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On Classical Representations of Finite-Dimensional Quantum Mechanics

P. Busch,[1] K.-E. Hellwig,[2] and W. Stulpe[2]

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In the case of a finite-dimensional Hilbert space, it is shown that quantum mechanics can be embedded into discrete classical probability theory. In particular, states can be represented as stochastic vectors and observables as random variables such that all probabilities and expectation values are given in classical terms.

1. INTRODUCTION

In our work (Stulpe, 1992, 1993; Singer and Stulpe, 1992; Bugajski *et al.*, 1992; Hellwig and Singer, 1990, 1991; Busch and Ruch, 1992) we investigated some aspects concerning the relation between quantum mechanics and classical statistical theories. A particularly interesting result is based on the fact that there exist injective affine mappings $W \mapsto TW = \rho$ from the density operators W on the Hilbert space $\mathscr{H} = L^2_{\mathbb{C}}(\mathbb{R}, dx)$ into the probability densities ρ on phase space. This fact was proved by Ali and Prugovečki (1977*a,b*), who called the maps T *phase-space representations of quantum mechanics*. Now our result (Stulpe, 1992; Singer and Stulpe, 1992) reads as follows. Given a phase-space representation T, then for every bounded self-adjoint operator $A \in \mathscr{B}_s(\mathscr{H})$, every $\varepsilon > 0$, and any finitely many density operators $W_1, \ldots, W_m$, there exists a function $f \in L^\infty_{\mathbb{R}}(\mathbb{R}^2, dq\, dp)$ such that

$$\left| \operatorname{tr} W_i A - \int \rho_i(q, p) f(q, p)\, dq\, dp \right| < \varepsilon \tag{1}$$

holds, where $\rho_i := TW_i$ $(i = 1, \ldots, m)$. That is, the quantum mechanical observables can be described by functions on phase space such that their

[1]Institut für Theoretische Physik, Universität zu Köln, D-5000 Köln 41, Germany.
[2]Institut für Theoretische Physik, Technische Universität Berlin, D-1000 Berlin 12, Germany.

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expectation values can, in arbitrarily good physical approximation, be calculated as in classical statistical mechanics.

There are also discrete versions of the result (1). In fact, one can prove the existence of injective affine mappings $W \mapsto TW = p$ from the density operators into the stochastic vectors $p \in l^1_{\mathbb{R}}$ (Singer and Stulpe, 1992; Stulpe, 1993). Given such a map T, then for every bounded self-adjoint operator $A \in \mathscr{B}_s(\mathscr{H})$, every $\varepsilon > 0$, and any finitely many density operators $W_1, \ldots, W_m$, there exists a discrete random variable $a \in l^\infty_{\mathbb{R}}$ such that

$$\left| \operatorname{tr} W_i A - \sum_{j=1}^{\infty} p_{ij} a_j \right| < \varepsilon \tag{2}$$

holds, where $p_i := TW_i$ $(i = 1, \ldots, m)$, P_{ij} is the jth component of p_i, and a_j is the jth component of a (Stulpe, 1993).

It is the aim of this paper to derive a sharpening of the result (2) if the Hilbert space is finite dimensional. In particular, we prove everything by use of some linear algebra and do not presuppose any previous results. In Section 2 we show the existence of injective affine mappings $W \mapsto TW = p$, where $p \in \mathbb{R}^N$ is a stochastic vector and N the square of dim $\mathscr{H}$. In Section 3 we present the analog of (1) and particularly of (2). Namely, given a *classical representation* $W \mapsto TW = p \in \mathbb{R}^N$, then a random variable $a \in \mathbb{R}^N$ can uniquely be assigned to every self-adjoint operator $A \in \mathscr{B}_s(\mathscr{H})$ such that for all density operators W

$$\operatorname{tr} WA = \sum_{j=1}^{N} p_j a_j \tag{3}$$

holds, where $p = TW$. It is crucial that neither p depends on A nor a on W. That is, the statistical scheme of finite-dimensional quantum mechanics can be embedded into discrete classical probability theory, and, in contrast to (1) and (2), the embedding (3) is exact.

2. CLASSICAL REPRESENTATIONS

We presuppose $n := \dim \mathscr{H} < \infty$. Let $\mathscr{B}_s(\mathscr{H})$ be the real vector space of all self-adjoint operators in $\mathscr{H}$; $\mathscr{B}_s(\mathscr{H})$ has dimension $n^2 =: N$ and can be thought of as the space of all Hermitian $n \times n$ matrices. We denote the set of all density operators by $K(\mathscr{H})$ and the set of all $A \in \mathscr{B}_s(\mathscr{H})$ satisfying $0 \le A \le 1$ by $[0, 1]$. Furthermore, let $K(\mathbb{R}^N)$ be the set of all stochastic vectors $p = (p_1, \ldots, p_N)$ in $\mathbb{R}^N$ (i.e., all $p_j \ge 0$ and $\sum_{j=1}^N p_j = 1$). Every stochastic vector $p \in \mathbb{R}^N$ corresponds bijectively to a probability measure on the power set of $\{1, \ldots, N\}$, and every arbitrary vector $a \in \mathbb{R}^N$ can be interpreted as a random variable on $\{1, \ldots, N\}$. Finally, let $e := (1, \ldots, 1)$ and let $[0, e]$ be the set of all $a \in \mathbb{R}^N$ satisfying $0 \le a_j \le 1$ for all $j = 1, \ldots, N$.

An injective affine mapping from the convex set $K(\mathscr{H})$ into the convex set $K(\mathbb{R}^N)$ can uniquely be extended to an injective (positive) linear map $T: \mathscr{B}_s(\mathscr{H}) \to \mathbb{R}^N$ fulfilling $TK(\mathscr{H}) \subseteq K(\mathbb{R}^N)$. Conversely, every such linear map T determines an injective affine mapping from $K(\mathscr{H})$ into $K(\mathbb{R}^N)$.

Definition 2.1. We call a linear map $T: \mathscr{B}_s(\mathscr{H}) \to \mathbb{R}^N$ a *classical representation of n-dimensional Hilbert-space quantum mechanics on* $\mathbb{R}^N$ if

(i) $TK(\mathscr{H}) \subseteq K(\mathbb{R}^N)$.
(ii) T is injective.

Because of $N = n^2$, T is even bijective. To prove the existence of such classical representations, we need the following lemma.

Lemma 2.2. The space $\mathscr{B}_s(\mathscr{H})$ has a Hamel basis $F_1, \ldots, F_N$ with $F_j \in [0, 1]$ for all $j = 1, \ldots, N$ and $\sum_{j=1}^N F_j = 1$.

Proof. Since the positive cone in $\mathscr{B}_s(\mathscr{H})$ is generating, it contains a basis $A_1, \ldots, A_N$. This basis can be chosen such that $A_j \in [0, 1]$ and, moreover, $\sum_{j=1}^N A_j \le 1$. Let

$$B := 1 - \sum_{j=1}^{N} A_j = \sum_{j=1}^{N} \alpha_j A_j \tag{4}$$

where $\alpha_j \in \mathbb{R}$. Because of $B \in [0, 1]$, we have $\alpha_j \neq -1$ for at least one j. Let $\alpha_{j_0} \neq -1$ and define

$$F_1 := A_1, \ldots, \qquad F_{j_0} := A_{j_0} + B, \ldots, \qquad F_N := A_N \tag{5}$$

Then $F_j \in [0, 1]$ and $\sum_{j=1}^N F_j = 1$ hold. It remains to show that $F_1, \ldots, F_N$ is a basis in $\mathscr{B}_s(\mathscr{H})$, i.e., that the elements $F_1, \ldots, F_N$ are linearly independent. Assume $\sum_{j=1}^N \lambda_j F_j = 0$. Inserting (5) and (4), we obtain

$$\sum_{j=1}^{N} (\lambda_j + \lambda_{j_0} \alpha_j) A_j = 0$$

From the linear independence of $A_1, \ldots, A_N$ it follows that

$$\lambda_j + \lambda_{j_0} = 0$$

for all j. Setting $j = j_0$, this equation implies $\lambda_{j_0} = 0$ since $\alpha_{j_0} \neq -1$. Hence, $\lambda_j = 0$ for all j, and the elements $F_1, \ldots, F_N$ are linearly independent. ■

Theorem 2.3. A basis $F_1, \ldots, F_N$ in $\mathscr{B}_s(\mathscr{H})$ with $F_j \in [0, 1]$ for all $j = 1, \ldots, N$, and $\sum_{j=1}^N F_j = 1$ defines a classical representation $T: \mathscr{B}_s(\mathscr{H}) \to \mathbb{R}^N$ by

$$TV := (\text{tr } VF_1, \ldots, \text{tr } VF_N) \tag{6}$$

Conversely, every classical representation T determines uniquely a basis $F_1, \ldots, F_N$ with the properties as above such that (6) holds.

Proof. The proof of the first statement is straightforward. To prove the converse, consider an arbitrary linear map $T: \mathscr{B}_s(\mathscr{H}) \to \mathbb{R}^N$ and the linear functional $V \mapsto (TV)_j$, where $(TV)_j$ denotes the jth component of TV. Since $\mathscr{B}_s(\mathscr{H})$ can be placed in duality to itself by $\langle A, B \rangle := \text{tr } AB$, it follows that $(TV)_j = \text{tr } VF_j$ with some $F_j \in \mathscr{B}_s(\mathscr{H})$. Hence, every linear map T from $\mathscr{B}_s(\mathscr{H})$ into $\mathbb{R}^N$ is of the form

$$TV = (\text{tr } VF_1, \ldots, \text{tr } VF_N)$$

Now let T be a classical representation. Then the property (i) of Definition 2.1 implies $F_j \in [0, 1]$ and $\sum_{j=1}^N F_j = 1$. From the property (ii) we obtain that $F_1, \ldots, F_N$ separate the elements of $\mathscr{B}_s(\mathscr{H})$. In consequence, the linear hull of $F_1, \ldots, F_N$ coincides with $\mathscr{B}_s(\mathscr{H})$, and the family $F_1, \ldots, F_N$ is a basis. ∎

Thus, we have proved the existence of classical representations of n-dimensional Hilbert-space quantum mechanics on $\mathbb{R}^N$ as well as their explicit form. Although such a classical representation $T: \mathscr{B}_s(\mathscr{H}) \to \mathbb{R}^N$ is bijective it does not act bijectively between the sets $K(\mathscr{H})$ and $K(\mathbb{R}^N)$ (provided that $n = \dim \mathscr{H} \geq 2$), i.e., $TK(\mathscr{H})$ is always a proper subset of $K(\mathbb{R}^N)$ (equivalently, T is a positive linear map, but not T^{-1}). Namely, if T restricted to $K(\mathscr{H})$ were a bijective affine map onto $K(\mathbb{R}^N)$, then the extreme points of the convex set $K(\mathscr{H})$ would be mapped onto the extreme points of the convex set $K(\mathbb{R}^N)$. This, however, is not possible, because $K(\mathscr{H})$ has infinitely many extreme points, whereas $K(\mathbb{R}^N)$ is a simplex with N extreme points. Hence, the classical representation T determines an injective embedding of the density operators into the probability measures on $\{1, \ldots, N\}$ which is never surjective [cf. the more general considerations in Singer and Stulpe (1993)].

The basis $F_1, \ldots, F_N$ constructed in Lemma 2.2 defines an *observable* F as a *POV-measure* on the power set of $\{1, \ldots, N\}$ by

$$F(B) := \sum_{i \in B} F_i \tag{7}$$

where $B \subseteq \{1, \ldots, N\}$. The probability distribution $\beta \mapsto P_W^F(B) := \text{tr } WF(B)$ of F in some state $W \in K(\mathscr{H})$ is just the probability measure that corresponds to the stochastic vector TW with T given by (6). Since accordingly the observable F distinguishes states by its respective probability distributions, F is called *informationally complete* (Ali and Prugovečki, 1977*a*,*b*). In fact, there is a general one-to-one correspondence between classical representations and informationally complete observables (see, e.g., Singer and Stulpe, 1933). Finally, we remark that an informationally complete observable cannot be a *PV-measure* (except for dim $\mathscr{H}=1$), as one can easily see in the special case (7). Namely, if F were projection valued, then the projections $F_1, \ldots, F_N$ would have to be mutually orthogonal, but a family of mutually orthogonal projections cannot have more than $n<N$ members.

3. THE DUALS OF CLASSICAL REPRESENTATIONS

By means of the scalar products

$$(A, B) \mapsto \langle A, B \rangle := \operatorname{tr} AB$$

$[A, B \in \mathscr{B}_s(\mathscr{H})]$ and

$$(x, y) \mapsto \langle x, y \rangle := \sum_{j=1}^{N} x_j y_j$$

$(x, y \in \mathbb{R}^N)$, the spaces $\mathscr{B}_s(\mathscr{H})$ and $\mathbb{R}^N$ are placed in duality to themselves, respectively. Hence, for a classical representation $T: \mathscr{B}_s(\mathscr{H}) \to \mathbb{R}^N$, the adjoint map $T': \mathbb{R}^N \to \mathscr{B}_s(\mathscr{H})$ is defined. It is not hard to show that the following hold:

(i) $T'x \geq 0$ for all $x \in \mathbb{R}^N$ with $x_j \geq 0$ $(j=1, \ldots, N)$ and $T'e=1$.

(ii) T' is bijective and $(T')^{-1} = (T^{-1})'$.

(iii) $T'[0, e] \subseteq [0, 1]$, where the inclusion is proper.

(iv) $(T')^{-1}$ is not a positive linear map, i.e., there are operators $A \geq 0$ such that $x := (T')^{-1}A$ has at least one component $x_j < 0$.

The following theorem now states how quantum observables can be described in the context of a classical representation.

Theorem 3.1. Let T be a classical representation of n-dimensional Hilbert-space quantum mechanics on $\mathbb{R}^N$. Then for every $A \in \mathscr{B}_s(\mathscr{H})$ there exists a uniquely determined element $a \in \mathbb{R}^N$ such that for all density operators $W \in K(\mathscr{H})$

$$\operatorname{tr} WA = \sum_{j=1}^{N} p_j a_j$$

holds, where $p = TW$. In particular, $a = (T')^{-1}A$.

Proof. Defining a by $A = T'a$, we obtain

$$\text{tr } WA = \langle W, T'a \rangle = \langle TW, a \rangle = \langle p, a \rangle = \sum_{j=1}^{N} p_j a_j$$

for all $W \in K(\mathscr{H})$. Since T is bijective, the set of all $p = TW$ generates $\mathbb{R}^N$, the latter implying the uniqueness of a. ■

According to Theorem 2.3, every classical representation T is of the form

$$TV = (\text{tr } VF_1, \ldots, \text{tr } VF_N)$$

where $V \in \mathscr{B}_s(\mathscr{H})$ and $F_1, \ldots, F_N$ is a suitable basis in $\mathscr{B}_s(\mathscr{H})$. From (6) it follows that T' is given by

$$T'a = \sum_{j=1}^{N} a_j F_j$$

In consequence, for $(T')^{-1}$ we obtain

$$(T')^{-1} A = a$$

where $A = \sum_{j=1}^{N} a_j F_j$ and $a := (a_1, \ldots, a_N)$.

Let $A = \sum_{j=1}^{N} \lambda_i |\phi_i\rangle\langle\phi_i|$ be the spectral representation of $A \in \mathscr{B}_s(\mathscr{H})$. For the expectation value $\langle A \rangle_W$ of the observable A in the state $W \in K(\mathscr{H})$, we then have, according to the usual statistical interpretation of quantum mechanics,

$$\langle A \rangle_W := \sum_{j=1}^{N} q_i \lambda_i = \text{tr } WA \tag{8}$$

where $q_i := \langle \phi_i | W\phi_i \rangle$. In contrast to the vector p occurring in (3), the stochastic vector $q := (q_1, \ldots, q_n)$ of (8) depends on A and does not characterize W uniquely (the latter means that the map $W \mapsto q$ is not injective, the reason for this being that the observable A, considered as a PV-measure, is not informationally complete). Similarly, in contrast to a, the vector $\lambda := (\lambda_1, \ldots, \lambda_n)$ does not characterize A. Note, however, that p, $a \in \mathbb{R}^N$, whereas q, $\lambda \in \mathbb{R}^n$.

Thus, we see that, by means of a classical representation of n-dimensional Hilbert-space quantum mechanics, the quantum states can be identified with stochastic vectors $p \in \mathbb{R}^N$ and the quantum observables with the discrete random variables $a \in \mathbb{R}^N$, where the expectation values can be calculated by the corresponding classical expression given in (3). Hence, we have obtained a classical reformulation of the statistical scheme of quantum mechanics or, more precisely, an embedding of finite-dimensional quantum mechanics into discrete classical probability theory.

Passing to the classical description of quantum observables, positivity and normalization properties are not conserved. According to point (iv) at the beginning of this section, for $A \geq 0$ it does not necessarily hold that $a = (T')^{-1}A \geq 0$. Similarly, according to (iii), if $A \in [0, 1]$, then a need not be an element of $[0, e]$. In particular, the elements of $[0, 1]$ can be interpreted as *effects*, i.e., as realistic 0–1 measurements, where the probability for the outcome 1 of $A \in [0, 1]$ in some state $W \in K(\mathscr{H})$ is given by tr WA. Hence, by Theorem 3.1, quantum mechanical effects $A \in [0, 1]$ can be described classically by vectors $a \in \mathbb{R}^N$, where, in general, $a \neq [0, e]$, i.e., a is not a classical effect.

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