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Chapter 4

Quantum physics on a general Hilbert space

In this chapter we generalize the results of Chapter 2 to infinite-dimensional Hilbert spaces. So let H be a Hilbert space and let $B(H)$ be the set of all *bounded* operators on H . Here a notable point is that linear operators on *finite-dimensional* Hilbert spaces are automatically bounded, whereas in general they are not. Thus we impose boundedness as an extra requirement, beyond linearity. This is very convenient, because as in the finite-dimensional case, $B(H)$ is a C^* -algebra, cf. §C.1. At the same time, assuming boundedness involves no loss of generality whatsoever, since we can always replace closed unbounded operators by bounded ones through the *bounded transform*, as explained in §B.21. Nonetheless, even the relatively easy setting of bounded operators leads to some technical complications we have to deal with. First, Definition 2.1 must be adjusted as follows:

Definition 4.1. *Let H be a Hilbert space.*

1. A **(quantum) event** is a closed linear subspace L of H .
2. A **density operator** is a positive trace-class operator ρ on H such that $\text{Tr}(\rho) = 1$; we continue to denote the set of all density operators on H by $\mathcal{D}(H)$.
3. A **(quantum) random variable** is a bounded self-adjoint operator on H .
4. The **spectrum** $\sigma(a)$ of a bounded operator a is the set of all $\lambda \in \mathbb{C}$ for which the operator $a - \lambda$ is not invertible in $B(H)$ (cf. Definition B.80).

As shown in Corollary B.88, if H is finite-dimensional this notion of a spectrum reduces to the set of eigenvalues of a . Even H is infinite-dimensional, the spectrum of a self-adjoint operator a is real (i.e., $\sigma(a) \subset \mathbb{R}$); this is also true if a is unbounded (see Theorem B.93). For any H , unit vectors ψ still define special density matrices e_ψ , as in (2.7); we will later see that these are pure states on $B(H)$, although the set of pure states is no longer exhausted by such density matrices. Finally, quantum events in H still bijectively correspond with projections on H ; see Proposition B.76. The Born rule as well as the correspondence between density matrices and states require a separate discussion, to which we now turn.

4.1 The Born rule from Bohrification (II)

In this section we extend the characterization of the Born rule in §2.5, which was restricted to finite phase spaces X and finite-dimensional Hilbert spaces H , to the general case. Recall that a **probability space** is a measure space (X, Σ, μ) for which $\mu(X) = 1$, and that, for compact X , a state on $C(X)$ is a positive map $\varphi : C(X) \rightarrow \mathbb{C}$ that is positive and satisfies $\varphi(1_X) = 1$. Theorem B.15 and Corollary (B.17) yield:

Theorem 4.2. *Let X be a compact Hausdorff space. There is a bijective correspondence between probability measures μ on X and states ω on $C(X)$, given by*

$$\omega(f) = \int_X d\mu f, \quad f \in C(X). \quad (4.1)$$

More precisely, the correspondence in question is between complete regular probability spaces (X, Σ, μ) and states on $C(X)$, and this is understood in what follows.

Second, we recall that if H is a Hilbert space and $a \in B(H)$, then $C^*(a)$ is the C^* -algebra generated by a and 1_H (i.e., the norm-closure of the algebra of all polynomials in a). Theorems B.84, B.94, and B.93 give the following spectral theorem:

Theorem 4.3. *If $a^* = a \in B(H)$, then $C^*(a)$ is commutative, $\sigma(a) \subset \mathbb{R}$ is compact, and there is an isomorphism of (commutative) C^* -algebras*

$$C(\sigma(a)) \cong C^*(a), \quad (4.2)$$

written $f \mapsto f(a)$, which is unique if it is subject to the following conditions:

1. the unit function $1_{\sigma(a)} : \lambda \mapsto 1$ corresponds to the unit operator 1_H ;
2. the identity function $\text{id}_{\sigma(a)} : \lambda \mapsto \lambda$ is mapped to the given operator a .

Furthermore, this **continuous functional calculus** satisfies the rules

$$(tf + g)(a) = tf(a) + g(a); \quad (4.3)$$

$$(fg)(a) = f(a)g(a); \quad (4.4)$$

$$f(a)^* = f^*(a). \quad (4.5)$$

Combining Theorems 4.2 and 4.3 gives a result of great importance:

Corollary 4.4. *Let H be a Hilbert space, let $a^* = a \in B(H)$, and let $\psi \in H$ be a unit vector. There exists a unique probability measure μ_ψ on the spectrum $\sigma(a)$ such that*

$$\langle \psi, f(a)\psi \rangle = \int_{\sigma(a)} d\mu_\psi f, \quad f \in C(\sigma(a)). \quad (4.6)$$

In terms of the spectral projections $e_\Delta = 1_\Delta(a)$ (defined for Borel sets $\Delta \subseteq \sigma(a)$) constructed in (B.305) - (B.307) and Theorem B.102, the Born measure is given by

$$\mu_\psi(\Delta) = \|e_\Delta \psi\|^2. \quad (4.7)$$

More generally, a density operator $\rho \in \mathcal{D}(H)$ induces a unique probability measure μ_ρ on $\sigma(a)$ for which

$$\mathrm{Tr}(\rho f(a)) = \int_{\sigma(a)} d\mu_\rho f, \quad f \in C(\sigma(a)); \quad (4.8)$$

$$\mu_\rho(\Delta) = \mathrm{Tr}(\rho e_\Delta). \quad (4.9)$$

This measure on $\sigma(a)$ is called the **Born measure** (defined by a and ψ or ρ).

Proof. The point is that the map $f \mapsto \langle \psi, f(a)\psi \rangle$ defines a state on $C(\sigma(a))$:

- Linearity follows from linearity of the continuous functional calculus $f \mapsto f(a)$;
- Positivity follows because if $f \geq 0$, then $f = \sqrt{f} \cdot \sqrt{f}$, so that by (4.4) and (4.5), $\langle \psi, f(a)\psi \rangle = \|\sqrt{f}(a)\psi\|^2 \geq 0$;
- Unitality follows from Theorem 4.3.1, i.e., $\langle \psi, 1_{\sigma(a)}(a)\psi \rangle = \langle \psi, 1_H\psi \rangle = 1$.

To prove (4.7), use Lemma B.97 to approximate 1_Δ by functions $f_n \in C(\sigma(a))$ as stated. By Theorem B.13.2 (i.e., the Lebesgue Monotone Convergence Theorem), we have $\int_{\sigma(a)} d\mu_\psi f_n \rightarrow \int_{\sigma(a)} d\mu_\psi 1_\Delta = \mu_\psi(\Delta)$, whereas by (B.315) with $a_n = f_n(a)$, one has $\langle \psi, f_n(a)\psi \rangle \rightarrow \langle \psi, e_\Delta\psi \rangle = \|e_\Delta\psi\|^2$. Hence (4.7) follows from (4.6).

The proof for density operators is analogous. \square

Defining the mean value $\langle a \rangle_\psi$ of a with respect to the Born measure μ_ψ by

$$\langle a \rangle_\psi = \int_{\sigma(a)} d\mu_\psi(x) x, \quad (4.10)$$

and similarly for ρ , using Theorem 4.3.2 we easily obtain

$$\langle a \rangle_\psi = \langle \psi, a\psi \rangle; \quad (4.11)$$

$$\langle a \rangle_\rho = \mathrm{Tr}(\rho a). \quad (4.12)$$

As an important special case, suppose that $\sigma(a) = \sigma_\rho(a)$ (i.e., each $\lambda \in \sigma(a)$ is an eigenvalue); this always happens if H is finite-dimensional. Eq. (A.57) then gives

$$\langle \psi, f(a)\psi \rangle = \sum_{\lambda \in \sigma(a)} f(\lambda) \cdot \|e_\lambda\psi\|^2,$$

where e_λ is the projection onto the eigenspace $H_\lambda = \{\psi \in H \mid a\psi = \lambda\psi\}$. Thus

$$\mu_\psi(\lambda) = \|e_\lambda\psi\|^2, \quad (4.13)$$

and using the notation $P_\psi(a = \lambda)$ for $\mu_\psi(\lambda)$, eq. (4.11) just becomes

$$\langle a \rangle_\psi = \sum_{\lambda \in \sigma(a)} \lambda \cdot P_\psi(a = \lambda). \quad (4.14)$$

It is customary to extend the Born measure on $\sigma(a) \subset \mathbb{R}$ to a (probability) measure μ'_ψ on all of \mathbb{R} by simply stipulating that

$$\mu'_\psi(\Delta) = \mu_\psi(\Delta \cap \sigma(a)); \quad (4.15)$$

we will often assume this and omit the prime. This obviously implies that $\mu_\psi(\Delta) = 0$ for any Borel set $\Delta \subset \mathbb{R}$ disjoint from $\sigma(a)$; in particular, if $\sigma(a)$ is discrete, then μ_ψ is concentrated on the eigenvalues λ of a , in that

$$\mu_\psi(\Delta) = \sum_{\lambda \in \Delta \cap \sigma(a)} \mu_\psi(\lambda). \quad (4.16)$$

To state an interesting property of the Born measure we need Hausdorff's solution to the relevant special case of the famous **Hamburger Moment Problem**:

Theorem 4.5. *If $K \subset \mathbb{R}$ is compact, then any finite measure μ on K is determined by its moments*

$$\alpha_n = \int_K d\mu(x) x^n. \quad (4.17)$$

Using $f(x) = x^n$ in (4.6), we therefore obtain:

Corollary 4.6. *The Born measure μ_ψ is determined by its moments*

$$\alpha_n = \langle \psi, a^n \psi \rangle. \quad (4.18)$$

More precisely, we need to be sure that numbers (α_n) of the kind (4.18) are the moments of some (probability) measure. This follows from the spectral theorem by running the above argument backwards, but one may also use the general solution of the Hamburger Moment Problem, which we here state without proof:

Theorem 4.7. *A sequence of real numbers (α_n) forms the moments of some measure μ on \mathbb{R} iff for all $N \in \mathbb{N}$ and $(\beta_1, \dots, \beta_N) \in \mathbb{C}^N$ one has $\sum_{n,m=0}^N \beta_n \beta_m \alpha^{n+m} \geq 0$. Furthermore, if there are constants C and D such that $|\alpha_n| \leq CD^n n!$, then μ is uniquely determined by its moments (α_n) .*

These conditions are easily checked from (4.18).

If a is unbounded, but still assumed to be self-adjoint (in the sense appropriate for unbounded operators, cf. Definition B.70), the spectrum $\sigma(a)$ remains real (see Theorem B.93) but it is no longer compact. Nonetheless, the Born measure on $\sigma(a)$ may be constructed in almost exactly the same way as in the bounded case, this time invoking Corollary B.21 and Theorem B.158 instead of Theorems 4.2 and B.94, respectively. Corollary 4.4 then holds almost *verbatim* for the unbounded case:

Corollary 4.8. *Let H be a Hilbert space, let $a^* = a$, and let $\psi \in H$ be a unit vector. There exists a unique probability measure μ_ψ on the spectrum $\sigma(a)$ such that*

$$\langle \psi, f(a) \psi \rangle = \int_{\sigma(a)} d\mu_\psi f, \quad f \in C_0(\sigma(a)). \quad (4.19)$$

Also, eqs. (4.7) and (4.9) hold, as does (4.8), with $f \in C_0(\sigma(a))$.

There is no need to worry about domains, since even if a is unbounded, $f(a)$ is bounded for $f \in C_b(\sigma(a))$, and hence also for $f \in C_0(\sigma(a))$.

The physical relevance of the Born measure is given by the **Born rule**:

If an observable a is measured in a state ρ , then the probability $P_\rho(a \in \Delta)$ that the outcome lies in $\Delta \subset \mathbb{R}$ is given by the Born measure μ_ρ defined by a and ρ , i.e.,

$$P_\rho(a \in \Delta) = \mu_\rho(\Delta). \tag{4.20}$$

As in the finite-dimensional case, the Born measure may be generalized to families (a_1, \dots, a_n) of commuting self-adjoint operators. Assuming these are bounded, the C^* -algebra $C^*(a_1, \dots, a_n)$ is defined in the obvious way, i.e., as the smallest C^* -algebra containing each a_i , or, equivalently, as the norm-closure of the algebra of all finite polynomials in the (a_1, \dots, a_n) . This C^* -algebra is commutative, as a simple approximation argument shows: polynomials in the a_i obviously commute, and this property extends to the closure by continuity of multiplication. However, even in the bounded case, the correct notion of a joint spectrum is not obvious. In order to motivate the following definition, it helps to recall Definition 1.4, Theorem C.24, and especially the last sentence before the proof of the latter, making the point that the spectrum $\sigma(a)$ of a single (bounded) self-adjoint operator coincides with the image of the Gelfand spectrum $\Sigma(C^*(a))$ in \mathbb{C} under the map $\omega \mapsto \omega(a)$.

Definition 4.9. *1. The joint spectrum $\sigma(\underline{a}) = \sigma(a_1, \dots, a_n) \subset \mathbb{R}^n$ of a finite family $\underline{a} = (a_1, \dots, a_n)$ of commuting bounded self-adjoint operators is the image of the Gelfand spectrum $\Sigma(C^*(a_1, \dots, a_n)) = \Sigma(C^*(\underline{a}))$ under the map*

$$\Sigma(C^*(a_1, \dots, a_n)) \rightarrow \mathbb{R}^n, \quad \omega \mapsto (\omega(a_1), \dots, \omega(a_n)). \tag{4.21}$$

Since $\omega(a_i)$ only utilizes the restriction of ω to $C^(a_i) \subset C^*(\underline{a})$, we have $\omega(a_i) \in \sigma(a_i) \subset \mathbb{R}$, so that $\Sigma(C^*(\underline{a})) \subseteq \sigma(a_1) \times \dots \times \sigma(a_n)$ is a compact subset of \mathbb{R}^n .*

To justify this definition, we note that:

- For $n = 1$, this definition reproduces the usual spectrum, cf. Theorem C.24.
- For $n > 1$ and $\dim(H) < \infty$, we recover the joint spectrum of Definition A.16.
- For $n > 1$ and $\dim(H) = \infty$, Weyl's Theorem B.91 generalizes in the obvious way: we have $\lambda \in \sigma(\underline{a})$ iff there exists a sequence (ψ_k) of unit vectors in H with

$$\lim_{k \rightarrow \infty} \|(a_i - \lambda_i)\psi_k\| = 0, \tag{4.22}$$

for each $i = 1, \dots, n$. The proof is similar.

One way to see the second claim is to use Proposition C.14 joined with the observation that, as in the case of $A = B(H)$ for finite-dimensional H , any pure state on a finite-dimensional C^* -algebra $A \subset B(H)$ is a vector state (2.42), too. To see this, we first specialize Theorem C.133 to the finite-dimensional case (where the proof becomes elementary), so that each state on $C^*(\underline{a})$ takes the form (2.33). Subsequently, we use the spectral decomposition (2.6), and use the definition of purity: suppose $\omega(b) = \text{Tr}(\rho b) = \sum_i p_i \langle v_i, b v_i \rangle \equiv \sum_i p_i \omega_{v_i}(b)$ is pure, where $b \in C^*(\underline{a})$.

Then $\omega_{v_i} = \omega$ for each i , so that ω is a vector state, say $\omega(b) = \langle \psi, b\psi \rangle$ where ψ is one of the v_i . Once we know this, suppose $\underline{\lambda} = (\lambda_1, \dots, \lambda_n) \in \sigma(\underline{a})$, with $\lambda_i = \omega(a_i)$. Multiplicativity of ω implies that for any finite polynomial in n real variables we have $\langle \psi, p(\underline{a})\psi \rangle = p(\underline{\lambda})$, which easily gives $a_i\psi = \lambda_i\psi$ for each i ; for example, take $p(\underline{x}) = (x_i - \lambda_i)^2$, so that the previous equation gives $\|(a_i - \lambda_i)\psi\|^2 = 0$.

Conversely, if $\underline{\lambda}$ is a joint eigenvalue of \underline{a} , then by definition there exists a joint eigenvector ψ whose vector state $\omega(b) = \langle \psi, b\psi \rangle$ on $C^*(\underline{a})$ is multiplicative.

Using this (perhaps contrived) notion of a joint spectrum, Theorem 2.19 now holds by construction also if $\dim(H) = \infty$, where the pertinent isomorphism $f \mapsto f(\underline{a})$ is given as in the single operator case, that is, by starting with polynomials and using a continuity argument to pass to arbitrary continuous functions.

Theorem 2.18 and Corollary 4.4 then generalize to:

Theorem 4.10. *Let H be a Hilbert space, let $\underline{a} = (a_1, \dots, a_n)$ be a finite family of commuting bounded self-adjoint operators, and let $\psi \in H$ be a unit vector. There exists a unique probability measure μ_ψ on the joint spectrum $\sigma(\underline{a})$ such that*

$$\langle \psi, f(\underline{a})\psi \rangle = \int_{\sigma(\underline{a})} d\mu_\psi f, \quad f \in C(\sigma(\underline{a})), \quad (4.23)$$

or, equivalently, for special Borel sets $\underline{\Delta} = \Delta_1 \times \dots \times \Delta_n \subseteq \sigma(\underline{a})$, where $\Delta_i \subset \sigma(a_i)$,

$$\mu_\psi(\underline{\Delta}) = \|e_{\Delta_1} \cdots e_{\Delta_n} \psi\|^2, \quad (4.24)$$

where the $e_{\Delta_i} = 1_{\Delta_i}(a_i)$ are the pertinent spectral projections (which commute).

Similarly for density operators instead of pure states.

If (some of) the operators a_i are unbounded, we use the trick of §B.21 and pass to their bounded transforms b_i , see Theorem B.152. We say that the b_i **commute** iff the corresponding bounded operators b_i do; this is equivalent to commutativity of all spectral projections of the a_i . We then define, in self-explanatory notation,

$$\sigma(\underline{a}) = \{ \underline{\lambda}(1 - \underline{\lambda}^2)^{-1/2} \mid \underline{\lambda} \in \sigma(\underline{b}) \cap (-1, 1)^n \}. \quad (4.25)$$

This leads to Born measures on $\sigma(\underline{a})$ defined either as in (4.23), with $f \in C(\sigma(\underline{a}))$ replaced by $f \in C_0(\sigma(\underline{a}))$, cf. (4.19), or as in (4.24).

For example, if $H = L^2(\mathbb{R}^n)$ and $a_i\psi(x) = x_i\psi(x)$, defined on the domain

$$D(a_i) = \{ \psi \in L^2(\mathbb{R}^n) \mid \int_{\mathbb{R}^n} d^n x x_i^2 |\psi(x)|^2 < \infty \}, \quad (4.26)$$

as in (B.242), then $b_i\psi(x) = x_i(1 + x_i^2)^{-1/2}\psi(x)$, so that $\sigma(\underline{b}) = [-1, 1]^n$ and hence $\sigma(\underline{a}) = \mathbb{R}^n$. For a measurable region $\underline{\Delta} \subset \mathbb{R}^n$ we then have Pauli's famous formula

$$\mu_\psi(\underline{\Delta}) = \int_{\underline{\Delta}} d^n x |\psi(x)|^2 \quad (4.27)$$

for finding the particle in the region $\underline{\Delta}$, given that the system is in a pure state ψ .

4.2 Density operators and normal states

Definition 2.4 of a state still makes good sense in the infinite-dimensional case, as it simply specializes the general definition of a state on a C^* -algebra A to the case $A = B(H)$. Thus we continue to say that a state on $B(H)$ is a complex-linear map $\omega : B(H) \rightarrow \mathbb{C}$ satisfying $\omega(b^*b) \geq 0$ for each $b \in B(H)$ and $\omega(1_H) = 1$. Despite this lack of novelty in the definition of a state (i.e., compared to finite-dimensional Hilbert spaces), Theorem 2.7 no longer holds if H is infinite-dimensional: although it (almost trivially) remains true that density operators ρ on H define states on $B(H)$ through the fundamental correspondence $\omega(a) = \text{Tr}(\rho a)$, $a \in B(H)$, cf. (2.33), there are (many) states that are *not* given in that way (see below). Fortunately, states that *do* arise through (2.33) can be characterized in a simple way.

Definition 4.11. A state $\omega : B(H) \rightarrow \mathbb{C}$ is called **normal** if for each orthogonal family (e_i) of projections (i.e., $e_i^* = e_i$ and $e_i e_j = \delta_{ij} e_i$) one has

$$\omega\left(\sum_i e_i\right) = \sum_i \omega(e_i). \quad (4.28)$$

Here $\sum_i e_i$ is defined as the projection on the smallest closed subspace K of H that contains each $e_i H$ (that is, $\sum_i e_i = \vee_i e_i$, i.e., the supremum in the poset $\mathcal{P}(H)$ of all projections on H with respect to the partial order $e \leq f$ iff $eH \subseteq fH$). Furthermore, the sum over i on the right-hand side is defined by (B.11), i.e., as the supremum (in \mathbb{R}) of the set of all sums $\sum_{i \in F} \omega(e_i)$ over finite subsets $F \subset I$ of the index set I in which i takes values. It is finite because $\sum_{i \in F} e_i \leq 1_H$ and hence, since ω is positive,

$$\sum_{i \in F} \omega(e_i) \leq \omega(1_H) = 1.$$

For example, let (v_i) be a basis of H with associated one-dimensional projections

$$e_i = |v_i\rangle\langle v_i|. \quad (4.29)$$

If ω is assumed to be a state, then the additivity condition (4.28) implies

$$\sum_i \omega(e_i) = 1, \quad (4.30)$$

or, equivalently, using Definition B.6 etc. as well as the notation $e_F \equiv \sum_{i \in F} e_i$,

$$\lim_F \omega(e_F) = 1. \quad (4.31)$$

If H is separable, any orthogonal family (e_i) of projections is necessarily countable, and (4.28) is analogous to the countable additivity condition defining a measure.

Theorem 4.12. A state ω on $B(H)$ takes the form $\omega(a) = \text{Tr}(\rho a)$ for some (unique) density operator $\rho \in \mathcal{D}(H)$ iff it is normal.

Proof. First, eq. (2.33) implies (4.28). To see this, take the trace with respect to some basis (v_j) of H that is *adapted* to the family (e_i) in the sense that for each j , either $e_i v_j = v_j$ (i.e., $v_j \in e_i H$) for one value of i , or $e_i v_j = 0$ for all i . Then

$$\omega\left(\sum_i e_i\right) = \text{Tr}\left(\rho \sum_i e_i\right) = \sum_j \langle v_j, \rho \sum_i e_i v_j \rangle = \sum_j \langle v_j, \rho v_j \rangle,$$

where the sum \sum_j is over those j for which $v_j \in K \equiv \bigvee_i e_i H$. On the other hand, since the basis is adapted, we have $v_j \in K$ iff there is an i for which $e_i v_j = v_j$ (since otherwise $e_i v_j = 0$ and hence $v_j \perp e_i H$ for each i , so that $v_j \in K^\perp$), so

$$\sum_i \omega(e_i) = \sum_i \text{Tr}(\rho e_i) = \sum_i \sum_j \langle v_j, \rho e_i v_j \rangle = \sup_{F \subset I} \sum_{j \in J_F} \langle v_j, \rho v_j \rangle = \sum_j \langle v_j, \rho v_j \rangle,$$

where J_F consists of those j for which $v_j \in \sum_{i \in F} e_i H$. This gives (4.28).

Conversely, assume ω is normal. For the e_i in (4.28) we now take the projections (4.29) determined by some basis (v_i) . For each $a \in B(H)$ we then have

$$\omega(a) = \lim_F \omega(e_F a). \quad (4.32)$$

Indeed, using Cauchy–Schwarz for the positive semi-definite form $(a, b) = \omega(a^* b)$, as in (C.197), and using $\sum_i e_i = 1_H$ and hence $\omega(a) = \omega(\sum_i e_i a)$ we have

$$|\omega(a) - \omega(e_F a)|^2 = |\omega(e_{F^c} a)|^2 \leq \omega(a^* a) \omega(e_{F^c}) \leq \|a\|^2 \omega(e_{F^c}), \quad (4.33)$$

since $e_{F^c} \equiv \sum_{i \notin F} e_i$ is a projection. Since $\omega(e_F) + \omega(e_{F^c}) = \omega(1_H) = 1$, eq. (4.31) gives $\lim_F \omega(e_{F^c}) = 0$, so that (4.33) gives (4.32). For each finite $F \subset I$, the operator $e_F a$ has finite rank and hence is compact. According to Theorem B.146, the restriction of $\omega : B(H) \rightarrow \mathbb{C}$ to the C*-algebra $B_0(H)$ of compact operators on H is induced by a trace-class operator ρ , which (from the requirement that ω be a state) must be a density operator. Hence $\omega(e_F a) = \text{Tr}(\rho e_F a)$, and we finally have

$$\omega(a) = \lim_F \omega(e_F a) = \lim_F \text{Tr}(\rho e_F a) = \text{Tr}(\rho a). \quad (4.34)$$

To derive the final equality, we rewrite $\text{Tr}(\rho e_F a) = \text{Tr}(e_F a \rho)$, cf. (A.78) and Proposition B.144, note that $a \rho \in B_1(H)$, as shown in Corollary B.147, and observe that for any $b \in B_1(H)$ we have $\lim_F \text{Tr}(e_F b) = \text{Tr}(b)$. To see this, simply compute the trace in the basis (v_i) defining the projections e_i through (4.29), so that $\text{Tr}(e_F b) = \sum_{i \in F} \langle v_i, b v_i \rangle$, and note that by Definition B.6,

$$\lim_F \sum_{i \in F} \langle v_i, b v_i \rangle = \sum_i \langle v_i, b v_i \rangle = \text{Tr}(b).$$

Finally, suppose $\omega(a) = \text{Tr}(\rho_1 a) = \text{Tr}(\rho_2 a)$ for each $a \in B(H)$ and hence for each $a \in B_0(H)$. It follows from (B.476) that $\text{Tr}(\rho a) = 0$ for all $a \in B_0(H)$ iff $\rho = 0$. Hence $\rho_1 = \rho_2$, i.e., a normal state ω uniquely determines a density operator ρ . \square

If ω is normal, we may therefore use the spectral resolution (2.6) of the corresponding density operator ρ , i.e., $\rho = \sum_i p_i |v_i\rangle\langle v_i|$, where (v_i) is some basis of H consisting of eigenvectors of ρ (which exists because ρ is compact and self-adjoint), and the corresponding eigenvalues satisfy $p_i \geq 0$ and $\sum_i p_i = 1$; see the explanation after Definition B.148. Computing the trace in the same basis gives

$$\mathrm{Tr}(\rho a) = \sum_i p_i \langle v_i, a v_i \rangle. \quad (4.35)$$

We may characterize normality in a number of other ways. First note that because of the duality $B_1(H)^* \cong B(H)$ of Theorem B.146, cf. (B.477), we may equip $B(H)$ with the w^* -topology in its role as the dual of the trace-class operators $B_1(H)$, see §B.9; this means that $a_\lambda \rightarrow a$ iff $\mathrm{Tr}(\rho a_\lambda) \rightarrow \mathrm{Tr}(\rho a)$ for each $\rho \in B_1(H)$, or, equivalently, for each $\rho \in \mathcal{D}(H)$, since each trace-class operator is a linear combination of at most four density operators, as follows from Lemma C.53 with (C.8) - (C.9). The w^* -topology on $B(H)$, seen as the dual of $B_1(H)$, is called the σ -weak topology. By Proposition B.46, the σ -weakly continuous linear functionals φ on $B(H)$ are just those given by $\varphi(a) = \mathrm{Tr}(\rho b)$ for some trace-class operator $b \in B_1(H)$.

Secondly, $B(H)$ is *monotone complete*, in the sense that each net (a_λ) of positive operators that is bounded (i.e., $0 \leq a_\lambda \leq c \cdot 1_H$ for some $c > 0$ and all $\lambda \in \Lambda$) and increasing (in that $a_\lambda \leq a_{\lambda'}$ whenever $\lambda \leq \lambda'$) has a supremum a with respect to the standard ordering \leq on $B(H)_+$, which supremum coincides with the strong limit of the net (i.e., $\lim_\lambda a_\lambda \psi = a\psi$ for each $\psi \in H$); the proof is the same as for Proposition B.98, and also here we write $a_\lambda \nearrow a$ to describe this entire situation.

Corollary 4.13. *The following conditions on a state $\omega \in S(B(H))$ are equivalent:*

1. ω is normal, cf. Definition 4.11;
2. $\omega(a) = \lim_\lambda \omega(a_\lambda)$ if $a_\lambda \nearrow a$;
3. $\omega(a) = \mathrm{Tr}(\rho a)$ for some density operator $\rho \in \mathcal{D}(H)$;
4. ω is σ -weakly continuous.

Proof. We have seen $1 \leftrightarrow 3 \leftrightarrow 4$, and $2 \rightarrow 1$ is obvious, so establishing $3 \rightarrow 2$ would complete the proof. To this effect, we first note that because the sum (4.35) is convergent, for $\varepsilon > 0$ we may find a finite subset $F \subset I$ for which $\sum_{i \notin F} p_i < \varepsilon/2 \|a\|$ (assuming $a \neq 0$). Since $0 \leq a_\lambda \leq a$ also implies $a_\lambda \leq \|a\| \cdot 1_H$ (since $a \leq \|a\| \cdot 1_H$), we therefore have $|\sum_{i \notin F} p_i \langle v_i, (a_\lambda - a) v_i \rangle| < 2\varepsilon/3$, uniformly in λ . Moreover, since F is finite and $a_\lambda \rightarrow a$ strongly, we can find λ_0 such that for all $\lambda \geq \lambda_0$ we have

$$|\sum_{i \in F} p_i \langle v_i, (a_\lambda - a) v_i \rangle| < \varepsilon/3. \quad (4.36)$$

Consequently, for such λ ,

$$|\mathrm{Tr}(\rho(a_\lambda - a))| \leq |\sum_{i \in F} p_i \langle v_i, (a_\lambda - a) v_i \rangle| + |\sum_{i \notin F} p_i \langle v_i, (a_\lambda - a) v_i \rangle| < \frac{2}{3}\varepsilon + \frac{1}{3}\varepsilon = \varepsilon.$$

This shows that $\lim_\lambda |\mathrm{Tr}(\rho(a_\lambda - a))| = 0$, so that assumption 3 implies no. 2. \square

We denote the **normal state space** of $B(H)$, i.e., the set of all normal states on $B(H)$ by $S_n(B(H))$. It is easy to see from Definition B.148 that $S_n(B(H))$ is a convex (but not necessarily compact!) subset of the total state space $S(B(H))$.

Corollary 4.14. *The relation $\omega(a) = \text{Tr}(\rho a)$ induces an isomorphism*

$$S_n(B(H)) \cong \mathcal{D}(H) \quad (4.37)$$

of convex sets (i.e., $\omega \leftrightarrow \rho$). Furthermore, for the corresponding pure states we have

$$P_n(B(H)) \cong \mathcal{P}_1(H), \quad (4.38)$$

i.e., any pure state ω on $B_0(H)$, as well as any normal pure state on $B(H)$, is given by $\omega = \omega_\psi$ for some unit vector $\psi \in H$, where $\omega(a) = \langle \psi, a\psi \rangle$, cf. (2.42).

The proof of (4.38) is practically the same as in the finite-dimensional case. From Theorem B.146 we obtain another characterization of $S_n(B(H))$ and hence of $\mathcal{D}(H)$:

Corollary 4.15. *If $B_0(H)$ is the C^* -algebra of compact operators on H , we have*

$$S(B_0(H)) = S_n(B(H)); \quad (4.39)$$

$$P(B_0(H)) = P_n(B(H)), \quad (4.40)$$

in the sense that any (pure) state ω on $B_0(H)$ has a unique normal extension to a (pure) state ω' on $B(H)$, given by the same density operator ρ that yields ω .

It can be shown that any state $\omega \in S(B(H))$ has a convex decomposition

$$\omega = t\omega_n + (1-t)\omega_s, \quad (4.41)$$

where $t \in [0, 1]$, ω_n is a normal state, and ω_s is called a **singular state**. In particular, since for $t \in (0, 1)$ the state ω is mixed, a *pure state is either normal or singular*.

Singular states are not as aberrant as the terminology may suggest: such states are routinely used in the physics literature and are typically denoted by $|\lambda\rangle$, where λ lies in the continuous spectrum of some self-adjoint operator (that has to be maximal for this notation to even begin to make sense, see §4.3 below). Examples of such “improper eigenstates” are $|x\rangle$ and $|p\rangle$, which many physicists regard as idealizations. However, mathematically such states are at least defined, namely as singular pure states on $B(H)$. The key to the existence of such states lies in Proposition C.15 and its proof, which should be reviewed now; we only need the case $a^* = a$.

Proposition 4.16. *Let $a = a^* \in B(H)$ have non-empty continuous spectrum, so that there is some $\lambda \in \sigma(a)$ that is not an eigenvalue of a . Then $\omega_\lambda(f(a)) = f(\lambda)$ defines a pure state on $A = C^*(a)$, whose extension to $B(H)$ by any pure state is singular.*

Proof. Normal pure states on $B(H)$ take the form $\omega_\psi(b) = \langle \psi, b\psi \rangle$, where $\psi \in H$ is a unit vector and $b \in B(H)$. We know from Proposition C.14 that ω_λ is multiplicative on $C^*(a)$. However, if some multiplicative state ω on $C^*(a)$ has the form $\omega = \omega_\psi$, then ψ must be eigenvector of a ; cf. the proof of Proposition 2.3. \square

4.3 The Kadison–Singer Conjecture

To obtain deeper insight into singular pure states, and as a matter of independent interest, we return to the Kadison–Singer problem, cf. §2.6. Recall that this problem asks if some abelian unital C^* -algebra $A \subset B(H)$ has the **Kadison–Singer property**, stating that a pure state ω_A on A has a *unique* pure extension ω to $B(H)$. Here the issue is uniqueness rather than existence, since at least one such extension exists: since A is necessarily unital (with $1_A = 1_H$) and ω_A is a state on A , so that in particular $\omega_A(1_A) = \|\omega_A\| = 1$, Corollary B.41 gives the existence of a bounded extension ω satisfying $\omega(1_H) = \|\omega\| = 1$, which by Proposition C.5 is a state on $B(H)$. Proposition 2.22 then gives the existence of a *pure* extension ω . As in the finite-dimensional case, the Kadison–Singer property forces A to be maximal (in the poset $\mathcal{C}(B(H))$ of all abelian unital C^* -subalgebras of $B(H)$, ordered by inclusion):

Proposition 4.17. *If some abelian unital C^* -subalgebra A of $B(H)$ has the Kadison–Singer property, then A is necessarily maximal.*

Proof. We use the Gelfand isomorphism $A \cong C(P(A))$, where $P(A)$ is the pure state space of A , cf. Theorem C.8 and Proposition C.14. If A has the Kadison–Singer property and $A \subseteq B \subset B(H)$, where B is an abelian unital C^* -subalgebra A of $B(H)$, then ω_A has a unique pure extension ω on $B(H)$, which restricts to some state ω_B on B . The same reasoning as in the proof of Proposition 2.22 shows that ω_B is a pure state on B , so that we obtain a unique map

$$P(A) \mapsto P(B); \tag{4.42}$$

$$\omega_A \mapsto \omega_B. \tag{4.43}$$

The inverse of this map is simply the pullback of the inclusion $A \hookrightarrow B$, i.e., $\omega_B \in P(B)$ defines $\omega_A \in P(A)$ by restriction, so that we have a bijection $P(A) \cong P(B)$, $\omega_A \leftrightarrow \omega_B$. Since for any pair of C^* -algebras $A \subseteq B$ the pullback $S(B) \rightarrow S(A)$ is continuous (in the pertinent w^* -topology), the map $\omega_B \mapsto \omega_A$ is continuous. As in Lemma C.20, this implies that it is in fact a homeomorphism, so that $A \cong B$ through the inclusion $A \hookrightarrow B$. This gives $A = B$, and hence A is maximal. \square

Maximality of A implies $A' = A$, so that A is a von Neumann algebra, sharing the unit of $B(H)$. To see the relevance of singular states for the Kadison–Singer problem, we first settle the normal case. We know what it means for a state on $B(H)$ to be normal (cf. Definition 4.11 and Corollary 4.13); for arbitrary von Neumann algebras $A \subset B(H)$ the situation is exactly the same: we *define* normality by (4.28) and *characterize* it by the equivalent properties in Corollary 4.13, where the σ -weak topology on A may be defined either as the one inherited from $B(H)$, or, more intrinsically, and the w^* -topology from the duality $A = A_*^*$, where the Banach space A_* is the so-called predual of A , e.g., $\ell_*^\infty \cong \ell^1$ and $L^\infty(0, 1)_* = L^1(0, 1)$, cf. §B.9.

Theorem 4.18. *Let H be a separable Hilbert space and let ω_A be a normal pure state on a maximal commutative unital C^* -algebra A in $B(H)$. Then ω_A has a unique extension to a state ω on $B(H)$, which is necessarily pure and normal.*

Proof. As noted after (4.41), a pure state on $B(H)$ is either normal or singular. The possibility that ω_A is normal whereas ω is singular is excluded by Corollary 4.13.3, so ω must be normal and hence given by a density operator. The proof of uniqueness is then the same as in the finite-dimensional case, cf. Theorem 2.21. \square

We now recall the classification of maximal maximal abelian $*$ -algebras (and hence of maximal abelian von Neumann algebras) A in $B(H)$ up to unitary equivalence (cf. Theorem B.118). This classification is the relevant one for the Kadison–Singer problem, since, as is easily seen, $A \subset B(H)$ has the Kadison–Singer property iff $uAu^{-1} \subset B(uH)$ has it. The uniqueness of the finite-dimensional case will be lost:

Theorem 4.19. *If H is separable and infinite-dimensional, and $A \subset B(H)$ is a maximal abelian $*$ -algebra, then A is unitarily equivalent to exactly one of the following:*

1. $L^\infty(0, 1) \subset B(L^2(0, 1))$;
2. $\ell^\infty \subset B(\ell^2)$;
3. $L^\infty(0, 1) \oplus \ell^\infty(\kappa) \subset B(L^2(0, 1) \oplus \ell^2(\kappa))$,

where $\ell^\infty \equiv \ell^\infty(\mathbb{N})$, $\ell^2 \equiv \ell^2(\mathbb{N})$, and κ is either $\{1, \dots, n\}$, in which case $\ell^2(\kappa) = \mathbb{C}^n$ and $\ell^\infty(\kappa) = D_n(\mathbb{C})$, or $\kappa = \mathbb{N}$, in which case $\ell^2(\kappa) = \ell^2$ and $\ell^\infty(\kappa) = \ell^\infty$.

This classification sheds some more light on Theorem 4.18. Since $L^\infty(0, 1)$ has no pure normal states and $D_n(\mathbb{C})$ has been dealt with in Theorem 2.21, the interesting case is ℓ^∞ . Using Corollary 4.13.3 (or the analysis below), it is easy to check that the normal pure states on ℓ^∞ are given by $\omega_A(f) = f(x)$ for some $x \in \mathbb{N}$; these are vector state of the kind $\omega_A(f) = \langle \psi, m_f \psi \rangle$ with $\psi = \delta_x$, or, in other words, they are given by $\omega_A(f) = \text{Tr}(\rho m_f)$ with $\rho = |\delta_x\rangle\langle \delta_x|$. We now invoke a fairly deep result:

Proposition 4.20. *A pure state ω on $B(H)$ is singular iff one (and hence all) of the following equivalent conditions is satisfied:*

- $\omega(a) = 0$ for each $a \in B_0(H)$;
- $\omega(e) = 0$ for each one-dimensional projection e ;
- $\sum_i \omega(e_i) = 0$ for the projections $e_i = |v_i\rangle\langle v_i|$ defined by some basis (v_i) .

One direction is easy: a normal pure state certainly does not satisfy the condition in question. For example, given (2.42) one may take $a = |\psi\rangle\langle \psi|$, which as a one-dimensional projection lies in $B_0(H)$, so that $\omega_\psi(a) = 1$. We omit the other direction of the proof. We conclude from this proposition that a pure singular state on $B(\ell^2)$ cannot restrict to a normal pure state on ℓ^∞ , which reconfirms Theorem 4.18.

We now study the Kadison–Singer property for each of the three cases in Theorem 4.19 (where the third will be an easy corollary of the first and the second). Since the proofs of the first two cases are formidable, we just sketch the argument.

Theorem 4.21. • *There exist (necessarily singular) pure states on $L^\infty(0, 1)$ that do not have a unique extension to $B(L^2(0, 1))$, and similarly for $L^\infty(0, 1) \oplus \ell^\infty(\kappa)$.*

- *Any pure state on ℓ^∞ has a unique extension to $B(\ell^2)$.*

The statement about ℓ^∞ is the **Kadison–Singer Conjecture**, which dates from 1959 but was only proved in 2013. The first claim (which was already known to Kadison and Singer themselves) is equally remarkable, however, as is the contrast between the two parts of Theorem 4.21. In particular, Dirac’s notation $|\lambda\rangle$ may be ambiguous.

The key to the proof of the first claim lies in the choice of a total countable family of normal states on $L^\infty(0, 1)$, from which all pure states may be constructed by a limiting operation. Here we call a (countable) family $(\omega_n)_{n \in \mathbb{N}}$ of states on some C^* -algebra A **total** if, for any self-adjoint $a \in A$, the conditions $\omega_n(a) \geq 0$ for each n imply $a \geq 0$ (the converse is trivial). For example, the well-known **Haar basis** (h_n) of $L^2(0, 1)$ provides such a family. The functions forming this basis are defined via some bijection β between the set of pairs (k, l) and \mathbb{N} , e.g., $\beta(k, l) = k + 2^l$, by

$$h_n = \chi_{\beta^{-1}(n)}, \quad (n \in \mathbb{N} = \{1, 2, \dots\}); \tag{4.44}$$

$$\chi_{k,l}(x) = 2^{k/2} g(2^k x - l), \quad (k \in \mathbb{N} \cup \{0\}, 0 \leq l < 2^k); \tag{4.45}$$

$$g(x) = 1_{[0,1/2)} - 1_{[1/2,1)}. \tag{4.46}$$

Basic analysis then shows that the Haar functions h_n form a basis of $L^2(0, 1)$ and that the associated vector states ω_n on $L^\infty(0, 1)$ form a total set, where obviously

$$\omega_n(f) = \langle h_n, m_f h_n \rangle = \int_0^1 h_n^2 f. \tag{4.47}$$

The relevance of total sets to the conjecture is explained by the following lemma.

Lemma 4.22. *If $T \subset S(A)$ is a total set of states on a unital C^* -algebra A , then*

$$S(A) = \text{co}(T)^-; \tag{4.48}$$

$$P(A) \subseteq T^-, \tag{4.49}$$

where $\text{co}(T)^-$ is the w^* -closure of the convex hull of T in A^* or in $S(A)$.

Proof. The inclusion $\text{co}(T)^- \subseteq S(A)$ is obvious, since $T \subseteq S(A)$ and $S(A)$ is a compact (and hence a closed) convex set. To prove the converse inclusion, suppose $a = a^* \in A$ and $s \in \mathbb{R}$ are such that $\omega(a) \geq s$ for each $\omega \in T$. Then $\omega(a - s \cdot 1_A) \geq 0$ and hence $\omega(a) \geq s$ for each $\omega \in S(A)$. Using Theorem B.43 (of Hahn–Banach type), this property would lead to a contradiction if $S(A)$ were not contained in $\text{co}(T)^-$.

The second claim, which is the one we will use, follows from the first through a corollary of the Krein–Milman Theorem B.50, stating that if $T \subset K$ is any subset of a compact convex set K such that $K = \text{co}(T)^-$, then $\partial_e K \subseteq T^-$. This corollary may be proved (by contradiction) from Theorem B.43 in a similar way. \square

Our next aim is to get rid of the closure in (4.49). The Haar basis yields a map

$$h : \mathbb{N} \rightarrow S(L^\infty(0, 1)); \tag{4.50}$$

$$n \mapsto \omega_n, \tag{4.51}$$

with image T , i.e., the set of Haar states. Since $S(A)$ is a compact Hausdorff space (in its w^* -topology), the universal property (B.135) of the Čech–Stone compactification $\beta\mathbb{N}$ of \mathbb{N} implies that h extends (uniquely) to a continuous map

$$\beta h : \beta\mathbb{N} \rightarrow S(A),$$

whose image is compact and hence closed (since $\beta\mathbb{N}$ is compact). Since $T = h(\mathbb{N}) \subset S(A)$ we have $T \subseteq \beta h(\beta\mathbb{N})$ and hence $T^- \subseteq \beta h(\beta\mathbb{N})$, so that, from (4.49),

$$P(L^\infty(0, 1)) \subseteq \beta h(\beta\mathbb{N}). \quad (4.52)$$

Hence each pure state $\omega_c \equiv \omega_{L^\infty(0,1)}$ on $L^\infty(0, 1)$ takes the form $\omega_c = \omega_c^{(U)}$, where

$$\omega_c^{(U)}(f) = \lim_U \omega_n(f) = \bigcap_{A \in U} \{\omega_n(f) \mid n \in A\}^-, \quad f \in L^\infty(0, 1), \quad (4.53)$$

and $U \in \beta\mathbb{N}$ is some ultrafilter on \mathbb{N} , cf. (B.136). The point of this analysis, then, is that ω_U can immediately be extended to $B(L^2(0, 1))$ by the same formula, i.e.,

$$\omega^{(U)}(a) = \lim_U \omega_n(a) = \bigcap_{A \in U} \{\omega_n(a) \mid n \in A\}^-, \quad a \in B(L^2(0, 1)), \quad (4.54)$$

where $\omega_n(a) = \langle h_n, ah_n \rangle$. If $L^\infty(0, 1)$ had the Kadison–Singer property, this were the unique extension of ω_U , and we will show that this leads to a contradiction.

Apart from the use of ultrafilters, the technically most challenging part of the argument disproving the Kadison–Singer property for $L^\infty(0, 1)$ is as follows. If $A = C([0, 1])$, for any $f \in A$ and any pure state $\omega \in P(A)$ there is some $x \in [0, 1]$ such that $\omega(f) = f(x)$; see Propositions C.14 and C.19. For $A = L^\infty(0, 1)$ the situation is not that simple due to measure zero complications. Nonetheless, it is easy to show that for each *positive* $f \in L^\infty(0, 1)$ and $\omega_c \in P(L^\infty(0, 1))$ and each $\varepsilon > 0$ one has

$$\mu(\{x \in (0, 1) \mid f(x) \in [\omega_c(f) - \varepsilon, \omega_c(f) + \varepsilon]\}) > 0. \quad (4.55)$$

where μ is Lebesgue measure on $(0, 1)$. Taking the projection

$$e = 1_{\{x \in (0, 1) \mid f(x) \in [\omega_c(f) - \varepsilon/2, \omega_c(f) + \varepsilon/2]\}},$$

it follows that for each positive $f \in L^\infty(0, 1)$, $\omega \in P(L^\infty(0, 1))$ and $\varepsilon > 0$ there exists a projection $e \in \mathcal{P}(L^\infty(0, 1))$ with $\omega(e) = 1$ and $\|ef - e\omega_c(f)\| < \varepsilon$. Hard analysis then generalizes this property from $L^\infty(0, 1)$ to $B(L^2(0, 1))$, as follows:

Lemma 4.23. *If $\omega_c \in P(L^\infty(0, 1))$ has a unique extension ω to $B(L^2(0, 1))$ (which is necessarily pure if it is unique), then for each $a \in B(L^2(0, 1))$ and $\varepsilon > 0$ there exists a projection $e \in \mathcal{P}(L^\infty(0, 1))$ with $\omega_c(e) = 1$ and*

$$\|ea - e\omega(a)\| < \varepsilon. \quad (4.56)$$

To derive a contradiction between (4.54) and (4.56), we use a bijection $b : \mathbb{N} \rightarrow \mathbb{N}$ that cyclically permutes the ordered subsets $(2^k + 1, \dots, 2^{k+1})$, $k = 0, 1, \dots$, that is, $(1, 2)$, $(3, 4)$, $(5, 6, 7, 8)$, $(9, \dots, 16)$, etc. This bijection induces a unitary operator

$$u : L^2(0, 1) \rightarrow L^2(0, 1); \quad (4.57)$$

$$uh_n = h_{b(n)}, \quad (4.58)$$

which is easily shown to have the following properties:

$$\omega_n(u) = 0, \quad n \in \mathbb{N}; \quad (4.59)$$

$$\|eue\| = 1, \quad e \in \mathcal{P}(L^\infty(0, 1)), e \neq 0. \quad (4.60)$$

To show that $L^\infty(0, 1)$ fails to have the Kadison–Singer property, suppose it does, so that any $\omega_c \in P(L^\infty(0, 1))$ has a unique extension $\omega \in P(B(L^2(0, 1)))$. As already noted, we may then assume that $\omega_c = \omega_c^{(U)}$, as in (4.53), whilst $\omega = \omega^{(U)}$, as in (4.54). Taking $a = u$ then gives $\omega(u) = 0$, see (4.59), so that $\|eu\| < \varepsilon$ by (4.56). But this contradicts (4.60), finishing the sketch of the proof of the first claim in Theorem 4.21. The remark about $L^\infty(0, 1) \oplus \ell^\infty(\kappa)$ follows from the one about $L^\infty(0, 1)$.

We now pass to the (even) more difficult case of $\ell^\infty \subset B(\ell^2)$. Although this will not be used in the proof, it gives some insight to know which states on ℓ^∞ we are actually talking about, i.e., the singular pure states, and compare this with (4.53).

Theorem 4.24. *There is a bijective correspondence*

$$\omega_d(f) = \int_{\mathbb{N}} d\mu f \quad (4.61)$$

between states ω_d on ℓ^∞ and finitely additive probability measures μ on \mathbb{N} , where:

1. ω_d is normal iff μ is countably additive (and hence is a probability measure).
2. ω_d is pure iff μ corresponds to some ultrafilter U on \mathbb{N} , in which case:
 ω_d is normal iff U is principal (and hence singular iff U is free).

This follows from case no. 5 in §B.9, notably eqs. (B.153) - (B.154). In other words, the pure states ω_d on ℓ^∞ are given by ultrafilters U on \mathbb{N} through

$$\omega_d^{(U)}(f) = \beta f(U) = \lim_U f(n); \quad (4.62)$$

the analogy with (4.53) is even clearer if we write $f(n) = \langle \delta_n, m_f \delta_n \rangle \equiv \omega_n(f)$. If $U = U_n$ is a principal ultrafilter, $n \in \mathbb{N}$, we thus recover the normal pure states

$$\omega_d^{(U_n)}(f) = f(n). \quad (4.63)$$

As in (4.54), we find at least one natural extension $\omega^{(U)}$ of $\omega_d^{(U)}$ to $B(\ell^2)$, namely

$$\omega^{(U)}(a) = \lim_U \omega_n(a). \quad (4.64)$$

We now show that that ℓ^∞ has the Kadison–Singer property, making $\omega^{(U)}$ the only extension of $\omega_d^{(U)}$. The proof relies on an extremely difficult lemma from linear algebra (formerly known as a **paving conjecture**). We first define a linear map $D : M_n(\mathbb{C}) \rightarrow D_n(\mathbb{C})$ by $D(a)_{ii} = a_{ii}$, $i = 1, \dots, n$, and $D(a)_{ij} = 0$ whenever $i \neq j$.

Lemma 4.25. *For any $\varepsilon > 0$ there exist $l \in \mathbb{N}$ such that for all $n \in \mathbb{N}$ and $a \in M_n(\mathbb{C})$ with $D(a) = 0$, there are l projections (e_1, \dots, e_l) in $D_n(\mathbb{C})$ such that*

$$\sum_{k=1}^l e_k = 1_n; \quad (4.65)$$

$$\|e_i a e_i\| \leq \varepsilon \|a\|, \quad i = 1, \dots, l. \quad (4.66)$$

Since this estimate is uniform in n , the lemma extends to ℓ^2 , where $D : B(\ell^2) \rightarrow \ell^\infty$ is defined analogously, i.e., $D(a)$ is diagonal in the canonical basis (δ_n) of ℓ^2 with

$$D(a)\delta_n = \omega_n(a)\delta_n, \quad n \in \mathbb{N}. \quad (4.67)$$

Lemma 4.26. *For any $\varepsilon > 0$ there exist $l \in \mathbb{N}$ such that for all $a \in B(\ell^2)$ with $D(a) = 0$, there are l projections (e_1, \dots, e_l) in ℓ^∞ such that*

$$\sum_{k=1}^l e_k = 1_H; \quad (4.68)$$

$$\|e_i a e_i\| \leq \varepsilon \|a\|, \quad i = 1, \dots, l. \quad (4.69)$$

Now suppose that $\omega_d \in P(\ell^\infty)$, that $\omega \in S(B(\ell^2))$ extends ω_d , and that $a \in B(\ell^2)$ has $D(a) = 0$. Let e_i be one of the projections in Lemma 4.26. Using Cauchy–Schwarz for the sesquilinear form $(a, b) = \omega(a^*b)$, we obtain (using $e_i^2 = e_i^* = e_i$)

$$|\omega(e_i a e_j)|^2 \leq \omega(e_i)\omega(e_j a^* a e_i); \quad (4.70)$$

$$|\omega(e_i a e_j)|^2 \leq \omega(a^* e_i a)\omega(e_j). \quad (4.71)$$

Since $\omega(e_i) = \omega_d(e_i)$ and ω_d is a pure state (and hence is multiplicative), we have $\omega(e_i) \in \{0, 1\}$, since e_i is a projection. Moreover, in view of (4.68) and the normalization $\omega(1_H) = 1$, there must be exactly one value of $i = 1, \dots, l$, say $i = i_0$, such that $\omega(e_{i_0}) = 1$, and $\omega(e_i) = 0$ for all $i \neq i_0$. Eqs. (4.70) - (4.71) therefore imply that $\omega(e_i a e_j) \neq 0$ iff $i = j = i_0$. Using (4.68) once more, we see that $\omega(a) = \sum_{i,j} \omega(e_i a e_j) = \omega(e_{i_0} a e_{i_0})$, so that $|\omega(a)| \leq \|\omega\| \|e_{i_0} a e_{i_0}\| \leq 1 \cdot \varepsilon \|a\|$ by (4.66). Letting $\varepsilon \rightarrow 0$, we proved:

Lemma 4.27. *If $\omega \in S(B(\ell^2))$ extends $\omega_d \in P(\ell^\infty)$, and $D(a) = 0$, then $\omega(a) = 0$.*

Since $D^2 = D$, we have $D(a - D(a)) = 0$, so that for any $a \in B(\ell^2)$, we have

$$\omega(a) = \omega(D(a)) = \omega_d(D(a)), \quad (4.72)$$

provided that ω extends ω_d , as before. This shows that ω is determined by ω_d and hence is unique, completing the proof (sketch) of Theorem 4.21.

4.4 Gleason's Theorem in arbitrary dimension

To a large extent the thrust and difficulty of the proof of Gleason's Theorem 2.28 already lies in its finite-dimensional version, but some care is needed in the general case, and also Corollary 2.29 needs to be refined. A major point here is that Definition 2.23 has no unambiguous generalization to arbitrary Hilbert spaces.

Definition 4.28. Let H be an arbitrary Hilbert space with unit sphere H_1 .

1. A **probability distribution** on $\mathcal{P}(H)$ is a map $p : H_1 \rightarrow [0, 1]$ that satisfies

$$\sum_{i \in I} p(v_i) = 1, \text{ for any basis } (v_i) \text{ of } H, \quad (4.73)$$

where, as in §B.12, the sum (over a possibly uncountable index set) is meant as in Definition B.6. In particular, if H is separable and the basis is labeled and ordered by $I = \mathbb{N}$, then it is an ordinary convergent sum of the kind $\sum_{i=1}^{\infty} \dots$.

2. A map $P : \mathcal{P}(H) \rightarrow [0, 1]$ that satisfies $P(1_H) = 1$ is called a:

a. **finitely additive probability measure** if

$$P\left(\sum_{j \in J} e_j\right) = \sum_{j \in J} P(e_j) \quad (4.74)$$

for any finite collection $(e_j)_{j \in J}$ of mutually orthogonal projections on H (i.e., $e_j H \perp e_k H$, or equivalently, $e_j e_k = 0$, whenever $j \neq k$); this is equivalent to the condition $P(e + f) = P(e) + P(f)$ whenever $ef = 0$, cf. Definition 2.23.2.

b. **probability measure** if (4.74) holds for any countable collection $(e_j)_{j \in J}$ of mutually orthogonal projections on H , where the first sum is defined in the strong operator topology; note that the strong sum $\sum_j e_j$ coincides with the supremum $\bigvee_j e_j$ of the given family, defined with respect to the usual ordering of projections (that is, $e \leq f$ iff $eH \subseteq fH$).

c. **completely additive probability measure** if (4.74) holds for arbitrary collections $(e_j)_{j \in J}$ of mutually orthogonal projections on H (the first sum again meant in the strong operator topology, with the same comment as above).

Thus a probability measure is by definition σ -additive in the usual sense of measure theory; the other two cases are unusual from that perspective. However, if H is separable, then J can be at most countable, so that complete additivity is the same as σ -additivity and hence any probability measure is completely additive. Surprisingly, assuming the *Continuum Hypothesis* (CH) of set theory, it can be shown that this is even the case for arbitrary Hilbert spaces. The fundamental distinction, then, is between *finitely* additive probability measures and probability measures (which by definition are *countably* additive). As we shall see, this reflects the distinction between *arbitrary* and *normal* states on $B(H)$, respectively, cf. §4.2. In what follows, in dealing with non-separable Hilbert spaces we assume CH, in which case probability distributions on H are equivalent to probability measures on $\mathcal{P}(H)$.

The proof is the same as in finite dimension (taking into account that infinite sums over projections are defined strongly). Even without CH, Gleason's Theorem still holds for non-separable Hilbert spaces if we assume P to be completely additive, and probability distributions are equivalent to completely additive probability measures on $\mathcal{P}(H)$. For separable Hilbert spaces, CH is irrelevant and unnecessary altogether.

We then have the following generalization (and bifurcation) of Theorem 2.28.

Theorem 4.29. *Let H be a Hilbert space of dimension > 2 .*

1. *Each probability measure P on $\mathcal{P}(H)$ is induced by a unique normal state on $B(H)$ via (2.122), i.e.,*

$$P(e) = \text{Tr}(\rho e), \quad (4.75)$$

where ρ is a density operator on H uniquely determined by P .

Equivalently, each probability distribution p on $\mathcal{P}(H)$ is given by (2.123), or

$$p(v) = \langle v, \rho v \rangle. \quad (4.76)$$

Conversely, each density operator ρ on H defines a probability measure P on $\mathcal{P}(H)$ via (4.75), as well as as a probability distribution p on $\mathcal{P}(H)$ via (4.76).

2. *Each finitely additive probability measure P on $\mathcal{P}(H)$ is induced by a unique state ω on $B(H)$ via*

$$P(e) = \omega(e), \quad (4.77)$$

and similarly each probability distribution p on $\mathcal{P}(H)$ is given by

$$p(v) = \omega(e_v). \quad (4.78)$$

Conversely, each state ω on H defines a probability measure P on $\mathcal{P}(H)$ via (4.77), as well as as probability distribution p on $\mathcal{P}(H)$ via (4.78).

Proof. The proof of part 1 is practically the same as in finite dimension, except for the fact that in the proof of Lemma 2.33 the reference to Proposition A.23 should be replaced by Proposition B.79, upon which one obtains a bounded positive operator ρ for which (2.123) holds. The normalization condition (2.110) then yields $\text{Tr}(\rho) = 1$ if the trace is taken over any basis of H , and since ρ is positive this implies $\rho \in B_1(H)$, see §B.20 (complete additivity of P is just necessary to relate it to p).

Unfortunately, the proof of part 2 exceeds the scope of this book (see Notes). \square

In infinite dimension, Corollary 2.29 becomes more complicated, too; for one thing, Definition 2.26 of a quasi-state bifurcates into two possibilities. The one given still makes perfect sense and is natural from the point of view of Bohrification; to avoid confusion we call a map $\omega : B(H) \rightarrow \mathbb{C}$ satisfying the conditions in Definition 2.26 a **strong quasi-state**. In the context of Gleason's Theorem, a slightly different notion is appropriate: a **weak quasi-state** on $B(H)$ satisfies Definition 2.26, except that linearity is only required on commutative C^* -algebras in $B(H)$ of the form $C^*(a)$, where $a = a^* \in B(H)$ (these are *singly generated*). Since commutative unital C^* -subalgebras of $B(H)$ are not necessarily singly generated, and a specific counterexample exists, weak quasi-states are not necessarily strong quasi-states.

Proposition 4.30. *The map $\omega \mapsto \omega|_{\mathcal{P}(H)}$ gives a bijective correspondence between weak quasi-states ω on $B(H)$ and finitely additive probability measures on $\mathcal{P}(H)$.*

Proof. For some finite family (e_1, \dots, e_n) of mutually orthogonal projections on H , add $e_0 = 1_H - \sum_j e_j$ if necessary and let $a = \sum_{j=0}^n \lambda_j e_j$, with all $\lambda_j \in \mathbb{R}$ different. Then $\sigma(a) = \{\lambda_0, \dots, \lambda_n\}$, so that $C^*(a) \cong C(\sigma(a)) \cong \mathbb{C}^{n+1}$ (cf. Theorem B.94) coincides with the linear span of the projections e_j . If ω is a weak quasi-state, then it is linear on $C^*(a)$ and hence also on the e_j , so that $\omega|_{\mathcal{P}(H)}$ is finitely additive.

Conversely, let μ be a finitely additive probability measure on $\mathcal{P}(H)$. If $a = a^* \in B(H)$ is given, using the notation (B.328) we symbolically define ω on a by

$$\omega(a) = \int_{\sigma(a)} d\mu(e_\lambda) \lambda. \tag{4.79}$$

More precisely, for any $\varepsilon > 0$ we use Corollary B.104 to define $\omega_\varepsilon(a) = \sum_{i=1}^n \lambda_i \mu(e_{A_i})$ and let $\omega(a) = \lim_{\varepsilon \rightarrow 0} \omega_\varepsilon(a)$; it follows from Lemma B.103 (or the theory underlying the Riemann–Stieltjes integral (4.79)) that this limit exists. Now let $b, c \in C^*(a)$, so that $b = f(a)$ and $c = g(a)$ for certain $f, g \in C(\sigma(a))$, and $b + c = (f + g)(a)$, cf. Theorem B.94. By (B.325) we therefore have $\omega_\varepsilon(b + c) = \sum_{i=1}^n (f + g)(\lambda_i) \mu(e_{A_i})$, which, since $(f + g)(\lambda_i) = f(\lambda_i) + g(\lambda_i)$, again by (B.325) equals $\omega_\varepsilon(b) + \omega_\varepsilon(c)$. Since this holds for every $\varepsilon > 0$, letting $\varepsilon \rightarrow 0$ we obtain $\omega(b + c) = \omega(b) + \omega(c)$, making ω linear on $C^*(a)$. It is clear that the quasi-state ω thus obtained, on restriction to $\mathcal{P}(H)$ reproduces μ , making the map $\omega \mapsto \omega|_{\mathcal{P}(H)}$ surjective. Finally, injectivity of this map follows from Corollary B.104. \square .

Corollary 4.31. *If $\dim(H) > 2$, then each weak quasi-state on $B(H)$ (and a fortiori each strong quasi-state) is linear and hence is actually a state.*

This is immediate from Theorem 4.29.2. and Proposition 4.30.

Another corollary of Gleason’s Theorem is the **Kochen–Specker Theorem**, which we will explain in detail in Chapter 6, where it will also be proved in a different way.

Theorem 4.32. *If $\dim(H) > 2$, there are no weak quasi-states $\omega : B(H) \rightarrow \mathbb{C}$ whose restriction to each C^* -subalgebra $C^*(a) \subset B(H)$ is pure (where $a = a^* \in B(H)$).*

Equivalently, there are no nonzero maps $\omega' : B(H)_{\text{sa}} \rightarrow \mathbb{R}$ that are:

- **Dispersion-free**, i.e., $\omega'(a^2) = \omega'(a)^2$ for each $a \in B(H)_{\text{sa}}$;
- **Quasi-linear**, i.e., linear on commuting operators.

Cf. Definitions 6.1 and 6.3. To see that these conditions are equivalent to those stated in Theorem 4.32 (despite the impression that linearity on all commuting self-adjoint operators seems stronger than linearity on each $C^*(a)$), extend ω' to $\omega : B(H) \rightarrow \mathbb{C}$ by complex linearity, as in Definition 2.26.1, and note that dispersion-freeness implies positivity and hence continuity on each subalgebra $C^*(a)$ (cf. Theorem C.52 and Lemma C.4). We then see that the two conditions just stated imply that ω is multiplicative on $C^*(a)$, and hence pure, see Proposition C.14, which conversely implies that pure states on $C^*(a)$ are dispersion-free. We now prove Theorem 4.32.

Proof. If e is a projection, then $e^2 = e$, so that $\omega(e^2) = \omega(e)$. Since ω is dispersion-free (as just explained), we also have $\omega(e^2) = \omega(e)^2$, whence $\omega(e)^2 = \omega(e)$ and hence $\omega(e) \in \{0, 1\}$. Furthermore, since ω is a state by Corollary 4.31, we may apply the GNS-construction, see Theorem C.88 (whose notation we use). In particular, for any projection e , using the fact that $\pi_\omega(e) = \pi_\omega(e)^* \pi_\omega(e)$, by (C.196) we have

$$\omega(e) = \langle \Omega_\omega, \pi_\omega(e) \Omega_\omega \rangle = \|\pi_\omega(e) \Omega_\omega\|^2. \quad (4.80)$$

If $\omega(e) = 0$, then $\pi_\omega(e) \Omega_\omega = 0$ from the second equality. If $\omega(e) = 1$, then $\pi_\omega(e) \Omega_\omega = \Omega_\omega$ from the first inequality and Cauchy–Schwarz (in which we have equality, so that $\pi_\omega(e) \Omega_\omega = z \Omega_\omega$ for some $z \in \mathbb{T}$, upon which (4.80) forces $z = 1$).

By the spectral theorem (e.g. in the form Corollary B.104) or the theory of von Neumann algebras, the linear span of $\mathcal{P}(H)$ is norm-dense in $B(H)$. Since Ω_ω is cyclic for $\pi_\omega(B(H))$ by the GNS-construction, it must be that $H_\omega = \mathbb{C} \cdot \Omega_\omega$, and hence $\pi_\omega(a) = \omega(a) \cdot 1_{H_\omega}$ for any $a \in B(H)$. Since $\pi_\omega(ab) = \pi_\omega(a) \pi_\omega(b)$ by the GNS-construction, this gives $\omega(ab) = \omega(a) \omega(b)$ for all $a, b \in B(H)$. However, such multiplicative states ω on $B(H)$ cannot exist if $\dim(H) > 1$. This is clear if ω is normal, cf. Proposition 2.10, so that the following argument (which also covers the normal case) is especially meant for the case where ω is singular.

1. If $\dim(H) = n < \infty$, there are n one-dimensional projections (e_1, \dots, e_n) such that $\sum_j e_j = 1_H$. (indeed, we may assume that $B(H) = M_n(\mathbb{C})$ and take diagonal matrices $e_1 = \text{diag}(1, 0, \dots, 0)$, etc.). Now for any pair (e_i, e_j) there is some $v \in B(H)$ (which by definition is a partial isometry) such that $e_i = vv^*$, $e_j = v^*v$ (in the above case e_i and e_j are thus related if $v_{ij} = 1$ and $v_{i'j'} = 0$ otherwise). Hence

$$\omega(e_i) = \omega(vv^*) = \omega(v) \omega(v^*) = \omega(v^*v) = \omega(e_j), \quad (4.81)$$

since ω is multiplicative. But ω is also additive, which implies

$$\sum_{j=1}^n \omega(e_i) = \omega \left(\sum_{j=1}^n e_j \right) = \omega(1_H) = 1. \quad (4.82)$$

Since also $\omega(e_i) \in \{0, 1\}$, eqs. (4.81) - (4.82) are clearly contradictory.

2. If $\dim(H) = \infty$, separable or not, a similar contradiction arises from the **halving lemma**, which states that there is a projection e and an operator v such that $e = vv^*$, $1_H - e = v^*v$. For example, in the separable case assume $H = \ell^2$ and take e the projection onto the closed linear span ℓ_e^2 of the basis vectors (δ_x) with $x \in \mathbb{N}$ even, so that $1_H - e$ projects onto the closed linear span ℓ_o^2 of the basis vectors (δ_x) with $x \in \mathbb{N}$ odd. Then $\ell^2 = \ell_e^2 \oplus \ell_o^2$; take $v = 0$ on ℓ_e^2 and $v : \ell_o^2 \rightarrow \ell_e^2$ any unitary operator. In general, a similar method works, for if I is a set indexing some basis of H one may find a subset $E \subset I$ that has the same cardinality as its complement $I \setminus E$, upon which $\ell^2(E) \cong \ell^2(I \setminus E)$, cf. Theorem B.63.

Multiplicativity of ω then leads to similar contradiction between the properties $\omega(e) = \omega(1_H - e)$, as in (4.81), and $\omega(e) + \omega(1_H - e) = \omega(1_H) = 1$, as in (4.82): if $\omega(e) = 0$ one finds $0 = 1$, whereas $\omega(e) = 1$ implies $2 = 1$. \square

Notes

§4.1. The Born rule from Bohrification (II)

The Born measure (and its construction along the lines of this section) is well known in functional analysis, cf. Pedersen (1989), §4.5. For the Hamburger Moment Problem see, for example, Reed, M. & Simon, B. (1975), *Methods of Modern Mathematical Physics. Vol II. Fourier Analysis, Self-adjointness* (New York: Academic Press), Theorem X.4, p. 145 and Example 4, p. 205. In fact, the proof uses spectral theory! Corollary 4.6 was suggested by the treatment of the Born rule in Hall (2013). Definition 4.9 of the joint spectrum goes back (at least) to Arens (1961) and Hörmander (1966), §3.1.13.

§4.2. Density operators and normal states

These are really results about von Neumann algebras and come from the pertinent literature; our proofs derive from Li (1992), §1.8 and Takesaki (2002), Ch. III.

§4.3. The Kadison–Singer Conjecture

As already mentioned in the notes to §2.6, the Kadison–Singer Conjecture was first discussed in Kadison & Singer (1959) and was finally proved by Marcus, Spielman, & Srivastava (2014ab), following important intermediate contributions by e.g. Anderson (1979) and Weaver (2004). For an introduction including a complete proof see Stevens (2016), and for applications of the conjecture and its proof to other areas of mathematics see Casazza et al (2005) as well as Casazza & Tremain (2016). Proposition 4.20 is due to Glimm (1960).

§4.4. Gleason’s Theorem in arbitrary dimension

The extension of Gleason’s Theorem to non-separable Hilbert space assuming complete additivity of P is due to Maeda (1980). Maeda (1990) generalizes this result to von Neumann algebras without summands of type I_2 . The proof that assuming CH countable additivity implies complete additivity (and hence Gleason’s Theorem) was given by Eilers & Horst (1975). Proposition 4.30 is due to Aarens (1970), whose Theorem 1 is wrong; see Aarens (1991). The proof of Theorem 4.32 is due to Döring (2004), using results of Hamhalter (1993).