U_1]_{jk} = n^{-1/2} \exp[(2\pi i/n)(j+k-1)^2], \\
&\quad\vdots \\
&[U_r]_{jk} = n^{-1/2} \exp[(2\pi i/n) r (j+k-1)^2], \\
&[U_{n-1}]_{jk} = n^{-1/2} \exp[(2\pi i/n)(n-1)(j+k-1)^2], \\
&[U_n]_{jk} = n^{-1/2} \exp[(2\pi i/n) jk], \\
&[U_{n+1}]_{jk} = \delta_{jk}.
\end{aligned} \tag{14}$$

That (14) are unitary operators follows from

$$\sum_{k=1}^{n} \exp[(2\pi i/n) a k] = 0$$

for integer $a \neq 0, \pm n, \pm 2n$. The unitarity of operators in (14) is equivalent to (13) for $s = r$. The equality in (13) for $s \neq r$ corresponds to $|[U_s U_r^+]_{jk}| = n^{-1/2}$, and that follows from

$$\left|\sum_{k=1}^{n} \exp[(2\pi i/n)(ak^2+bk)]\right| = n^{-1/2}$$

for a, b integers, $a \neq 0, \pm n, \pm 2n$, and n prime. The set of CPS (9) is $\{U_r P_k U_r^+\}$, $k = 1, 2, \ldots, n$ and $r = 1, 2, \ldots, n+1$, where $\{P_k\}$ is CPS diagonal in the basis used to express (14). What is achieved for prime n is orthogonal decomposition $V_h(C^n) = 1 \oplus \bar{V}_h(C^n) = 1 \oplus V(\{\bar{P}_k^{(1)}\}) \oplus \ldots \oplus V(\{\bar{P}_k^{(n+1)}\})$. Having this in mind, any $A \in V_h(C^n)$ may be represented by $A = \Sigma_{r=1}^{n+1} \boldsymbol{M}^{(r)} A - \operatorname{Tr} A$, whose special case is (12).

When n is not prime and $n = \Pi_k n_k$ is its prime decomposition, in analogy with (14) one may construct $n_m \leqslant n_k$ CPS satisfying (9).

5. Conclusions

In this formal and geometrised approach to the state determination, the span of $V_h(C^n)$ has a role similar to that of the C^n span in the state preparation, and the concept of quantum measurement becomes more 'visible' than in the ordinary approach.

However, a real state determination is completely dependent on the number of available measurement procedures, and this may serve to compare the possibilities allowed by the Hilbert space formulation of quantum mechanics, with the measurable properties of the inspected ensemble.

The orthogonal decomposition of $\bar{V}_h(C^n)$ is in fact a generalisation of the spin $j = \frac{1}{2}$ example, when (9) is satisfied by the eigen-projectors of s_x, s_y and s_z, and (12) becomes

$$W = W_x + W_y + W_z - 1,$$

where W_i are post-measurement states of the analysed ensemble after the passage through the appropriately oriented Stern–Gerlach set-up.

For higher dimensions this orthogonalisation may have, perhaps, an aesthetic value, but the important fact is that the number of measurements necessary for the state determination increases linearly with n, which together with (3) gives, at least in principle, a possibility for the state determination to be made even for large n.

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