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The Simplex Structure of the Classical States of the Quantum Harmonic Oscillator

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Abstract. It is shown that the convex set of classical states of the quantum harmonic oscillator is a simplex generated as the closed convex hull of the coherent states in the weak topology of the Banach space of trace class operators.

1. Introduction

Let $\psi(x,y)\in H$, where $(x,y)\in\mathbb{R}^2$, denote a coherent state vector of the one-dimensional quantum harmonic oscillator

$$\psi(x,y)=\exp\left(-\frac{x^2+y^2}{2}\right)\sum_{n=0}^{\infty}\frac{(x+iy)^n}{\sqrt{n!}}\varphi_n. \tag{1}$$

Here $\varphi_n, n\in\mathbb{Z}_+$, are the eigenvectors of the number operator which constitute a complete orthonormal set of the Hilbert space H under consideration.

In the following $L^1(H)$ denotes the Banach space of trace class operators on H equipped with the trace norm $\|\cdot\|_1$, and $S(H)$ is the set of statistical operators

$$S(H)=\{W\in L^1(H);\quad W\geqq 0,\ \mathrm{tr}(W)=1\}. \tag{2}$$

A state on $L(H)$, the Banach space of bounded linear operators on H, is called a *coherent state* if it can be identified with a statistical operator of the form

$$P(x,y)=(\psi(x,y),\cdot)\psi(x,y), \tag{3}$$

where $(x,y)\in\mathbb{R}^2$ and $\psi(x,y)$ is defined in (1). For information concerning the physical and mathematical properties of coherent states we refer to [1,2]. There the P-representation of a statistical operator W is introduced as an integral representation in terms of coherent states

$$W=\int_{\mathbb{R}^2} dxdyp(x,y)P(x,y), \tag{4}$$

where $p(x,y)$ is called a quasi-probability insofar as it is discerned from a probability density on $\mathbb{R}^2$ by the fact that it is admitted that

i) $p(x, y)$ takes negative values,
ii) $p(x, y)$ is a distribution.

Besides the fact that the integral in (4) is defined in a weak sense only, we see the shortcomings of this approach to an integral representation of statistical operators in the application of quasi-probabilities which are unnatural from a probabilistic point of view.

In this note we attack the representation problem by means of a different strategy. We focus on representations of the form (cf. [3])

$$W = \int d\mu(x, y) P(x, y) \tag{5}$$

(which are rigorously defined below) where μ is a probability measure on $\mathbb{R}^2$, i.e. $\mu \in M_+^1(\mathbb{R}^2)$. Obviously, in this approach not very statistical operator is representable. On the other hand it turns out that the set of statistical operators which are representable has a, in the sense of classical statistical mechanics, typical classical structure: it is a simplex. Here a convex set is defined to be a simplex provided the cone generated by it is a lattice in its own order.

2. Classical States

Our aim is to give a rigorous meaning to the integral (5). To this end we recall that due to the fact that $(x, y) \to \psi(x, y)$ is continuous (cf. [2]) the mapping $\Phi: \mathbb{R}^2 \to L^1(H)$ defined by

$$\Phi(x, y) = P(x, y) \tag{6}$$

is continuous, too. This implies that the range of Φ is a separable subset of $L^1(H)$ and, in turn, that Φ is strongly measurable. Moreover, by virtue of $\| P(x, y) \|_1 = 1$, for any $\mu \in M_+^1(\mathbb{R}^2)$,

$$\int d\mu(x, y) \| P(x, y) \|_1 = 1 \tag{7}$$

holds. These facts entail that Φ is Bochner integrable with respect to any $\mu \in M_+^1(\mathbb{R}^2)$ (cf. [4]). Obviously, for any $\mu \in M_+^1(\mathbb{R}^2)$ the integral $\int d\mu(x, y) P(x, y) \in S(H)$ such that the following definition makes sense.

Definition. Whenever there exists a probability measure $\mu \in M_+^1(\mathbb{R}^2)$ such that a statistical operator $W \in S(H)$ is representable as a Bochner integral via $W = \int d\mu(x, y) P(x, y)$, the state on $L(H)$ determined by W is called a *classical state.*

It is evident that the set of classical states which we denote by $CS(H)$ is a convex subset of the convex set $S(H)$ and it is our goal to show that $CS(H)$ is a simplex contained in $S(H)$. To this end we need some properties of the mapping $D: M_+^1(\mathbb{R}^2) \to CS(H)$ defined by

$$D(\mu) = \int d\mu(x, y) P(x, y). \tag{8}$$

Let us introduce for all $\mu \in M_+^1(\mathbb{R}^2)$ a positive bounded measure $\nu[\mu] \in M_+^b(\mathbb{R}^2)$ by

$$\frac{d\nu[\mu]}{d\mu}(x, y) = \exp(-(x^2 + y^2)), \tag{9}$$

so that $\nu[\mu](\mathbb{R}^2) \leqq 1$, and denote the characteristic function of $\nu[\mu]$ by $\hat{\nu}[\mu]$,

$$\hat{\nu}[\mu](x, y) = \int d\nu[\mu](x', y') \exp(ixx' + iyy'). \tag{10}$$

For any $(x, y) \in \mathbb{R}^2$ and any $\mu \in M_+^1(\mathbb{R}^2)$ we have, by the properties of Bochner integrals,

$$\begin{aligned}(\psi(x, y), D(\mu)\psi(-x, -y)) &= \int d\mu(x', y')(\psi(x, y), P(x', y')\psi(-x, -y)) \\ &= \int d\mu(x', y')(\psi(x, y), \psi(x', y'))(\psi(x', y'), \psi(-x, -y)). \end{aligned} \tag{11}$$

Taking into account Eq. (1) this yields for any $(x, y) \in \mathbb{R}^2$ and any $\mu \in M_+^1(\mathbb{R}^2)$,

$$\begin{aligned}&(\psi(x, y), D(\mu)\psi(-x, -y)) \\ &\quad = \int d\mu(x', y') \exp\{-(x^2 + y^2) - (x'^2 + y'^2)\} \exp\{i(-2y)x' + i(2x)y'\} \\ &\quad = \exp\{-(x^2 + y^2)\}\hat{\nu}[\mu](-2y, 2x). \end{aligned} \tag{12}$$

Next we associate with any $W \in S(H)$ a mapping $w: \mathbb{R}^2 \to \mathbb{R}$ defined by

$$w(x, y) = (\psi(x, y), W\psi(x, y)). \tag{13}$$

Obviously, for all $(x, y) \in \mathbb{R}^2$ we have $0 \leqq w(x, y) \leqq 1$ and $w \in C_b(\mathbb{R}^2; \mathbb{R})$ for any $W \in S(H)$. Due to the fact that the coherent state vectors are a total set in H (cf. e.g. [3]) $w_1 = w_2$ implies $W_1 = W_2$. Moreover, since

$$\int dx dy \frac{1}{\pi} w(x, y) = 1 \tag{14}$$

holds (cf. e.g. [2]), $(1/\pi)w$ can be considered as a probability density with respect to the Lebesgue measure λ^2 on $\mathbb{R}^2$. This fact allows us to associate with any $W \in S(H)$ a uniquely determined element $\rho_W \in M_+^1(\mathbb{R}^2)$ defined such that

$$\frac{d\rho_W}{d\lambda^2}(x, y) = \frac{1}{\pi} w(x, y). \tag{15}$$

Let us denote by $\gamma, \gamma \in M_+^1(\mathbb{R}^2)$, the probability measure with density

$$\frac{d\gamma}{d\lambda^2}(x, y) = g(x, y) = \frac{1}{\pi} \exp(-(x^2 + y^2)) \tag{16}$$

and characteristic function

$$\hat{\gamma}(x, y) = \exp\left\{-\frac{x^2 + y^2}{4}\right\}. \tag{17}$$

For any $W \in S(H)$ we define the *quasicharacteristic function* $\hat{\sigma}_W$ of W by $\hat{\sigma}_W: \mathbb{R}^2 \to \mathbb{C}$,

$$\hat{\sigma}_W(x, y) = \exp\left(\frac{x^2 + y^2}{4}\right)\hat{\rho}_W(x, y). \tag{18}$$

Obviously, $\hat{\sigma}_W$ is continuous and $\hat{\sigma}_W(0, 0) = 1$ holds.

With these prerequisites we state our first lemma.

Lemma 1. *For $W \in S(H)$ the quasicharacteristic function $\hat{\sigma}_W$ defined by Eq. (18) is a characteristic function of an element of $M^1_+(\mathbb{R}^2)$ if and only if $W \in CS(H)$. Moreover, for* $D(\mu) \in CS(\mathrm{H})$

$$\hat{\sigma}_{D(\mu)} = \hat{\mu} \tag{19}$$

holds.

Proof.
i) Assume $W \in CS(H)$. Then there exists a $\mu \in M^1_+(\mathbb{R}^2)$ such that $W = D(\mu)$ and $w = d[\mu]$. But for any $\mu \in M^1_+(\mathbb{R}^2)$,

$$\frac{1}{\pi} d[\mu](x, y) = (g * \mu)(x, y) \tag{20}$$

holds for all $(x, y) \in \mathbb{R}^2$, where $*$ denotes the convolution.
Fourier transformation yields

$$\hat{\rho}_{D(\mu)}(x, y) = \hat{\gamma}(x, y)\hat{\mu}(x, y) \tag{21}$$

for all $\mu \in M^1_+(\mathbb{R}^2)$ and all $(x, y) \in \mathbb{R}^2$. From the definition (18) we have

$$\hat{\sigma}_W(x, y) = \hat{\sigma}_{D(\mu)}(x, y) = (\hat{\gamma}(x, y))^{-1} \hat{\rho}_{D(\mu)}(x, y). \tag{22}$$

Comparing this with (21), the first part of the assertion and Eq. (19) follow.
ii) Assume $\hat{\sigma}_W$ is a characteristic function. Then there exists an uniquely determined probability measure $\mu_W \in M^1_+(\mathbb{R}^2)$ such that $\hat{\sigma}_W = \hat{\mu}_W$. It remains to be proved that $D(\mu_W) = W$. But by the assumption

$$\hat{\rho}_W(x, y) = \hat{\gamma}(x, y)\hat{\sigma}_W(x, y) = \hat{\gamma}(x, y)\hat{\mu}_W(x, y), \tag{23}$$

and by (19)

$$\hat{\rho}_{D(\mu_W)}(x, y) = \hat{\gamma}(x, y)\hat{\mu}_W(x, y). \tag{24}$$

Therefore we have

$$\hat{\rho}_W(x, y) = \hat{\rho}_{D(\mu_W)}(x, y) \tag{25}$$

for all $(x, y) \in \mathbb{R}^2$. This implies

$$\frac{1}{\pi} w(x, y) = \frac{1}{\pi} d[\mu_W](x, y) \tag{26}$$

for all $(x, y) \in \mathbb{R}^2$ since both functions are continuous.
This ends the proof of the lemma.

Our conclusion is as follows. Whereas it is possible to associate with any statistical operator $W \in S(H)$ a probability measure, namely ρ_W, Lemma 1 shows that only for the classical states it is possible to define another characteristic probability measure in terms of $\hat{\sigma}_W$. And this one is just the mixing measure in the integral representation of these states.

3. The Simplex of Classical States

To prove the simplex structure of $CS(H)$ we need a preliminary lemma.

Lemma 2. *The mapping D defined in Eq. (8) is an affine homeomorphism,* i.e. *D is affine and*

i) *injective,*

ii) *continuous with respect to the weak topologies, and*

iii) *if $\{\mu_n\}$ is a sequence in $M^1_+(\mathbb{R}^2)$ such that $D(\mu_n) \to W \in S(H)$ weakly, then there exists a uniquely determined element $\mu \in M^1_+(\mathbb{R}^2)$ such that $\mu_n \to \mu$ weakly and $W = D(\mu)$.*

Proof.
i) Assume $D(\mu_1) = D(\mu_2)$ where $\mu_1, \mu_2 \in M^1_+(\mathbb{R}^2)$. For all $(x, y) \in \mathbb{R}^2$ this implies that

$$(\psi(x, y), D(\mu_1)\psi(-x, -y)) = (\psi(x, y), D(\mu_2)\psi(-x, -y)). \tag{27}$$

From Eq. (12) we infer that

$$\hat{v}[\mu_1](x, y) = \hat{v}[\mu_2](x, y) \tag{28}$$

holds for all $(x, y) \in \mathbb{R}^2$. From the uniqueness of characteristic functions $v[\mu_1] = v[\mu_2]$ follows which, in turn, implies $\mu_1 = \mu_2$ as the density (14) is strictly positive for all $(x, y) \in \mathbb{R}^2$.

ii) Under the duality $L^1(H) \times L(H) \in (T, A) \to \mathrm{tr}(AT)$ the topological dual of $L^1(H)$ can be identified with $L(H)$. Given a sequence $\{D(\mu_n)\}$ in $CS(H)$ with $\mu_n \to \mu$ weakly, for any continuous linear functional f on $L^1(H)$ there exists an uniquely determined element $A_f \in L(H)$ such that

$$\begin{aligned} {}_n)) &= \int d\mu_n(x, y) f(P(x, y)) = \int d\mu_n(x, y)\, \mathrm{tr}(A_f P(x, y)) \\ &= \int d\mu_n(x, y)(\psi(x, y), A_f\psi(x, y)). \end{aligned} \tag{29}$$

As $(x, y) \to (\psi(x, y), A_f\psi(x, y)) \in C_b(\mathbb{R}^2; \mathbb{C})$ we conclude that

$$f(D(\mu_n)) \to f(D(\mu)) \tag{30}$$

for all linear continuous functionals on $L^1(H)$.

iii) As $D(\mu_n) \to W \in S(H)$ weakly we have for all $A \in L(H)$

$$\lim_{n\to\infty} \mathrm{tr}(D(\mu_n)A) = \mathrm{tr}(WA). \tag{31}$$

Setting $A = P(x, y)$, for all $(x, y) \in \mathbb{R}^2$ we obtain by means of Eq. (20)

$$\lim_{n\to\infty} (g * \mu_n)(x, y) = \frac{1}{\pi} w(x, y). \tag{32}$$

Accordingly, in the weak topology

$$\lim_{n\to\infty} \rho_{D(\mu_n)} = \rho_W. \tag{33}$$

This implies (cf. e.g. [5])

$$\lim_{n\to\infty} \hat{\gamma}(x, y)\hat{\mu}_n(x, y) = \hat{\rho}_W(x, y) \tag{34}$$

for all $(x, y) \in \mathbb{R}^2$. This is equivalent to the fact that for all $(x, y) \in \mathbb{R}^2$,

$$\lim_{n \to \infty} \hat{\mu}_n(x, y) = (\hat{\gamma}(x, y))^{-1} \hat{\rho}_W(x, y). \tag{35}$$

Since the mapping

$$(x, y) \to (\hat{\gamma}(x, y))^{-1} \hat{\rho}_W(x, y) \tag{36}$$

is continuous and normalized to 1 in $(0, 0) \in \mathbb{R}^2$ we eventually obtain, using Theorem 48.7 II of ref. [5], that i) there exists an uniquely determined element $\mu \in M_+^1(\mathbb{R}^2)$ such that $\mu_n \to \mu$ weakly, and ii)

$$\hat{\mu}(x, y) = (\hat{\gamma}(x, y))^{-1} \hat{\rho}_W(x, y) \tag{37}$$

for all $(x, y) \in \mathbb{R}^2$.

It remains to show that $W = D(\mu)$. But this is obvious from Lemma 1 as we have shown that $\hat{\sigma}_W = \hat{\mu}$ is a characteristic function and from the uniqueness part of this lemma. This ends the proof of Lemma 2.

Our central result is contained in the following theorem.

Theorem. *Let $CS(H)$ be the convex set of classical states of the harmonic oscillator, then*

i) *$CS(H)$ is a simplex and the set of extreme points is the set of coherent states*

$$\mathrm{ex}(CS(H)) = \{P(x, y); (x, y) \in \mathbb{R}^2\}, \tag{38}$$

ii) *$CS(H)$ is the closed convex hull of its extreme points*

$$CS(H) = \mathrm{cl}(\mathrm{con}(\mathrm{ex}(CS(H)))), \tag{39}$$

where the closure refers to the weak topology of the Banach space $L^1(H)$,

iii) *each $D(\mu) \in CS(H)$ is the barycenter of an uniquely determined probability measure π_μ on $L^1(H)$ (equipped with the weak Borel σ-field) satisfying $\pi_\mu(\mathrm{ex}(CS(H))) = 1$, i.e.*

$$\mathrm{tr}\,(AD(\mu)) = \int_{\mathrm{ex}(CS(H))} d\pi_\mu(T)\,\mathrm{tr}(AT) \tag{40}$$

holds for all $A \in L(H)$.

Proof.

i) Due to the fact that $M_+^1(\mathbb{R}^2)$ is a simplex the same holds for $CS(H)$ as, according to Lemma 2, part i) the mapping D is an affine bijection and preserves, therefore, order properties. Accordingly, the set $\mathrm{ex}(CS(H))$ is the image of $\mathrm{ex}(M_+^1(\mathbb{R}^2)) = \{\delta_{(x,y)}; (x, y) \in \mathbb{R}^2\}$ under this mapping where $\delta_{(x,y)}$ denotes the Dirac measure on $\mathbb{R}^2$ concentrated at $(x, y) \in \mathbb{R}^2$. From this (38) follows.

ii) Firstly, we prove that

$$\int d\mu(x, y) P(x, y) \in \mathrm{cl}(\mathrm{con}(\{P(x, y); (x, y) \in \mathbb{R}^2\})) \tag{41}$$

for all $\mu \in M_+^1(\mathbb{R}^2)$. Suppose that there is a $\mu \in M_+^1(\mathbb{R}^2)$ such that $D(\mu)$ does not satisfy (41). The geometric version of the Hahn–Banach theorem then ensures the existence of a strictly separating hyperplane, i.e. there exists a selfadjoint $A \in L(H)$ and a real number α such that

$$\operatorname{tr}(AD(\mu)) = \int d\mu(x', y') \operatorname{tr}(AP(x', y')) < \alpha \leqq \operatorname{tr}(AP(x, y)) \tag{42}$$

for all $P(x, y) \in L^1(H)$, $(x, y) \in \mathbb{R}^2$. Integration yields

$$\int d\mu(x', y') \operatorname{tr}(AP(x', y')) < \alpha\mu(\mathbb{R}^2) \leqq \int d\mu(x, y) \operatorname{tr}(AP(x, y)) \tag{43}$$

which is a contradiction.

Accordingly, we have

$$\operatorname{con}(\{P(x, y); (x, y) \in \mathbb{R}^2\}) \subset CS(H) \subset \operatorname{cl}(\operatorname{con}(\{P(x, y); (x, y) \in \mathbb{R}^2\})). \tag{44}$$

By part iii) of Lemma 2 the set $CS(H)$ is weakly closed such that (39) follows if we take into account Eq. (38).

iii) The mapping Φ defined in Eq. (6) is continuous and therefore Borel measurable. For any $D(\mu) \in CS(H)$ the probability measure $\pi_\mu = \Phi \circ \mu$, the image of μ under Φ, satisfies for all $A \in L(H)$

$$\operatorname{tr}(AD(\mu)) = \int d\mu(x, y) \operatorname{tr}(AP(x, y)) = \int_{L^1(H)} d\pi_\mu(T) \operatorname{tr}(AT). \tag{45}$$

As $\operatorname{ex}(CS(H))$ is weakly closed and therefore measurable, we obtain

$$\pi_\mu(\operatorname{ex}(CS(H))) = 1, \tag{46}$$

which proves the existence of the integral representation (40). Uniqueness of this integral representation follows from the uniqueness part of Lemma 2 together with the property that Φ considered as a mapping from $\mathbb{R}^2$ onto $\operatorname{ex}(CS(H))$ is a homeomorphism which, in turn, follows from Lemma 2 where we also need part ii). This ends the proof of the theorem.

4. Remarks

1. In the present situation an application of classical Choquet theory is not possible as $CS(H)$ is the homeomorphic image of the non-compact set $M_+^1(\mathbb{R}^2)$. Nevertheless, part i) and part iii) of the theorem are equivalent.

This is due to the fact that the separability of H implies that $L^1(H)$ is a separable dual space which according to [4, Th. III. 3.1.] has the RN-property. We therefore can use the results of [6, 7] which contain an exact analogue of the classical existence and uniqueness theorems for barycentric integral representations of closed and bounded convex subsets of a Banach space with RN-property.

2. The coherent state vectors are intimately connected with the (trivial) Bose–Fock–space structure of the Hilbert space of the harmonic oscillator (cf. [3]), namely

$$H = F_+(\mathbb{C}). \tag{47}$$

A generalization of our results to the simplex structure of the classical states on $F_+(\mathbb{C}^k)$, $k \in \mathbb{N}$, is quite straightforward. Technical difficulties, due to our method and obviously not specific to the problem, arise in the case of the boson field with state space $F_+(K)$, K an infinite dimensional separable complex Hilbert space, by virtue of the fact that on K there exists neither an analogue of the Lebesgue measure nor a rotation invariant Gaussian measure.

3. It is well known that $S(H)$ is a convex set with extremals (pure states)

$$\mathrm{ex}(S(H)) = P(H), \tag{48}$$

where $P(H)$ denotes the set of orthogonal projections onto one-dimensional subspaces of H.

This fact implies

$$\mathrm{ex}(CS(H)) = CS(H) \cap \mathrm{ex}(S(H)) \tag{49}$$

and shows that the coherent states are the only pure states which are representable according to our definition.

4. A convenient possibility to characterize the fundamental difference between a system in classical mechanics and quantum mechanics is provided by the structure of the convex set of states of these systems. Whereas the state space of a classical system, the set of all probability measures on its phase space is always a simplex, the state space of a quantum system, here $S(H)$, is never a simplex. This is due to the fact that for any $W \in S(H)$, $W \notin P(H)$, there exist (infinitely many) different representations of the form

$$W = \sum_i p_i P_i, \tag{50}$$

where $P_i \in P(H)$, $p_i \geqq 0$, $\sum_i p_i = 1$, (cf. e.g. [8]).

Considering the quantum harmonic oscillator in a pure state, it is well known that only in a coherent state the quantum harmonic oscillator exhibits a structural analogy to the classical harmonic oscillator. In this work we have shown that, in addition, the closed convex hull of these states has a structure which is characteristic for a classical system.

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