TRANSITION PROBABILITIES OF POSITIVE LINEAR FUNCTIONALS ON *-ALGEBRAS

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Abstract. Using unbounded Hilbert space representations basic results on the transition probability of positive linear functionals \( f \) and \( g \) on a unital *-algebra are obtained. The main assumption is the essential self-adjointness of GNS representations \( \pi_f \) and \( \pi_g \). Applications to functionals given by density matrices and by integrals and to vector functionals on the Weyl algebra are given.

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1. Introduction

Let \( f \) and \( g \) be states on a unital *-algebra \( A \). Suppose that these states are realized as vectors states of a common *-representation \( \pi \) of \( A \) on a Hilbert space with unit vectors \( \varphi \) and \( \psi \), respectively, that is, \( f(a) = \langle \pi(a)\varphi, \varphi \rangle \) and \( g(a) = \langle \pi(a)\psi, \psi \rangle \) for \( a \in A \). In quantum physics the number \( |\langle \varphi, \psi \rangle|^2 \) is then interpreted as the transition probability from \( f \) to \( g \) in these vector states. The (abstract) transition probability \( P_A(f, g) \) is defined as the supremum of values \( |\langle \varphi, \psi \rangle|^2 \), where the supremum is taken over all realizations of \( f \) and \( g \) as vectors states in some common *-representation of \( A \). This definition was introduced by A. Uhlmann [17]. The square root \( \sqrt{P_A(f, g)} \) is often called fidelity in the literature [3], [10].

The transition probability is related to other important topics such as the Bures distance [8], Sakai’s non-commutative Radon-Nikodym theorem [5] and the geometric mean of Pusz and Woronowicz [12]. It was extensively studied in the finite dimensional case (see e.g. the monograph [7]) and a number of results have been derived for \( C^* \)-algebras and von Neumann algebras (see e.g. [3], [6], [1], [2], [4], [3], [19]).

The aim of the present paper is to study the transition probability \( P_A(f, g) \) for positive linear functionals \( f \) and \( g \) on a general unital
*-algebra $A$. Then, in contrast to the case of $C^*$-algebras, the corresponding $*$-representations of $A$ act by unbounded operators in general and a number of technical problems of unbounded representation theory on Hilbert space come up. Dealing with these difficulties in a proper way is a main purpose of this paper. In section 2 we therefore collect all basic definitions and facts on unbounded Hilbert space representations that will be used throughout this paper.

In section 3 we state and prove our main theorems about the transition probability $P_A(f,g)$ for a general $*$-algebras. The crucial assumption for these results is the essential self-adjointness of the GNS representations $\pi_f$ and $\pi_g$. This means that we restrict ourselves to a class of "nice" functionals. In contrast we do not restrict the $*$-representation $\pi$ where the functionals $f$ and $g$ are realized as vector functionals. (In some results it is assumed that $\pi$ is closed or biclosed, but this is no restriction of generality, since any $*$-representation has a closed or biclosed extension.)

In section 4 we apply Theorem 8 from section 3 to generalize two standard formulas (24) and (33) for the transition probability to the unbounded case; these formulas concern trace functionals $f(\cdot) = \text{Tr} \rho(\cdot)t$ and functionals on commutative $*$-algebras given by integrals. A simple counter-example based on the Hamburger moment problem shows that these formulas can fail if the assumption of essential self-adjointness of GNS representations is omitted. In section 5 we determine the transition probability of positive functionals on the Weyl algebra given by certain functions from $C^\infty_0(\mathbb{R})$. In this case both GNS representations $\pi_f$ and $\pi_g$ are not essentially self-adjoint and the corresponding formula for $P_A(f,g)$ is in general different from the standard formula (24).

Throughout this paper we suppose that $A$ is a complex unital $*$-algebra. The involution of $A$ is denoted by $a \to a^+$ and the unit element of $A$ by 1. Let $\mathcal{P}(A)$ be the set of all positive linear functionals on $A$. Recall that a linear functional $f$ on $A$ is called positive if $f(a^+a) \geq 0$ for all $a \in A$. Let $\sum A^2$ be the set of all finite sum of squares $a^+a$, where $a \in A$. All notions and facts on von Neumann algebras and on unbounded operators used in this paper can be found in [11] and [16], respectively.

2. Basics on Unbounded Representations

Proofs of all unproven facts stated in this section and more details can be found in the author’s monograph [15]. Proposition 11 below is a new result that might of interest in itself.
Let $\langle \mathcal{D}, \langle \cdot, \cdot \rangle \rangle$ be a unitary space and $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ the Hilbert space completion of $(\mathcal{D}, \langle \cdot, \cdot \rangle)$. We denote by $L(\mathcal{D})$ the algebra of all linear operators $a : \mathcal{D} \to \mathcal{D}$, by $I_D$ the identity map of $\mathcal{D}$ and by $B(\mathcal{H})$ the $*$-algebra of all bounded linear operators on $\mathcal{H}$.

**Definition 1.** A representation of $A$ on $\mathcal{D}$ is an algebra homomorphism $\pi$ of $A$ into the algebra $L(\mathcal{D})$ such that $\pi(1) = I_D$ and $\pi(a)$ is a closable operator on $\mathcal{H}$ for $a \in A$. We then write $\mathcal{D}(\pi) := \mathcal{D}$ and $\mathcal{H}(\pi) := \mathcal{H}$.

A $*$-representation $\pi$ of $A$ on $\mathcal{D}$ is a representation $\pi$ satisfying

(1) $\langle \pi(a)\varphi, \psi \rangle = \langle \varphi, \pi(a^+)(\psi) \rangle$ for $a \in A$, $\varphi, \psi \in \mathcal{D}(\pi)$.

Let $\pi$ be a representation of $A$. Then

(2) $\mathcal{D}(\pi^*) := \cap_{a \in A} \mathcal{D}(\pi(a)^*)$ and $\pi^*(a) := \pi(a^+)^* [\mathcal{D}(\pi^*)]$ for $a \in A$,

defines a representation $\pi^*$ of $A$ on $\mathcal{D}(\pi^*)$, called the adjoint representation to $\pi$. Clearly, $\pi$ is a $*$-representation if and only if $\pi \subseteq \pi^*$.

If $\pi$ is a $*$-representation of $A$, then

(3) $\mathcal{D}(\pi) := \cap_{a \in A} \mathcal{D}(\pi(a))$ and $\pi(a) := \overline{\pi(a)} [\mathcal{D}(\pi)]$, $a \in A$,

(4) $\mathcal{D}(\pi^{**}) := \cap_{a \in A} \mathcal{D}(\pi^*(a))$ and $\pi^{**}(a) := \pi^*(a^+)^* [\mathcal{D}(\pi^{**})]$, $a \in A$,

are $*$-representations $\pi^*$ and $\pi^{**}$ of $A$, called the closure resp. the biclosure of $\pi$. Then

$$\pi \subseteq \pi^* \subseteq \pi^{**} \subseteq \pi^*.$$ 

If $\pi$ is a $*$-representation, then $\mathcal{H}(\pi) = \mathcal{H}(\pi^*)$. But for a representation $\pi$ it may happen that the domain $\mathcal{D}(\pi^*)$ is not dense in $\mathcal{H}(\pi)$, that is, $\mathcal{H}(\pi^*) \neq \mathcal{H}(\pi)$.

**Proposition 1.** Let $\pi$ and $\rho$ be representations of a $*$-algebra $A$ such that $\rho \subseteq \pi$. Then:

(i) $P_{\mathcal{H}(\rho)}\pi^*(a) \subseteq \rho^*(a) P_{\mathcal{H}(\rho)}$, where $P_{\mathcal{H}(\rho)}$ is the projection of $\mathcal{H}(\pi)$ onto $\mathcal{H}(\rho)$.

(ii) If $\mathcal{H}(\rho) = \mathcal{H}(\pi)$, then $\pi^* \subseteq \rho^*$.

(iii) $\rho^{**} \subseteq \pi^{**}$.

**Proof.** (i): Let $P$ denote the projection $P_{\mathcal{H}(\rho)}$ and fix $\psi \in \mathcal{D}(\pi^*)$. Let $\varphi \in \mathcal{D}(\rho)$ and $a \in A$. Using the assumption $\rho \subseteq \pi$ we obtain

$$\langle \rho(a^+)\varphi, P\psi \rangle = \langle P\rho(a^+)\varphi, \psi \rangle = \langle \rho(a^+)\varphi, \psi \rangle = \langle \pi(a^+)\varphi, \psi \rangle = \langle \varphi, \pi(a^+)^*\psi \rangle = \langle \varphi, \pi^*(a)^*\psi \rangle = \langle P\varphi, \pi^*(a)^*\psi \rangle = \langle \varphi, P\pi^*(a)^*\psi \rangle.$$ 

From this equality it follows that $P\psi \in \mathcal{D}(\rho(a^+)^*)$ and $\rho(a^+)^*P\psi = P\pi^*(a)^*\psi$. Hence $\psi \in \cap_{b \in A} \mathcal{D}(\rho(b)^*) = \mathcal{D}(\rho^*)$ and $\rho^*(a)P\psi = P\pi^*(a)^*\psi$. This proves that $P\pi^*(a) \subseteq \rho^*(a) P.$
(ii) follows at once from (i), since $P = I$ by the assumption $\mathcal{H}(\rho) = \mathcal{H}(\pi)$.

(iii): Let $\xi \in \mathcal{D}(\rho^{**})$ and $\psi \in \mathcal{D}(\pi^*)$. Since $\mathcal{H}(\rho^{**}) \subseteq \mathcal{H}(\rho^*) \subseteq \mathcal{H}(\rho)$ by definition, $P\xi = \xi$. By (i), $P\psi \in \mathcal{D}(\rho^*)$ and $\rho^*(a)P\psi = P\rho^*(a)\psi$. Therefore, we derive

$$\langle \pi^*(a)\psi, \xi \rangle = \langle \pi^*(a)\psi, P\xi \rangle = \langle P\pi^*(a)\psi, \xi \rangle = \langle \rho^*(a)\pi^*(a)\psi, \xi \rangle = \langle \psi, \rho^{**}(a^+)\xi \rangle$$

for $a \in A$. Hence $\xi \in \mathcal{D}(\pi^*(a)^*)$ and $\pi^*(a)^*\xi = \rho^{**}(a^+)\xi$ for $a \in A$. This implies that $\xi \in \mathcal{D}(\pi^{**})$ and $\pi^{**}(a^+)\xi = \pi^*(a)^*\xi = \rho^{**}(a^+)\xi$. Thus we have proved that $\rho^{**} \subseteq \pi^{**}$. □

**Definition 2.** A $\ast$-representation $\pi$ of a $\ast$-algebra $A$ is called

- closed if $\pi = \overline{\pi}$, or equivalently, if $\mathcal{D}(\pi) = \mathcal{D}(\overline{\pi})$,
- biclosed if $\pi = \pi^{**}$, or equivalently, if $\mathcal{D}(\pi) = \mathcal{D}(\pi^{**})$,
- self-adjoint if $\pi = \pi^*$, or equivalently, if $\mathcal{D}(\pi) = \mathcal{D}(\pi^*)$,
- essentially self-adjoint if $\pi^*$ is self-adjoint, that is, if $\pi^* = \pi^{**}$, or equivalently, if $\mathcal{D}(\pi^{**}) = \mathcal{D}(\pi^*)$.

Remark. It should be emphasized that the preceding definition of essential self-adjointness is different from the definition given in [15].

In [15, Definition 8.1.10], a $\ast$-representation was called essentially self-adjoint if $\overline{\pi}$ is self-adjoint, that is, if $\overline{\pi} = \pi^*$.

Let $\pi$ be a $\ast$-representation. Then the $\ast$-representations $\overline{\pi}$ and $\pi^{**}$ are closed, $\pi^{**}$ is biclosed and $(\overline{\pi})^* = \pi^*$. It may happen that $\overline{\pi} \neq \pi^{**}$, so that $\overline{\pi}$ is closed, but not biclosed. The locally convex topology on $\mathcal{D}(\pi)$ defined by the family of seminorms $\{\| \cdot \|_a := \| \pi(a) \cdot \| : a \in A\}$ is called the graph topology and denoted by $t_{\pi(A)}$. Then the $\ast$-representation $\pi$ is closed if and only if the locally convex space $\mathcal{D}(\pi)[t_{\pi(A)}]$ is complete.

**Proposition 2.** If $\pi_1$ is a self-adjoint $\ast$-subrepresentation of a $\ast$-representation $\pi$ of $A$, then there exists a $\ast$-representation $\pi_2$ of $A$ on the Hilbert space $\mathcal{H}(\pi) \ominus \mathcal{H}(\pi_1)$ such that $\pi = \pi_1 \oplus \pi_2$.

**Proof.** [15, Corollary 8.3.3]. □

For a $\ast$-representation of $A$ we define two commutants

$$\pi(A)^\prime_s = \{ T \in \mathbf{B}(\mathcal{H}(\pi)) : T \varphi \in \mathcal{D}(\pi), T\pi(a)\varphi = \pi(a)T\varphi \text{ for } a \in A, \varphi \in \mathcal{D}(\pi) \},$$

$$\pi(A)^\prime_{ss} = \{ T \in \mathbf{B}(\mathcal{H}(\pi)) : T\overline{\pi(a)} \subseteq \overline{\pi(a)}T, T^*\overline{\pi(a)} \subseteq \overline{\pi(a)}T^* \}.$$

The symmetrized commutant $\pi(A)^\prime_{ss}$ is always a von Neumann algebra. If $\pi$ is closed, then

$$\pi(A)^\prime_{ss} = \pi(A)^\prime_s \cap (\pi(A)^\prime_s)^*.$$
If \( \pi_1 \) and \( \pi_2 \) are representations of \( A \), the intertwining space \( I(\pi_1, \pi_2) \) consists of all bounded linear operators \( T \) of \( \mathcal{H}(\pi_1) \) into \( \mathcal{H}(\pi_2) \) satisfying
\[
T \varphi \in \mathcal{D}(\pi_2) \quad \text{and} \quad T \pi_1(a) \varphi = \pi_2(a) T \varphi \quad \text{for} \quad a \in A, \varphi \in \mathcal{D}(\pi_1).
\]

The \(*\)-representation \( \pi_f \) in the following proposition is called the GNS representation associated with the positive linear functional \( f \).

**Proposition 3.** Suppose that \( f \in \mathcal{P}(A) \). Then there exists a \(*\)-representation \( \pi_f \) with algebraically cyclic vector \( \varphi_f \), that is, \( \mathcal{D}(\pi_f) = \pi_f(A) \varphi_f \), such that
\[
f(a) = \langle \pi_f(a) \varphi_f, \varphi_f \rangle, \quad a \in A.
\]
If \( \pi \) is another \(*\)-representation of \( A \) with algebraically cyclic vector \( \varphi \) such that \( f(a) = \langle \pi(a) \varphi, \varphi \rangle \) for all \( a \in A \), then there exists a unitary operator \( U \) of \( \mathcal{H}(\pi) \) onto \( \mathcal{H}(\pi_f) \) such that \( U \mathcal{D}(\pi) = \mathcal{D}(\pi_f) \) and \( \pi_f(a) = U^* \pi(a) U \) for \( a \in A \).

**Proof.** [15, Theorem 8.6.4]. \( \square \)

We study some of the preceding notions by a simple but instructive example.

**Example 1.** *(One-dimensional Hamburger moment problem)*

Let \( A \) by the polynomial \(*\)-algebra \( \mathbb{C}[x] \) with involution determined by \( x^+ := x \). We denote by \( M(\mathbb{R}) \) the set of positive Borel measures \( \mu \) such that \( p(x) \in L^1(\mathbb{R}, \mu) \) for all \( p \in \mathbb{C}[x] \). The number \( s_n = \int x^n d\mu(x) \) is the \( n \)-th moment and the sequence \( s(\mu) = (s_n)_{n \in \mathbb{N}_0} \) is called the moment sequence of a measure \( \mu \in M(\mathbb{R}) \). The moment sequence \( s(\mu) \), or likewise the measure \( \mu \), is called *determinate*, if the moment sequence \( s(\mu) \) determines the measure \( \mu \) uniquely, that is, if \( s(\mu) = s(\nu) \) for some \( \nu \in M(\mathbb{R}) \) implies that \( \nu = \mu \).

For \( \mu \in M(\mathbb{R}) \) we define a \(*\)-representation \( \pi_\mu \) of \( A = \mathbb{C}[x] \) by \( \pi_\mu(p) q = p \cdot q \) for \( p \in A \) and \( q \in \mathcal{D}(\pi_\mu) := \mathbb{C}[x] \) on the Hilbert space \( \mathcal{H}(\pi_\mu) := L^2(\mathbb{R}, \mu) \). Put \( f_\mu(p) = \int p(x) d\mu(x) \) for \( p \in \mathbb{C}[x] \). Obviously, the vector \( 1 \in \mathcal{D}(\pi_\mu) := \mathbb{C}[x] \) is algebraically cyclic for \( \pi_\mu \). Therefore, since \( f_\mu(p) = \langle \pi_\mu(p), 1 \rangle \) for \( p \in \mathbb{C}[x] \), \( \pi_\mu \) is (unitarily equivalent to) the GNS representation \( \pi_{f_\mu} \) of the positive linear functional \( f_\mu \) on \( A = \mathbb{C}[x] \).

**Statement:** The \(*\)-representation \( \pi_\mu \) is essentially self-adjoint if and only if the moment sequence \( s(\mu) \) is determinate.

**Proof.** By a well-known result on the Hamburger moment problem (see e.g. [16, Theorem 16.11]), the moment sequence \( s(\mu) \) is determinate if and only if the operator \( \pi_\mu(x) \) is essentially sel-adjoint. By [15]
Proposition 8.1(v)], the latter holds if and only if the \(\ast\)-representation \((\pi_\mu)\ast\) is self-adjoint, that is, if \(\pi_\mu\) is essentially self-adjoint.

By [15, Proposition 8.1(vii)], the closure \(\overline{\pi_\mu}\) of the \(\ast\)-representation \(\pi_\mu\) is self-adjoint if and only if all powers of the operator \(\pi_\mu(x)\) are essentially self-adjoint. This is a rather strong condition. It is fulfilled (for instance) if 1 is an analytic vector for the symmetric operator \(\pi_\mu(x)\), that is, if there exists a constant \(M > 0\) such that

\[
\|\pi_\mu(x)^n1\| = s_{2n}^{1/2} \leq M^n n! \quad \text{for} \quad n \in \mathbb{N}.
\]

From the theory of moment problems it is well-known that there are examples of measures \(\mu \in \mathcal{M}(\mathbb{R})\) for which \(\pi_\mu(x)\) is essentially self-adjoint, but \(\pi_\mu(x^2)\) is not. In this case \(\pi_\mu\) is essentially self-adjoint (which means that \((\pi_\mu)\ast\) is self-adjoint), but the closure \(\overline{\pi_\mu}\) of \(\pi_\mu\) is not self-adjoint.

3. Main Results on Transition Probabilities

Let \(\text{Rep}A\) denote the family of all \(\ast\)-representations of \(A\). Given \(\pi \in \text{Rep}A\) and \(f \in \mathcal{P}(A)\), let \(S(\pi, f)\) be the set of all representing vectors for the functional \(f\) in \(\mathcal{D}(\pi)\), that is, \(S(\pi, f)\) is the set of vectors \(\varphi \in \mathcal{D}(\pi)\) such that \(f(a) = \langle \pi(a)\varphi, \varphi \rangle\) for \(a \in A\). Note that \(S(\pi, f)\) may be empty, but by Proposition 3 for each \(f \in \mathcal{P}(A)\) there exists a \(\ast\)-representation \(\pi\) of \(A\) for which \(S(\pi, f)\) is not empty. If \(f\) is a state, that is, if \(f(1) = 1\), then all vectors \(\varphi \in S(\pi, f)\) are unit vectors.

**Definition 3.** For \(f, g \in \mathcal{P}(A)\) the transition probability \(P_A(f, g)\) of \(f\) and \(g\) is defined by

\[
P_A(f, g) = \sup_{\pi \in \text{Rep}A} \sup_{\varphi \in S(\pi, f), \psi \in S(\pi, g)} |\langle \varphi, \psi \rangle|^2.
\]

If \(A\) is a unital \(\ast\)-subalgebra of \(B\) and \(f, g \in \mathcal{P}(B)\), then it is obvious that

\[
P_B(f, g) \leq \mathcal{P}_A(f[A], g[A]),
\]

because the restriction of any \(\ast\)-representation of \(B\) is a \(\ast\)-representation of \(A\).

Let \(\mathcal{G}(f, g)\) denote the set of all linear functionals on \(A\) satisfying

\[
|F(b^+a)|^2 \leq f(a^+a)g(b^+b) \quad \text{for} \quad a, b \in A.
\]

Any vector \(\varphi \in S(\pi, f)\) is called an amplitude of \(f\) in the representation \(\pi\) and any linear functional of \(\mathcal{G}(f, g)\) is called a transition form from \(f\)
to $g$. If $\varphi \in S(\pi, f)$ and $\psi \in S(\pi, g)$, then the functional $F_{\varphi, \psi}$ defined by

$$F_{\varphi, \psi}(a) := \langle \pi(a)\varphi, \psi \rangle, \quad a \in A,$$

is a transition form from $f$ to $g$. Indeed, for $a, b \in A$ we have

$$|F_{\varphi, \psi}(b^+a)|^2 = |\langle \pi(b^+a)\varphi, \psi \rangle|^2 = |\langle \pi(a)\varphi, \pi(b)\psi \rangle|^2 \leq \|\pi(a)\varphi\|^2 \|\pi(b)\psi\|^2 = f(a^+a)g(b^+b)$$

which proves that $F_{\varphi, \psi} \in \mathcal{G}(f, g)$. By Theorem 4 below, each functional $F \in \mathcal{G}(f, g)$ arises in this manner. The number $|F_{\varphi, \psi}(1)|^2 = |\langle \varphi, \psi \rangle|^2$ is called the transition probability of the amplitudes $\varphi$ and $\psi$ and by definition the transition probability $P_A(f, g)$ is the supremum of all such transition amplitudes.

The following description of the transition probability was proved by P.M. Alberti for $C^*$-algebras [1] and by A. Uhlmann for general $*$-algebras [18].

**Theorem 4.** Suppose that $f, g \in \mathcal{P}(A)$. Then

$$P_A(f, g) = \sup_{F \in \mathcal{G}(f, g)} |F(1)|^2. \tag{11}$$

There exist a $*$-representation $\pi$ of $A$ and vectors $\varphi \in S(\pi, f)$ and $\psi \in S(\pi, g)$ such that

$$P_A(f, g) = |\langle \varphi, \psi \rangle|^2. \tag{12}$$

Next we express the transition forms of $\mathcal{G}(f, g)$ and hence the transition probability in terms of intertwiners of the corresponding GNS representations. This provides a powerful tool for computing the transition probability. Recall $\pi_f$ denotes the GNS representation of $A$ associated with $f \in \mathcal{P}(A)$ and $\varphi_f$ is the corresponding algebraically cyclic vector.

**Proposition 5.** Suppose that $f, g \in \mathcal{P}(A)$. Then there a one-to-one correspondence between the sets $\mathcal{G}(f, g)$ and $I(\pi_f, (\pi_g)^*)$ given by

$$F(b^+a) = \langle T\pi_f(a)\varphi_f, \pi_g(b)\varphi_g \rangle \quad \text{for} \quad a, b \in A, \quad \tag{13}$$

where $F \in \mathcal{G}(f, g)$ and $T \in I(\pi_f, (\pi_g)^*)$. In particular, $F(1) = \langle T\varphi_f, \varphi_g \rangle$.

**Proof.** Let $F \in \mathcal{G}(f, g)$. Then

$$|F(b^+a)|^2 \leq f(a^*a)g(b^*b) = \|\pi_f(a)\varphi_f\|^2 \|\pi_g(b)\varphi_g\|^2 \quad \text{for} \quad a, b \in A.$$
Hence there exists a bounded linear operator $T$ of $\mathcal{H}(\pi_g)$ into $\mathcal{H}(\pi_f)$ such that $\|T\| \leq 1$ and (13) holds. Let $a, b, c \in A$. Using (13) we obtain

$$
\langle T\pi_f(a)\varphi_f, \pi_g(c^+\pi_g(b)\varphi_g \rangle = F((c^+)b^+a) = F(b^+(ca))
$$

Hence $T\pi_f(b)\varphi_f \in D(\pi_g(c^*))$ and $\pi_g(c^+)T\pi_f(a)\varphi_f = T\pi_f(c^+)\pi_f(a)\varphi_f$. Because $c \in A$ was arbitrary, $T\pi_f(a)\varphi_f \in D((\pi_g)^*)$. Then

$$(\pi_g)(c^+)T\pi_f(a)\varphi_f = T\pi_f(c^+)\pi_f(a)\varphi_f \quad \text{for} \quad a \in A,$$

which means that $T \in I(\pi_f, (\pi_g)^*)$.

Conversely, let $T \in I(\pi_f, (\pi_g)^*)$ and $\|T\| \leq 1$. Define $F(a) = \langle T\pi_f(a)\varphi_f, \varphi_g \rangle$ for $a \in A$. It is straightforward to check that (13) holds and hence (5), that is, $F \in \mathcal{G}(f, g)$.

Clearly, by (13), $F = 0$ is equivalent to $T = 0$. Thus we have a one-to-one correspondence between functionals $F$ and operators $T$. □

Combining Theorem 4 and Proposition 5 and using the formula $F(1) = \langle T\varphi_f, \varphi_g \rangle$ we obtain

**Corollary 6.** For any $f, g \in \mathcal{P}(A)$ we have

(14) $P_A(f, g) = \sup_{T \in I(\pi_f, (\pi_g)^*), \|T\| \leq 1} |\langle T\varphi_f, \varphi_g \rangle|^2$.

If the GNS representations of $f$ and $g$ are essentially self-adjoint, a number of stronger results can be obtained.

**Theorem 7.** Suppose that $f$ and $g$ are positive linear functionals on $A$ such that their GNS representations $\pi_f$ and $\pi_g$ are essentially self-adjoint. Let $\pi$ be a biclosed $\ast$-representation of $A$ such that the sets $S(\pi, f)$ and $S(\pi, g)$ are not empty. Fix vectors $\varphi \in S(\pi, f)$ and $\psi \in S(\pi, g)$. Then

(15) $P(f, g) = \sup_{T \in \pi(A)^\prime \ast, \|T\| \leq 1} |\langle T\varphi, \psi \rangle|^2$.

**Proof.** Let $T \in \pi(A)^\prime \ast$ and $\|T\| \leq 1$. Similarly, as in the proof of Proposition 5, we define $F(a) = \langle T\pi(a)\varphi, \psi \rangle$, $a \in A$. Since $\pi(A)^\prime \ast \subseteq \pi(A)^\prime$, we obtain

$$
|F(b^+a)|^2 = |\langle T\pi(b^+a)\varphi, \psi \rangle|^2 = |\langle \pi(b^+)T\pi(a)\varphi, \psi \rangle|^2
$$

$$
= |\langle T\pi(a)\varphi, \pi(b)\psi \rangle|^2 \leq \|\pi(a)\varphi\|^2 \|\pi(b)\psi\|^2 = f(a^+a)g(b^+b)
$$

for $a, b \in A$, that is, $F \in \mathcal{G}(f, g)$. Clearly, we have $\langle T\varphi, \psi \rangle = F(1)$. Let $\rho_f$ and $\rho_g$ denote the restrictions $\pi[\pi(A)\varphi$ and $\pi[\pi(A)\psi$, respectively. Since $\rho_f \subseteq \pi$ and $\rho_g \subseteq \pi$ and $\pi$ is biclosed, it follows
from Proposition 1(iii) that \((\rho_f)^{**} \subseteq \pi^{**} = \pi\) and \((\rho_g)^{**} \subseteq \pi^{**} = \pi\).

Since \(\phi \in S(\pi, f)\) and \(\psi \in S(\pi, g)\), the representations \(\rho_f\) and \(\rho_g\) are unitarily equivalent to the GNS representations \(\pi_f\) and \(\pi_g\), respectively. For notational simplicity we identify \(\rho_f\) with \(\pi_f\) and \(\rho_g\) with \(\pi_g\). Since \(\rho_f\) and \(\rho_g\) are essentially self-adjoint by assumption, \((\rho_f)^{**}\) and \((\rho_g)^{**}\) are self-adjoint. Therefore, by Proposition 2, there are subrepresentations \(\rho_1\) and \(\rho_2\) of \(\pi\) such that \(\pi = (\rho_f)^{**} \oplus \rho_1\) and \(\pi = (\rho_g)^{**} \oplus \rho_2\).

Conversely, suppose that \(F \in \mathcal{G}(f, g)\). By Proposition 3 there is an intertwiner \(T_0 \in I(\rho_f, (\rho_g)^*) \cong I(\pi_f, (\pi_g)^*)\) such that \(\|T_0\| \leq 1\) and (13) holds with \(T\) replaced by \(T_0\). Define \(T : \mathcal{H}(\rho_f) \oplus \mathcal{H}(\rho_1) \rightarrow \mathcal{H}(\rho_g) \oplus \mathcal{H}(\rho_2)\) by \(T(\xi_f, \xi_1) = (T_0\xi_f, 0)\). Clearly, \(T^*\) acts by \(T^*(\eta_g, \eta_2) = (T_0^*\eta_1, 0)\). Since \((\rho_f)^{**} = (\rho_f)^*\) and \((\rho_g)^{**} = (\rho_f)^*\) by assumption and \(T_0 \in I(\rho_f, (\rho_g)^*)\), it follows from Proposition 8.2.3(iii) and (iv), in (15) that

\[
T_0 \in I((\rho_f)^{**}, (\rho_g)^*) = I((\rho_f)^*, (\rho_g)^*),
T_0^* \in I((\rho_g)^{**}, (\rho_f)^*) = I((\rho_g)^*, (\rho_f)^*).
\]

From these relations we easily derive that the operators \(T\) and \(T^*\) are in \(\pi(A)'_s\), so that \(T \in \pi(A)'_s\) by (5). Then we have \(\|T\| = \|T_0\| \leq 1\) and \(F(1) = \langle T_0\phi, \psi \rangle = \langle T\phi, \psi \rangle\). Together with the first paragraph of this proof we have shown that the supremum over the operators \(T \in \pi(A)'_s\), \(\|T\| \leq 1\), is equal to the supremum over the functionals \(F \in \mathcal{G}(f, g)\). Since the latter is equal to \(P_A(f, g)\) by Theorem 4 this proves (15). \(\square\)

Remark. A slight modification of the preceding proof shows the following: If we assume that the closures \(\pi_f\) and \(\pi_g\) of the GNS representations \(\pi_f\) and \(\pi_g\) are self-adjoint, then the assertion of Theorem 7 remains valid if it is only assumed that \(\pi\) is \(\text{closed}\) rather than biclosed. A similar remark applies also for the subsequent applications of Theorem 7 given below.

Theorem 8. Suppose that \(f,g \in \mathcal{P}(A)\) and the GNS representations \(\pi_f\) and \(\pi_g\) are essentially self-adjoint. Suppose that \(\pi\) is a biclosed *-representation of \(A\) and there exist vectors \(\phi \in S(\pi, f)\) and \(\psi \in S(\pi, g)\). Let \(F_\phi\) and \(F_\psi\) denote the vector functionals on the von Neumann algebra \(\mathcal{M} := (\pi(A)'_s)'\) given by \(F_\phi(x) = \langle x\phi, \phi \rangle\) and \(F_\psi(x) = \langle x\psi, \psi \rangle\),
Further, there exist vectors $\varphi' \in S(\pi, f)$ and $\psi' \in S(\pi, g)$ such that

$$\langle x \varphi', \varphi' \rangle = \langle x \varphi, \varphi \rangle \quad \text{and} \quad \langle x \psi', \psi' \rangle = \langle x \psi, \psi \rangle \quad \text{for } x \in \mathcal{M} \quad \text{and}$$

$$P_A(f, g) = P_{\mathcal{M}}(F_\varphi, F_\psi). \quad \text{(16)}$$

**Proof.** Since $\pi(A)_{ss}'$ is a von Neumann algebra, we have $T \in \pi(A)_{ss}'$ if and only if $T \in (\pi(A)_{ss}')'' = \mathcal{M}'. \quad \text{Therefore, applying formula (15) to the } \ast\text{-representation } \pi \text{ of } A \text{ and to the identity representation of the von Neumann algebra } \mathcal{M}, \text{it follows that the supremum of } \|T \varphi, \psi\|^2 \quad \text{over all operators } T \in \pi(A)_{ss}' = \mathcal{M}', \quad \text{with } \|T\| \leq 1, \quad \text{is equal to } P_A(f, g) \quad \text{and also to } P_{\mathcal{M}}(F_\varphi, F_\psi). \quad \text{This yields the equality (16).}$$

Now we prove the existence of vectors $\varphi'$ and $\psi'$ having the desired properties. In order to do so we go into the details of the proof of [2, Appendix 7]. Besides we use some facts from von Neumann algebra theory [11]. We define a normal linear functional on the von Neumann algebra $\mathcal{M}$ by $h(\cdot) = \langle \cdot, \varphi \rangle$. Let $h = R_u \cdot h$ be the polar decomposition of $h$, where $u$ is a partial isometry from $\mathcal{M}'$. Then we have $|h| = R_u \cdot h$ and hence $\|h\| = \|\cdot h\| = |h|(1) = h(u^*) = \langle u^* \varphi, \psi \rangle$. Therefore, we obtain

$$P_{\mathcal{M}}(F_\varphi, F_\psi) = \sup_{T \in \mathcal{M}', \|T\| \leq 1} |\langle T \varphi, \psi \rangle|^2 = \|h\|^2 = \langle u^* \varphi, \psi \rangle^2, \quad \text{(18)}$$

where the first equality follows formula (15) applied to the von Neumann algebra $\mathcal{M}$. In the proof of [2, Appendix 7] it was shown that there exist partial isometries $v, w \in \mathcal{M}'$ satisfying

$$\langle u^* \varphi, \psi \rangle = \langle v^* w \varphi, \psi \rangle, \quad \text{(19)}$$

$$w^* w \geq p(\varphi), \quad v^* v \geq p(\psi), \quad \text{(20)}$$

where $p(\varphi)$ and $p(\psi)$ are the projections of $\mathcal{M}'$ onto the closures of $\mathcal{M} \varphi$ and $\mathcal{M} \psi$, respectively. Set $\varphi' := w \varphi$ and $\psi' := v \psi$. Comparing (19) with (18) and (19) we obtain (17).

From (20) it follows that $\langle x \varphi', \varphi' \rangle = \langle x \varphi, \varphi \rangle$ and $\langle x \psi', \psi' \rangle = \langle x \psi, \psi \rangle$ for $x \in \mathcal{M}$ and that $w^* w \varphi = \varphi$ and $v^* v \psi = \psi$. Since $w, w^* \in \mathcal{M}' = \pi(a)'_{ss}$ and $\pi$ is closed, we have $w, w^* \in \pi(a)'_{ss}$ by (15). Therefore, $w$ and $w^*$ leave the domain $\mathcal{D}(\pi)$ invariant, so that $\varphi' = w \varphi \in \mathcal{D}(\pi)$ and $\psi' = v \psi \in \mathcal{D}(\pi)$. For $a \in A$ we derive

$$\langle \pi(a) \varphi', \varphi' \rangle = \langle \pi(a) x \varphi, w \varphi \rangle = \langle w^* \pi(a) w \varphi, \varphi \rangle$$

$$= \langle \pi(a) w^* w \varphi, \varphi \rangle = \langle \pi(a) \varphi, \varphi \rangle = f(a).$$

That is, $\varphi' \in S(\pi, f)$. Similarly, $\psi' \in S(\pi, g). \quad \square$
Theorem 16 allows us to reduce the computation of the transition probability of the functionals $f$ and $g$ on $A$ to that of the vector functionals $F_\varphi$ and $F_\psi$ of the von Neumann algebra $\mathcal{M} = (\pi(A)_{ss})'$. In the next section we will apply this result in two important situations.

The following theorem generalizes a classical result of A. Uhlmann [17] to the unbounded case.

**Theorem 9.** Let $f, g \in \mathcal{P}(A)$ be such that the GNS representations $\pi_f$ and $\pi_g$ are essentially self-adjoint. Suppose that there exist a positive linear functional $h$ on $A$ and elements $b, c \in A$ such that $f(a) = h(b^+ ab)$ and $g(a) = h(c^+ ac)$ for $a \in A$. Assume that $c^+ b \in \sum A^2$. Then

$$P_A(f, g) = h(c^+ b)^2.$$ 

**Proof.** Recall that $\pi_h$ is the GNS representation of $h$ with algebraically cyclic vector $\varphi_h$. By the assumptions $f(\cdot) = h(b^+ \cdot b)$ and $g(\cdot) = h(c^+ \cdot c)$ we have $\pi_h(b)\varphi_h \in S(\pi, f)$ and $\pi_h(c)\varphi_h \in S(\pi, g)$. Therefore,

$$h(c^+ b)^2 = \langle \pi_h(b)\varphi_h, \pi_h(c)\varphi_h \rangle^2 \leq P_A(f, g).$$

To prove the converse inequality we want to apply Theorem 7 to the biclosed representation $\pi := (\pi_h)^{**}$. Suppose that $T \in \pi(A)_{ss}'$ and $\|T\| \leq 1$. Set $R := \pi(c^+ b)$. Since $c^+ b \in \sum A^2$ by assumption, $R$ is a positive, hence symmetric, operator. Since $\pi := (\pi_h)^{**}$ is closed, we have $T \in \pi(A)'_s$. Using these facts and the Cauchy-Schwarz inequality we derive

$$\langle T\pi_h(b)\varphi_h, \pi_h(c)\varphi_h \rangle^2 = \langle T\pi(b)\varphi_h, \pi(c)\varphi_h \rangle^2 = \langle \pi(b)T\varphi_h, \pi(c)\varphi_h \rangle^2 = \langle RT\varphi_h, \varphi_h \rangle^2 \leq \langle RT\varphi_h, T\varphi_h \rangle \langle R\varphi_h, \varphi_h \rangle = \langle RT\varphi_h, T\varphi_h \rangle h(c^+ b).$$

Since $T \in \pi(A)'_{ss}$, we have $TR \subseteq RT$. There exists a positive self-adjoint extension $\tilde{R}$ of $R$ on $\mathcal{H}(\pi)$ such that $T\tilde{R} \subseteq \tilde{R}T$ [16 Exercise 14.14]. The latter implies that $T\tilde{R}^{1/2} \subseteq \tilde{R}^{1/2}T$ and hence

$$\langle RT\varphi_h, T\varphi_h \rangle = \langle \tilde{R}T\varphi_h, \tilde{T}\varphi_h \rangle = \langle \tilde{R}^{1/2}T\varphi_h, \tilde{R}^{1/2}T\varphi_h \rangle = \langle T\tilde{R}^{1/2}\varphi_h, T\tilde{R}^{1/2}\varphi_h \rangle \leq \langle \tilde{R}^{1/2}\varphi_h, \tilde{R}^{1/2}\varphi_h \rangle = \langle R\varphi_h, \varphi_h \rangle = \langle \pi_h(c^+ b)\varphi_h, \varphi_h \rangle = h(c^+ b)$$

Inserting (22) into (21) we get

$$\langle T\pi_h(b)\varphi_h, \pi_h(c)\varphi_h \rangle^2 \leq h(c^+ b).$$

Hence $P_A(f, g) \leq h(c^+ b)$ by Theorem 7. \qed
Remarks. 1. The assumption $c^*b \in \sum A^2$ was only needed to ensure that the operator $R = \pi(c^*b) \equiv (\pi_h)^{**}(c^*b)$ is positive. Clearly, this is satisfied if $F(c^*b) \geq 0$ for all positive linear functionals $F$ on $A$.

2. If the closures of the GNS representations $\pi_f$ and $\pi_g$ are self-adjoint, we can set $\pi := \pi_h$ in the preceding proof and it suffices to assume that $h(a^*c^*ba) \geq 0$ for all $a \in A$ instead of $c^*b \in \sum A^2$.

4. Two Applications

To formulate our first application we begin with some preliminaries.

Let $\rho$ be a closed $\ast$-representation of $A$. We denote by $B_1(\rho(A))_+$ the set of positive trace class operators on $H(\rho)$ such that $tH(\rho) \subseteq D(\rho)$ and the closure of $\rho(a)t\rho(b)$ is trace class for all $a, b \in A$.

Now let $t \in B_1(\rho(A))_+$. We define a positive linear functional $f_t$ by

$$f_t(a) := \text{Tr} \rho(a) t, \quad a \in A,$$

where $\text{Tr}$ always denotes the trace on the Hilbert space $H(\rho)$. Note that $f_t(a) \geq 0$ if $\rho(a) \geq 0$ (that is, $\langle \rho(a) \varphi, \varphi \rangle \geq 0$ for all $\varphi \in D(\rho)$).

In unbounded representation theory a large class of positive linear functionals is of the form $f_t$. We illustrate this by restating the following theorem proved in [14]. Recall that a Frechet–Montel space is a complete metrizable locally convex space such that each bounded sequence has a convergent subsequence.

**Theorem 10.** Let $f$ be a linear functional on $A$ and let $\rho$ be a closed $\ast$-representation of $A$. Suppose that the locally convex space $D(\rho)[t_{\rho(A)}]$ is a Frechet–Montel space and $f(a) \geq 0$ whenever $\rho(a) \geq 0$ for $a \in A$. Then there exists an operator $t \in B(\rho(A))_+$ such that $f = f_t$, that is, $f(a) = \text{Tr} \rho(a) t$ for $a \in A$.

Further, let $\mathcal{M}$ be a type I factor acting on the Hilbert space $H(\rho)$ and let $\text{tr}_\mathcal{M}$ denote its canonical trace. Since in particular $t$ is of trace class, $F_t(x) = \text{Tr} xt, \ x \in \mathcal{M}$, defines a positive normal linear functional $F_t$ on $\mathcal{M}$. Hence there exists a unique positive element $\hat{t} \in \mathcal{M}$ such that $\text{tr}_\mathcal{M}(\hat{t}) < \infty$ and

$$F_t(x) \equiv \text{Tr} xt = \text{tr}_\mathcal{M} xt \quad \text{for} \quad x \in \mathcal{M}. \quad (23)$$

The element $\hat{t}$ can be obtained as follows. Since $\mathcal{M}$ is a type I factor, there exist Hilbert spaces $H_0$ and $H_1$ such that, up to unitary equivalence, $H(\pi) = H_0 \otimes H_1$ and $\mathcal{M} = B(H_0) \otimes \mathbb{C} \cdot I_{H_1}$. The canonical trace of $\mathcal{M}$ is then given by $\text{tr}_\mathcal{M}(y \otimes \lambda \cdot I_{H_1}) := \text{Tr} \lambda y$, where $\text{Tr}$ denotes the trace on the Hilbert space $H_1$. Now $\tilde{F}_t(y) := F_t(y \otimes I_{H_1}), \ y \in B(H_0)$, defines a positive normal linear functional $\tilde{F}_t$ on $B(H_0)$. Hence there exists a unique positive trace class operator $\tilde{t}$ on the Hilbert space $H_0$...
Theorem 11. Let $\rho$ be a closed $*$-representation of $A$ such that the von Neumann algebra $\mathcal{M} := (\rho(A)_{ss})'$ is a type I factor. For $s, t \in \mathcal{B}(\rho(A))_+$, let $f_s, f_t$ denote the positive linear functionals on $A$ defined by

$$f_s(a) = \text{Tr} \rho(a)s, \quad f_t(a) = \text{Tr} \rho(a)t \quad \text{for} \quad a \in A.$$  

Suppose that the GNS representations $\pi_s$ and $\pi_t$ are essentially self-adjoint. Then

$$P_A(f_s, f_t) = (\text{Tr}_M |\tilde{t}|^{1/2} \tilde{s}^{1/2}|)^2 = (\text{Tr}_M (\tilde{s}^{1/2} \tilde{t} \tilde{s}^{1/2})^{1/2})^2.$$  

Proof. Let $\rho_\infty$ be the orthogonal sum $\bigoplus_{n=0}^\infty \rho$ on $\mathcal{H}_\infty = \bigoplus_{n=0}^\infty \mathcal{H}(\rho)$. Since $\rho$ is biconed, so is the $*$-representation $\rho_\infty$ of $A$. We want to apply Theorem 8. First we will describe the GNS representations $\pi_s$ and $\pi_t$ as $*$-subrepresentations of $\rho_\infty$.

The result is well-known if $\mathcal{H}(\rho)$ is finite dimensional [17], so we can assume that $\mathcal{H}(\rho)$ is infinite dimensional. Since $s \in \mathcal{B}_1(\rho(A))_+$, there are a sequence $(\lambda_n)_{n \in \mathbb{N}}$ of nonnegative numbers and an orthonormal sequence $(\varphi_n)_{n \in \mathbb{N}}$ of $\mathcal{H}(\rho)$ such that $\varphi_n \in \mathcal{D}(\rho)$ for $n \in \mathbb{N}$,

$$s\varphi = \sum_n \langle \varphi, \varphi_n \rangle \lambda_n \varphi_n \quad \text{for} \quad \varphi \in \mathcal{H}(\rho),$$

and $(\rho(a)\lambda_n^{1/2} \varphi_n)_{n \in \mathbb{N}} \in \mathcal{H}_\infty$ for all $a \in A$. Further, for $a \in A$ we have

$$f_s(a) = \sum_{n=1}^\infty \langle \rho(a)\varphi_n, \lambda_n \varphi_n \rangle.$$  

All these facts are contained in Propositions 5.1.9 and 5.1.12 in [15]. Hence

$$\rho_\Phi(a)(\rho(b)\lambda_n^{1/2} \varphi_n) := (\rho(ab)\lambda_n^{1/2} \varphi_n), \quad a, b \in A,$$

defines a $*$-representation $\rho_\Phi$ of $A$ on the domain

$$\mathcal{D}(\rho_\Phi) := \{(\rho(a)\lambda_n^{1/2} \varphi_n)_{n \in \mathbb{N}}; a \in A\}$$

with algebraically cyclic vector $\Phi := (\lambda_n^{1/2} \varphi_n)_{n \in \mathbb{N}}$. From (25) we derive

$$f_s(a) = \sum_{n=1}^\infty \langle \rho(a)\lambda_n^{1/2} \varphi_n, \lambda_n^{1/2} \varphi_n \rangle = \langle \rho_\Phi(a)\Phi, \Phi \rangle =: f_\Phi(a), \quad a \in A,$$

that is, $f_s$ is equal to the vector functional $f_\Phi$ in the representation $\rho_\Phi$. Therefore, by the uniqueness of the GNS representation, $\pi_s$ is unitarily equivalent to $\rho_\Phi$. Likewise, the GNS representation $\pi_t$ is
unitarily equivalent to the corresponding \(*\)-representation \(\rho_\Psi\), where
\[ t\varphi = \sum_n \langle \varphi, \psi_n \rangle \mu_n \psi_n \]
is a corresponding representation of the operator \( t \) and \( \Psi := (\mu_n^{1/2} \psi_n)_{n \in \mathbb{N}} \). Clearly, since \( \rho_\Psi \subseteq \rho_\infty \) and \( \rho_\Psi \subseteq \rho_\infty \), we have \( \Phi \in S(\rho_\infty, f_s) \) and \( \Psi \in S(\rho_\infty, f_1) \).

Let \( \mathcal{M}_\infty \) denote the von Neumann algebra \((\rho_\infty(A)'_{ss})'\). Then, by Theorem \[ \ref{main1} \] we have

\[ (26) \quad P_\Lambda(f_s, f_1) \equiv P_\Lambda(f_\Phi, f_\Psi) = P_{\mathcal{M}_\infty}(F_\Phi, F_\Psi). \]

Let \( x \in \mathcal{B}(\mathcal{H}_\infty) \). We write \( x \) as a matrix \((x_{jk})_{j,k \in \mathbb{N}}\) with entries \( x_{jk} \in \mathcal{B}(\mathcal{H}(\rho)) \). Clearly, \( x \) belongs to in \( \rho_\infty(A)'_{ss} \) if and only if each entry \( x_{jk} \) is in \( \rho(A)'_{ss} \). Further, it is easily verified that \( x \) is in \((\rho_\infty(A)'_{ss})'\) if and only if there is a (uniquely determined) operator \( x_0 \in (\rho(A)'_{ss})' \) such that \( x_{jk} = \delta_{jk} x_0 \) for all \( j, k \in \mathbb{N} \). The map \( \pi(x_0) := x \) defines a \(*\)-isomorphism of von Neumann algebras \( \mathcal{M} := (\rho(A)'_{ss})' \) and \( \mathcal{M}_\infty = (\rho_\infty(A)'_{ss})' \), that is, \( \pi \) is a \(*\)-representation of \( \mathcal{M} \).

As above, we let \( F_s \) and \( F_t \) denote the normal functionals on \( \mathcal{M} \) defined by \( F_s(x) := \text{Tr} x s \) and \( F_t(x) := \text{Tr} x t \), \( x \in \mathcal{M} \). Repeating the preceding reasoning with \( \rho \) and \( A \) replaced by \( \pi \) and \( \mathcal{M} \), respectively, we obtain \( F_s(\cdot) = \langle \pi_0(\cdot) \Phi, \Phi \rangle = F_\Phi(\cdot) \) and \( F_t = F_\Psi \). Hence \( P_\mathcal{M}(F_s, F_t) = P_{\mathcal{M}_\infty}(F_\Phi, F_\Psi) \), so that

\[ (27) \quad P_\Lambda(f_s, f_1) = P_\mathcal{M}(F_s, F_t) \]

by \((26)\). It is proved in \[ \cite{3} \] Corollary 1 (see also \[ \cite{17} \]) that

\[ P_\mathcal{M}(F_s, F_t) = (\text{tr}_\mathcal{M} |\hat{s}^{1/2} \hat{s}^{1/2}|)^2. \]

Combined with \((27)\) this yields \((30)\) and completes the proof. \( \square \)

Let us remain the assumptions and the notations of Theorem \[ \ref{main1} \].

In general, \( P_\Lambda(f_s, f_1) \) is different from \((\text{Tr} (s^{1/2} t s^{1/2})^2)^2\) a simple examples show. However, if in addition \( \rho \) is \textit{irreducible} (that is, if \( \rho(A)'_{ss} = \mathbb{C} \cdot I \)), then \( s = \hat{s} \) and \( t = \hat{t} \) as noted above and therefore by \((24)\) we have

\[ (28) \quad P_\Lambda(f_s, f_1) = (\text{Tr} (s^{1/2} t s^{1/2})^2)^2. \]

We now apply the preceding theorem to an interesting example.

**Example 2.** \textit{(Schrödinger representation of the Weyl algebra)}

Let \( A \) be the Weyl algebra, that is, \( A \) is the unital \(*\)-algebra generated by two hermitian generators \( p \) and \( q \) satisfying

\[ pq - qp = -i1, \]
and let \( \rho \) be the Schrödinger representation of \( A \), that is,

\[
(\rho(q)\varphi)(x) = x\varphi(x), \quad (\rho(p)\varphi)(x) = -i\frac{d}{dx}\varphi(x), \quad \varphi \in D(\rho) := \mathcal{S}(\mathbb{R}),
\]
on \( L^2(\mathbb{R}) \). Since \( \rho \) is irreducible, \( \rho_\infty(A)_{ss} = \mathbb{C} \cdot I \). Hence \( \mathcal{M} = \mathcal{B}(\mathcal{H}(\rho)) \) and \( \text{tr}_\mathcal{M} = \text{Tr} \). Therefore, if \( s, t \in \mathcal{B}(\pi(A))_+ \) and the GNS representations \( \pi_{f_s} \) and \( \pi_{f_t} \) are essentially self-adjoint, it follows from Theorem 11 and formula (28) that

\[
P_A(f_s, f_t) = (\text{Tr}|ts^{1/2}s^{1/2}|)^2 = (\text{Tr}(s^{1/2}ts^{1/2})^{1/2})^2.
\]

Let us specialize this to the rank one case, that is, let \( s = \varphi \otimes \varphi \) and \( t = \psi \otimes \psi \) with \( \varphi, \psi \in D(\rho) \), so that \( f_s(a) = \langle \rho(a)\varphi, \varphi \rangle \) and \( f_t(a) = \langle \rho(a)\psi, \psi \rangle \) for \( a \in A \). Then formula (30) yields

\[
P_A(f_s, f_t) = |\langle \varphi, \psi \rangle|^2.
\]

Recall that (31) holds under the assumption that the GNS representations \( \pi_{f_s} \) and \( \pi_{f_t} \) are essentially self-adjoint. We shall see in section 5 below that (31) is no longer true if the latter assumption is omitted.

Now we turn to the second main application.

**Theorem 12.** Let \( X \) be a locally compact topological Hausdorff space and let \( A \) be a \( \ast \)-subalgebra of \( C(X) \) which contains the constant function 1 and separates the points of \( X \). Let \( \mu \) be a positive regular Borel measure on \( X \) such that \( A \subseteq L^1(X, \mu) \) and let \( \eta, \xi \in L^\infty(X, \mu) \) be non-negative functions. Define positive linear functionals \( f_\eta \) and \( f_\xi \) on \( A \) by

\[
f_\eta(a) = \int_X a(x)\eta(x) \, d\mu(x), \quad f_\xi(a) = \int_X a(x)\xi(x) \, d\mu(x) \quad \text{for} \quad a \in A.
\]

Suppose that the GNS representations \( \pi_{f_\eta} \) and \( \pi_{f_\xi} \) are essentially self-adjoint. Then

\[
P_A(f_\eta, f_\xi) = \left( \int_X \eta(x)^{1/2} \xi(x)^{1/2} \, d\mu(x) \right)^2.
\]

**Proof.** We define a closed \( \ast \)-representation \( \pi \) of the \( \ast \)-algebra \( A \) on \( L^2(X, \mu) \) by \( \pi(a)\varphi = a \cdot \varphi \) for \( a \in A \) and \( \varphi \) in the domain

\[
\mathcal{D}(\pi) := \{ \varphi \in L^2(X, \mu) : a \cdot \varphi \in L^2(X, \mu) \quad \text{for} \quad a \in A \}.
\]

First we prove that \( \pi(A)_{ss}' = L^\infty(X, \mu) \), where the functions of \( L^\infty(X, \mu) \) act as multiplication operators on \( L^2(X, \mu) \). Let \( \mathfrak{A} \) denote the \( \ast \)-subalgebra of \( L^\infty(X, \mu) \) generated by the functions \( (a \pm i)^{-1} \),
where \( a = a^+ \in A \). Obviously, \( L^\infty(X, \mu) \subseteq \pi(A)'_{ss} \). Conversely, let \( x \in \pi(A)_{ss}' \). It is straightforward to show that for any \( a = a^+ \in A \) the operator \( \overline{\pi(a)} \) is self-adjoint and hence equal to the (self-adjoint) multiplication operator by the function \( a \). By definition \( x \) commutes with \( \overline{\pi(a)} \), hence with \( (\pi(a) \pm iI)^{-1} = (a \pm i)^{-1} \), and therefore with the whole algebra \( \mathfrak{A} \). The *-algebra \( A \) separates the points of \( X \), so does the *-algebra \( \mathfrak{A} \). Therefore, from the Stone–Weierstrass theorem [9 Corollary 8.2], applied to the one point compactification of \( X \), it follows that \( \mathfrak{A} \) is norm dense in \( C_0(X) \). Hence \( x \) commutes with \( C_0(X) \) and so with its closure \( L^\infty(X, \mu) \) in the weak operator topology. Thus, \( x \in L^\infty(X, \mu)' \). Since \( L^\infty(X, \mu)' = L^\infty(X, \mu) \), we have shown that \( \pi(A)'_{ss} = L^\infty(X, \mu) \). Therefore, \( \mathcal{M} := (\pi(A)'_{ss})' = L^\infty(X, \mu) \).

Let \( F_\eta \) and \( F_\xi \) denote the positive linear functionals on \( \mathcal{M} \) defined by \(|32|\) with \( A \) replaced by \( \mathcal{M} \). For \( \mathcal{M} = L^\infty(X, \mu) \) it is well-known (see e.g. formula (14) in \([1]\)) that \( P_{\mathcal{M}}(F_\eta, F_\xi) = (\int_X \eta(x)1/2 \xi(x)1/2 \, d\mu(x))^2 \). Since \( P_A(f_\eta, f_\xi) = P_\mathcal{M}(F_\eta, F_\xi) \) by Theorem 8, we obtain \(|33|\). \( \square \)

In the following two examples we reconsider the one dimensional Hamburger moment problem (see Example 11) and we specialize the preceding theorem to the case where \( X = \mathbb{R} \) and \( A = \mathbb{C}[x] \).

**Example 3.** **Determinate Hamburger moment problems**

Let \( \mu_\eta \) and \( \mu_\xi \) be the positive Borel measures on \( \mathbb{R} \) defined by \( d\mu_\eta = \eta \, d\mu \) and \( d\mu_\xi = \xi \, d\mu \). Since \( \mathbb{C}[x] \in L^1(\mathbb{R}, \mu) \) and \( \eta, \xi \in L^\infty(\mathbb{R}, \mu) \), we have \( \mu_\eta, \mu_\xi \in M(\mathbb{R}) \). If both measures \( \mu_\eta \) and \( \mu_\xi \) are determinate, then the GNS representations \( \pi_{f_\mu_\eta} \) and \( \pi_{f_\mu_\xi} \) are essentially self-adjoint (as shown in Example 11) and hence formula \(|33|\) holds by Theorem 12.

**Example 4.** **Indeterminate Hamburger moment problems**

Suppose \( \nu \in M(\mathbb{R}) \) is an indeterminate measure such that \( \nu(\mathbb{R}) = 1 \).

Let \( V_\nu \) denote the set of all positive Borel measures \( \mu \in M(\mathbb{R}) \) which have the same moments as \( \nu \), that is, \( \int x^n \, d\nu(x) = \int x^n \, d\mu(x) \) for all \( n \in \mathbb{N}_0 \). Since \( \nu \) is indeterminate and \( V_\nu \) is convex and weakly compact, there exists a measure \( \mu \in \mathbb{V}_\nu \) which is not an extreme point of \( V_\nu \), that is, there are measures \( \mu_1, \mu_2 \in \mathbb{V}_\nu \), \( \mu_j \neq \mu \) for \( j = 1, 2 \), such that \( \mu = \frac{1}{2}(\mu_1 + \mu_2) \). Since \( \mu_j(M) \leq 2\mu(M) \) for all measurable sets \( M \) and \( \mu_1 + \mu_2 = 2\mu \), there exists functions \( \eta, \xi \in L^\infty(\mathbb{R}, \nu) \) satisfying

\[
(34) \quad \eta(x) + \xi(x) = 2, \quad \|\xi\|_\infty \leq 2, \quad \|\eta\|_\infty \leq 2, \quad d\mu_1 = \eta \, d\mu, \quad d\mu_2 = \xi \, d\mu.
\]

Define \( f(p) = \int p(x) \, d\mu(x) \) for \( p \in \mathbb{C}[x] \). Since \( \mu_1, \mu_2, \mu \in \mathbb{V}_\nu \), the functionals \( f_\eta \) and \( f_\xi \) defined by \(|32|\) are equal to \( f \). Therefore, since \( f(1) = \mu(\mathbb{R}) = \nu(\mathbb{R}) = 1 \), we have \( P_A(f_\eta, f_\xi) = P_A(f, f) = 1 \).
Put $J := \left( \int_X \eta(x)^{1/2} \xi(x)^{1/2} \, d\mu(x) \right)^2$. From (34) we obtain $\eta(x)\xi(x) = \eta(x)(2 - \eta(x)) \leq 1$ and hence $J \leq 1$, since $\mu(\mathbb{R}) = 1$. If $J$ would be equal to 1, then $\eta(x)(2 - \eta(x)) = 1$ a.e. on $\mathbb{R}$ which implies that $\eta(x) = 1$ a.e. on $\mathbb{R}$ by (34). But then $\mu_1 = \mu_2 = \mu$ which contradicts the choice of measures $\mu_1$ and $\mu_2$. Thus we have proved that $J \neq 1 = P_A(f_\eta, f_\xi)$, that is, formula (33) does not hold in this case.

The classical moment problem leads to a number of open problems concerning transition probabilities. We will state three of them.

Let $M(\mathbb{R}^d)$, $d \in \mathbb{N}$, denote the set of positive Borel measures $\mu$ on $\mathbb{R}^d$ such that all polynomials $p(x_1, \ldots, x_d) \in \mathbb{C}[x_1, \ldots, x_d]$ are $\mu$-integrable. For $\mu \in M(\mathbb{R}^d)$ we define a positive linear functional $g_\mu$ on the $\ast$-algebra $A := \mathbb{C}[x_1, \ldots, x_d]$ by

$$g_\mu(p) = \int p \, d\mu, \quad p \in \mathbb{C}[x_1, \ldots, x_d].$$

Then the main problem is the following:

**Problem 1:** Given $\mu, \nu \in M(\mathbb{R}^d)$, what is $P_A(g_\mu, g_\nu)$?

This seems to be a difficult problem and it is hard to expect a sufficiently complete answer. For $d = 1$ Example 3 contains some answer under the assumption that both measures $\mu_\eta$ and $\mu_\xi$ are determinate. This suggests the following questions:

**Problem 2:** What about the case when the measures $\mu_\eta$ and/or $\mu_\xi$ in Example 3 are not determinate?

**Problem 3:** Is formula (33) still valid in the multi-dimensional case $d > 1$ if $\mu_\eta$ and $\mu_\xi$ are determinate?

It can be shown that the answer to problem 3 is affirmative if all multiplication operators $\pi_\mu(x_j)$, $j = 1, \ldots, d$, are essentially self-adjoint. The latter assumption is sufficient, but not necessary for $\mu$ being determinate [13]. In the multi-dimensional case determinacy turns out to be much more difficult than in the one-dimensional case, see e.g. [13].

5. **Vector Functionals of the Schrödinger Representation**

The crucial assumption for the results in preceding sections was the essential self-adjointness of GNS representations $\pi_f$ and $\pi_g$. In this section we consider the simplest situation where $\pi_f$ and $\pi_g$ are not essentially self-adjoint.

In this section $A$ denotes the Weyl algebra (see Example 2) and $\pi$ is the Schrödinger representation of $A$ given by (29). For $\eta \in \mathcal{D}(\pi) = \mathcal{S}(\mathbb{R})$ let $f_\eta$ denote the positive linear functional $f_\eta$ on $A$ given by

$$f_\eta(x) = \langle \pi(x) \eta, \eta \rangle, \quad x \in A.$$
Consider the following condition on the function $\eta$:

\[ (*) \text{ There are finitely many mutually disjoint open intervals } J_l(\eta) = (\alpha_l, \beta_l), \; l = 1, \ldots, r, \text{ such that } \eta(t) \neq 0 \text{ for } t \in J(\eta) \triangleq \cup_l J_l(\eta) \text{ and } \eta^{(n)}(t) = 0 \text{ for } t \in \mathbb{R}/J(\eta) \text{ and all } n \in \mathbb{N}_0. \]

The main result of this section is the following theorem.

**Theorem 13.** Suppose that $\varphi$ and $\psi$ are functions of $C_0^\infty(\mathbb{R})$ satisfying condition $(*)$. Then

\[ P_A(f_\varphi, f_\psi) = \left( \sum_{k,l} \left| \int_{J_k(\varphi) \cap J_l(\psi)} \varphi(x)\overline{\psi(x)} \, dx \right| \right)^2. \tag{35} \]

(If $J_k(\varphi) \cap J_l(\psi)$ is empty, the corresponding integral is set zero.)

Before we turn to the proof of the theorem let us discuss formula (35) in two simple cases.

- If both sets $J(\varphi)$ and $J(\psi)$ consist of a single interval, then
  \[ P_A(f_\varphi, f_\psi) = \left| \int_{\mathbb{R}} \varphi(x)\overline{\psi(x)} \, dx \right|^2 = |\langle \varphi, \psi \rangle|^2, \]
  that is, in this case formula (31) holds.

- Let $\varphi, \psi \in C_0^\infty(\mathbb{R})$ be such that $J(\varphi) = J(\psi)$, $J_k(\varphi) = J_k(\psi)$ and $\varphi(x) = \epsilon_k \psi(x)$ on $J_k(\varphi)$ for $k = 1, \ldots, r$, where $\epsilon_k \in \{1, -1\}$. Then formula (35) yields $P_A(f_\varphi, f_\psi) = \|\varphi\|^4$. It is easy to choose $\varphi \neq 0$ and the numbers $\epsilon_k$ such that $\langle \varphi, \psi \rangle = 0$, so formula (31) does not hold in this case.

The proof of Theorem 13 requires a number of technical preparations. The first aim is to describe the closure $\overline{\pi f_\eta}$ of the GNS representation $\pi f_\eta$ for a function $\eta \in C_0^\infty(\mathbb{R})$ satisfying condition $(*)$.

Let $\rho_\eta$ denote the restriction of $\pi$ to the dense domain

\[ \mathcal{D}(\rho_\eta) = \{ \xi \in \bigoplus_{l=1}^r C^\infty((\alpha_l, \beta_l)) : \xi^{(k)}(\alpha_l) = \xi^{(k)}(\beta_l) = 0, \; k \in \mathbb{N}_0, \; l = 1, \ldots, r \} \]

in the Hilbert space $L^2(\mathcal{J}(\eta))$. The following lemma says that $\rho_\eta$ is unitarily equivalent to $\overline{\pi f_\eta}$.

**Lemma 14.** There is a unitary operator $U$ of $\mathcal{H}(\pi f_\eta)$ onto $L^2(\mathcal{J}(\eta))$ given by $U(\pi f_\eta(a)\eta) = \rho_\eta(a)\eta$, $a \in A$, such that $\rho_\eta = U\overline{\pi f_\eta}U^*$.

**Proof.** From the properties of GNS representations it follows easily that the unitary operator $U$ defined by $U(\pi f_\eta(a)\eta) = \rho_\eta(a)\eta$, $a \in A$, provides unitary equivalences $\tau_\eta = U\pi f_\eta U^*$ and $\overline{\pi_\eta} = U\overline{\pi f_\eta}U^*$, where $\tau_\eta$ denotes the restriction of $\pi$ to $\mathcal{D}(\rho_\eta) = \pi(A)\eta$. Clearly, $\tau_\eta \subseteq \rho_\eta$ and hence $\overline{\pi_\eta} \subseteq \overline{\pi f_\eta}$. \hfill \ensuremath{\blacksquare}
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ρ_η, since ρ_η is obviously closed. To prove the statement it therefore suffices to show that ρ_η is the closure of τ_η, that is, π(Λ)η is dense in D(ρ_η) in the graph topology of ρ_η(A). For this the auxiliary Lemmas 15 and 16 proved below are essentially used.

Each element a ∈ A is of a finite sum of terms f(q)p^n, where n ∈ N and f ∈ C[q]. Since η ∈ C_0^∞(R), the set J(η) and hence the operators π_0(f(q)) are bounded. Therefore, the graph topology τ_{min}(A) is generated by the seminorms ∥ρ_η(p^n)∥, n ∈ N_0, on D(ρ_η). Let ψ ∈ D(ρ_η).

First assume that ψ vanishes in some neighbourhoods of the end points α_l, β_l. Then, by Lemma 16, for any m ∈ N there is sequence (f_n)_{n∈N} of polynomials such that

\[
\lim_{n} \rho_η((ip)^k)(\rho_η(f(q))η - ψ) = \lim_{n} ((f_n η)^{(k)} - ψ^{(k)}) = 0
\]

in L^2(J(η)) for k = 0, \ldots, m. This shows that ψ is in the closure of ρ_η(A)η with respect the graph topology of ρ_η(A).

The case of a general function ψ is reduced to the preceding case as follows. Suppose that ε > 0 and 2ε < min_l |β_l - α_l|. We define

ψ_ε(x) = ψ(x - ε + 2ε(x - α_l - ε)(β_l - α_l - 2ε)^{-1}) for x ∈ (α_l, β_l)

and l = 1, \ldots, r and ψ_ε(x) = 0 otherwise. Then ψ_ε vanishes in some neighbourhoods of the end points α_l, β_l, so ψ_ε is in the closure of ρ_η(A)η as shown in the preceding paragraph. Using the dominated Lebesgue convergence theorem it follows that

\[
\lim_{ε \to 0} \rho_η((ip)^k)(ψ_ε - ψ) = \lim_{ε \to 0} (ψ_ε^{(k)} - ψ^{(k)}) = 0
\]

in L^2(J(η)) for k ∈ N_0. Therefore, since ψ_ε is in the closure of ρ_η(A)η, so is ψ.

Lemma 15. Suppose that g ∈ C^{(k)}([α, β]), where α, β ∈ R and k ∈ N. Then there exists a sequence (f_n)_{n∈N} of polynomials such that f_n(j)(x) → g(j)(x) uniformly on [α, β] for j = 0, \ldots, k as n → ∞.

Proof. By the Weierstrass theorem there is a sequence (h_n)_{n∈N} of polynomials such that h_n(x) → g(k)(x) uniformly on [α, β]. Fix γ ∈ [α, β] and set h_{n,k} := h_n. Then

\[
h_{n,k-1}(x) := g(k)(γ) + \int_γ^x h_{n,k}(s) ds → g(k-1)(x) = g(k)(γ) + \int_γ^x g(k)(s) ds.
\]

Clearly, (h_{n,k-1})_{n∈N} is sequence of polynomials and we have h_{n,k-1}(x) = h_{n,k}(x) on [α, β]. Proceeding by induction we obtain sequences (h_{n,k-j})_{n∈N}, j = 0, \ldots, k, of polynomials such that h_{n,k-j}(x) → g(k-j)(x) and h_{n,k-j}(x) = h_{n,k+1-j}(x) on [α, β]. Setting f_n := h_{n,0} the sequence (f_n)_{n∈N} has the desired properties. □
Lemma 16. Suppose that $\eta \in C_0^\infty(\mathbb{R})$ satisfies condition (\ast). Let $\psi \in \bigoplus_{r=1}^\infty C_0^{(m)}((\alpha_1, \beta_1))$, where $m \in \mathbb{N}$. Then there exists a sequence $(f_n)_{n \in \mathbb{N}}$ of polynomials such that $\lim_{n \to \infty} (f_n \psi)^{(k)} = \psi^{(k)}$ in $L^2(\mathcal{J} \psi)$ for $k = 0, \ldots, m$.

Proof. By the assumption $\psi$ vanishes in some neighbourhoods of the end points $\alpha_l$ and $\beta_l$. Set $\psi(x) = 0$ on $\mathbb{R}/\mathcal{J} \psi$. Then, $\psi \eta^{-1}$ becomes a function of $C^{(m)}([\alpha, \beta])$, where $\alpha := \min_l \alpha_l$ and $\beta := \max_l \beta_l$. Therefore, by Lemma 14 there exists a sequence $(f_n)_{n \in \mathbb{N}}$ of polynomials such that $f_n^{(j)}(x) \to (\psi \eta^{-1})^{(j)}(x)$ for $j = 0, \ldots, m$ uniformly on $[\alpha, \beta]$. Then

$$(f_n \eta)^{(k)} = \sum_{j=0}^k \binom{k}{j} f_n^{(j)} \eta^{(k-j)} \to \sum_{j=0}^k \binom{k}{j} (\psi \eta^{-1})^{(j)} \eta^{(k-j)} = \psi^{(k)}$$

as $n \to \infty$ uniformly on $[\alpha, \beta]$ and hence in $L^2(\mathcal{J} \psi)$.

Now we are able to give the

Proof of Theorem 13. Let us abbreviate $\pi_\varphi = \pi_{f_\varphi}$ and $\pi_\psi = \pi_{f_\psi}$. By Lemma 14 the closure $\pi_\psi = \pi_{f_\psi}$ of the GNS representation $\pi_{f_\psi}$ is unitarily equivalent to the representation $\rho_\psi$. For notational simplicity we shall identify the representations $\pi_\psi$ and $\rho_\psi$ via the unitary $U$ defined in Lemma 14. Using this description of $\pi_\psi \cong \rho_\psi$ it is straightforward to check that the domain $\mathcal{D}(\pi_\psi^*)$ consists of all functions $g \in C^\infty(\mathcal{J} \psi)$ such that their restrictions to $\mathcal{J}_l \psi$ extend to functions of $C^\infty(\mathcal{J}_l \psi)$ and $g(t) = 0$ on $\mathbb{R}/\mathcal{J} \psi$. Further, we have $(\pi_\psi^* f \psi g) = f \cdot g$ and $(\pi_\psi^* \psi g) = -ig'$ for $g \in \mathcal{D}(\pi_\psi^*)$ and $f \in \mathbb{C}[q]$.

Suppose that $T \in I(\pi_\varphi, (\pi_\psi)^*)$ and $\|T\| \leq 1$. Set $\xi := T \varphi$. By the intertwining property of $T$, for each polynomial $f$ we have

$$(36) \quad T(f \cdot \varphi) = T \pi_\varphi(f \psi \varphi) = (\pi_\psi)^*(f \psi) T \varphi = (\pi_\psi)^*(f \psi) \xi = f \cdot \xi.$$  

Therefore, since $\|T\| \leq 1$, we obtain

$$(37) \quad \int_{\alpha}^\beta |f(x)|^2 |\xi(x)|^2 dx = \int_{\alpha}^\beta |T(f \cdot \varphi)(x)|^2 dx \leq \int_{\alpha}^\beta |f(x)|^2 |\varphi(x)|^2 dx$$

for all polynomials $f$ and hence for all functions $f \in C(\alpha, \beta)$ by the Weierstrass theorem. Hence (37) implies that

$$(38) \quad |\xi(x)| \leq |\varphi(x)| \text{ on } [\alpha, \beta].$$

Therefore, $\xi(x) = 0$ if $x \in \mathbb{R}/\mathcal{J} \varphi$. Clearly, $\xi(x) = 0$ if $x \in \mathbb{R}/\mathcal{J} \psi$, since $\xi \in \mathcal{D}(\pi_\psi^*)$. Since $\varphi$ satisfies condition (\ast), the set $\{f \cdot \varphi : f \in \mathbb{C}[x]\}$ is dense in $L^2(\mathcal{J} \varphi) = \mathcal{H}(\pi_\varphi)$. Therefore, it follows from (36)
that $T$ is equal to the multiplication operator by the bounded function $\xi \varphi^{-1}$. (Note that $\xi \varphi^{-1}$ is bounded by (38).) In particular, we obtain

$$\varphi' \cdot \xi \varphi^{-1} = T \varphi' = T \pi_\varphi(ip) \varphi = (\pi_\psi)^* (ip) T \varphi = (\pi_\psi)^* (ip) \xi = \xi'$$

Thus, $\varphi'(x)\xi(x) = \varphi(x)\xi'(x)$ which in turn implies that $(\xi')'(x) = 0$ for all $x \in \mathcal{J}(\varphi) \cap \mathcal{J}(\psi)$. Hence $\xi(x) = \lambda \varphi(x)$ for some constant $\lambda \in \mathbb{C}$ on each connected component of $\mathcal{J}(\varphi) \cap \mathcal{J}(\psi)$. By (38), $|\lambda| \leq 1$. The connected components of the open set $\mathcal{J}(\varphi) \cap \mathcal{J}(\psi)$ are precisely the intervals $\mathcal{J}_l(\varphi) \cap \mathcal{J}_k(\psi)$ provided the latter is not empty.

Conversely, suppose that for all indices $l, k$ such that $\mathcal{J}_l(\varphi) \cap \mathcal{J}_k(\psi) \neq \emptyset$ a complex number $\lambda_{k, l}$, where $|\lambda_{k, l}| \leq 1$, is given. Set $\xi(x) = \lambda_{k, l} \varphi(x)$ for $x \in \mathcal{J}_l(\varphi) \cap \mathcal{J}_k(\psi)$ and $\xi(x) = 0$ otherwise. From the description of the domain $D((\pi_\psi)^*)$ given in the first paragraph of this proof it follows that $\xi \in D((\pi_\psi)^*)$. Define $T(\pi_\varphi(a) \varphi) := (\pi_\psi)^* (a) \xi$, $a \in \mathbb{A}$. It is easily checked that $T$ extends by continuity to an operator $T$ of $\mathcal{H}(\pi_\varphi) = L^2(\mathcal{J}(\varphi))$ into $\mathcal{H}((\pi_\psi)^*) = L^2(\mathcal{J}(\psi))$ such that $T \in I(\pi_\varphi, (\pi_\psi)^*)$ and $\|T\| \leq 1$. Since $T \varphi = \xi$, we have

$$\langle T \varphi, \psi \rangle = \sum_{k, l} \lambda_{k, l} \int_{\mathcal{J}_l(\varphi) \cap \mathcal{J}_k(\psi)} \varphi(x) \overline{\psi(x)} \, dx.$$ 

Therefore, the supremum of expressions $|\langle T \varphi, \psi \rangle|$ is obtained if we choose $\lambda_{k, l}$ such that the number $\lambda_{k, l} \int_{\mathcal{J}_l(\varphi) \cap \mathcal{J}_k(\psi)} \varphi \overline{\psi} \, dx$ is equal to its modulus $|\int_{\mathcal{J}_k(\varphi) \cap \mathcal{J}_l(\psi)} \varphi \overline{\psi} \, dx|$. This implies formula (35). $\square$

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