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TRANSITION PROBABILITIES OF POSITIVE FUNCTIONALS ON $*$-ALGEBRAS

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ABSTRACT. The transition probability $P_A(f,g)$ of positive linear functionals f and g on a unital $*$-algebra A was defined by A. Uhlmann, *Rep. Math. Phys.* **9**(1976), 273–279. In this paper we study this notion in the context of *unbounded* Hilbert space representations of the $*$-algebra A and derive a number of basic results. The main technical assumption is the essential self-adjointness of the GNS representations π_f and π_g. Applications to functionals given by density matrices or by integrals and to vector functionals on the Weyl algebra are given.

KEYWORDS: *Transition probability, non-commutative probability, unbounded representations.*

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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 π of A on a Hilbert space with unit vectors φ and ψ, 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 vector states in some common $*$-representation of A. This definition was introduced by A. Uhlmann [18]. The square root $\sqrt{P_A(f,g)}$ is also called fidelity in the literature [3], [11].

The transition probability is related to other important topics such as Bures' distance [9], Sakai's non-commutative Radon–Nikodym theorem [6], and the geometric mean of Pusz and Woronowicz [13]. There are an extensive literature about the finite dimensional case (see e.g. the monograph [8]) and a number of results for C^*-algebras and von Neumann algebras (see e.g. [1], [2], [3], [4], [6], [7], [20]). In contrast it seems that the case of *unbounded* representations has been not yet studied. The aim of the present paper is to fill this gap and to study the transition probability $P_A(f,g)$ for positive linear functionals f and g on a general unital $*$-algebra A.

Since the $*$-representations of A act by unbounded operators on Hilbert spaces, a number of technical problems of unbounded representation theory [16] come up. Dealing with these difficulties in a proper way is a main purpose of this paper.

In Section 2 we 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 π_f and π_g. This means that we restrict ourselves to a class of "nice" functionals. Let π be a fixed biclosed $*$-representation π of A such that the functionals f and g are realized as vector functionals by vectors φ and ψ, respectively. (The assumption that π is biclosed is no restriction of generality, since any $*$-representation has a biclosed extension.)

Our first main result (Theorem 3.5) states that the transition probability $P_A(f,g)$ is the supremum of $|\langle T\varphi,\psi\rangle|^2$ taken over all operators T in the commutant $\pi(A)'_{ss}$ with norm $\|T\| \leqslant 1$.

The second main result (Theorem 3.7) says that the supremum in the definition of $P_A(f,g)$ is always attained, that is, there are vectors φ' and ψ' in the domain of π representing the functionals f and g, respectively, such that $P_A(f,g) = |\langle\varphi',\psi'\rangle|^2$.

The third main result (Theorem 3.8) gives a generalization of Uhlmann's formula $P_A(f,g) = h(c^+b)^2$ for positive functionals of the form $f(\cdot) = h(b^+\cdot b)$ and $g(\cdot) = h(c^+\cdot c)$.

In Section 4 we apply Theorem 3.7 from Section 3 to generalize two standard formulas (4.2) and (4.11) for transition probabilities to the unbounded case; these formulas concern trace functionals $f_t(a) = \operatorname{Tr}\rho(a)t$ and functionals of the form $f_\eta(a) = \int a\eta\, \mathrm{d}\mu$ on $*$-algebras of functions. 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 $C_0^\infty(\mathbb{R})$. In this case both GNS representations π_f and π_g are *not* essentially self-adjoint and the corresponding formula for $P_A(f,g)$ is in general different from the standard formula (4.2).

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 $f(a^+a) \geqslant 0$ 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 [12] and [17], respectively.

2. BASICS ON UNBOUNDED REPRESENTATIONS

Proofs of all unproven facts stated in this section and more details can be found in the monograph [16], see e.g. [5]. Proposition 2.2 below is a new result that might be of interest in itself.

Let $(\mathcal{D}, \langle\cdot,\cdot\rangle)$ 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 $I_{\mathcal{D}}$ the identity map of $\mathcal{D}$ and by $\mathbf{B}(\mathcal{H})$ the $*$-algebra of all bounded linear operators on $\mathcal{H}$.

DEFINITION 2.1. A *representation* of A on $\mathcal{D}$ is an algebra homomorphism π of A into the algebra $L(\mathcal{D})$ such that $\pi(1) = I_{\mathcal{D}}$ 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* π of A on $\mathcal{D}$ is a representation π satisfying

$$\langle \pi(a)\varphi, \psi\rangle = \langle \varphi, \pi(a^+)\psi\rangle \quad \text{for } a \in A,\ \varphi, \psi \in \mathcal{D}(\pi). \tag{2.1}$$

Let π be a representation of A. Then

$$\mathcal{D}(\pi^*) := \bigcap_{a\in A} \mathcal{D}(\pi(a)^*) \quad \text{and} \quad \pi^*(a) := \pi(a^+)^* \lceil \mathcal{D}(\pi^*) \quad \text{for } a \in A, \tag{2.2}$$

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

If π is a $*$-representation of A, then

$$\mathcal{D}(\overline{\pi}) := \bigcap_{a\in A} \mathcal{D}(\overline{\pi(a)}) \quad \text{and} \quad \overline{\pi}(a) := \overline{\pi(a)} \lceil \mathcal{D}(\overline{\pi}), \quad a \in A, \tag{2.3}$$

$$\mathcal{D}(\pi^{**}) := \bigcap_{a\in A} \mathcal{D}(\pi^*(a)^*) \quad \text{and} \quad \pi^{**}(a) := \pi^*(a^+)^* \lceil \mathcal{D}(\pi^{**}), \quad a \in A, \tag{2.4}$$

are $*$-representations π^* and π^{**} of A, called the *closure* respectively the *biclosure* of π. Then

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

If π is a $*$-representation, then $\mathcal{H}(\pi) = \mathcal{H}(\pi^*)$. But for a representation π 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 2.2. *Let π and ρ 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

$$\begin{aligned}\langle \rho(a^+)\varphi, P\psi\rangle &= \langle P\rho(a^+)\varphi, \psi\rangle = \langle \rho(a^+)\varphi, \psi\rangle = \langle \pi(a^+)\varphi, \psi\rangle \\ &= \langle \varphi, \pi(a^+)^*\psi\rangle = \langle \varphi, \pi^*(a)\psi\rangle = \langle P\varphi, \pi^*(a)\psi\rangle = \langle \varphi, P\pi^*(a)\psi\rangle.\end{aligned}$$

From this equality it follows that $P\psi \in \mathcal{D}(\rho(a^+)^*)$ and $\rho(a^+)^*P\psi = P\pi^*(a)\psi$. Hence $\psi \in \bigcap_{b\in A} \mathcal{D}(\rho(b)^*) = \mathcal{D}(\rho^*)$ 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 $\rho^*(a)P\psi = P\pi^*(a)\psi$. Therefore, we derive

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

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 2.3. A $*$-representation π of a $*$-algebra A is called

(i) *closed* if $\pi = \overline{\pi}$, or equivalently, if $\mathcal{D}(\pi) = \mathcal{D}(\overline{\pi})$,

(ii) *biclosed* if $\pi = \pi^{**}$, or equivalently, if $\mathcal{D}(\pi) = \mathcal{D}(\pi^{**})$,

(iii) *self-adjoint* if $\pi = \pi^*$, or equivalently, if $\mathcal{D}(\pi) = \mathcal{D}(\pi^*)$,

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

REMARK 2.4. It should be emphasized that the preceding definition of *essential self-adjointness* is different form the definition given in [16]. In Definition 8.1.10 of [16], a $*$-representation was called essentially self-adjoint if $\overline{\pi}$ is self-adjoint, that is, if $\overline{\pi} = \pi^*$.

Let π be a $*$-representation. Then the $*$-representations $\overline{\pi}$ and π^{**} are closed, π^{**} 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 $\mathrm{t}_{\pi(A)}$. Then the $*$-representation π is closed if and only if the locally convex space $\mathcal{D}(\pi)[\mathrm{t}_{\pi(A)}]$ is complete.

PROPOSITION 2.5. *If π_1 is a self-adjoint $*$-subrepresentation of a $*$-representation π of A, then there exists a $*$-representation π_2 of A on the Hilbert space $\mathcal{H}(\pi) \ominus \mathcal{H}(\pi_1)$ such that $\pi = \pi_1 \oplus \pi_2$.*

For the proof see Corollary 8.3.3 of [16].

For a $*$-representation of A we define two *commutants*:

$$\pi(A)'_s = \{T \in \mathbf{B}(\mathcal{H}(\pi)) : T\varphi \in \mathcal{D}(\pi),$$
$$T\pi(a)\varphi = \pi(a)T\varphi \text{ for } a \in A, \varphi \in \mathcal{D}(\pi)\},$$
$$\pi(A)'_{ss} = \{T \in \mathbf{B}(\mathcal{H}(\pi) : T\overline{\pi(a)} \subseteq \overline{\pi(a)}T, T^*\overline{\pi(a)} \subseteq \overline{\pi(a)}T^*\}.$$

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

$$\pi(A)'_{ss} = \pi(A)'_s \cap (\pi(A)'_s)^*. \tag{2.5}$$

If π_1 and π_2 are representations of A, the *interwining space* $I(\pi_1, \pi_2)$ consists of all bounded linear operators T of $\mathcal{H}(\pi_1)$ into $\mathcal{H}(\pi_2)$ satisfying

$$T\varphi \in \mathcal{D}(\pi_2) \quad \text{and} \quad T\pi_1(a)\varphi = \pi_2(a)T\varphi \quad \text{for } a \in A, \varphi \in \mathcal{D}(\pi_1). \tag{2.6}$$

The $*$-representation π_f in the following proposition is called the *GNS representation* associated with the positive linear functional f.

PROPOSITION 2.6. *Suppose that $f \in \mathcal{P}(A)$. Then there exists a $*$-representation π_f with algebraically cyclic vector φ_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 π is another $*$-representation of A with algebraically cyclic vector φ 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 $a \in A$.

For the proof see Theorem 8.6.4. of [16].

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

EXAMPLE 2.7 (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 μ such that $p(x) \in L^1(\mathbb{R}, \mu)$ for all $p \in \mathbb{C}[x]$. The number $s_n = \int x^n \mathrm{d}\mu(x)$ 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 μ, is called *determinate*, if the moment sequence $s(\mu)$ determines the measure μ 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 π_μ 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 $f_\mu(p) = \int p(x)\mathrm{d}\mu(x)$ for $p \in \mathbb{C}[x]$. Obviously, the vector $1 \in \mathcal{D}(\pi_\mu) := \mathbb{C}[x]$ is algebraically cyclic for π_μ. Therefore, since $f_\mu(p) = \langle \pi_\mu(p)1, 1 \rangle$ for $p \in \mathbb{C}[x]$, π_μ is (unitarily equivalent to) the GNS representation π_{f_μ} of the positive linear functional f_μ on $A = \mathbb{C}[x]$.

STATEMENT 2.8. *The $*$-representation π_μ 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. Theorem 16.11 of [17]), the moment sequence $s(\mu)$ is determinate if and only if the operator $\pi_\mu(x)$ is essentially self-adjoint. By Proposition 8.1(v) of [16], the latter holds if and only if the $*$-representation $(\pi_\mu)^*$ is self-adjoint, that is, if π_μ is essentially self-adjoint. ∎

By Proposition 8.1(vii) of [16], the closure $\overline{\pi}_\mu$ of the $*$-representation π_μ 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

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

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

3. MAIN RESULTS ON TRANSITION PROBABILITIES

Let Rep$A$ denote the family of all $*$-representations of A. Given $\pi \in \mathrm{Rep}A$ 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 2.6 for each $f \in \mathcal{P}(A)$ there exists a $*$-representation π 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 3.1. For $f, g \in \mathcal{P}(A)$ the *transition probability* $P_A(f, g)$ of f and g is defined by

$$P_A(f,g) = \sup_{\pi \in \mathrm{Rep}A} \; \sup_{\varphi \in \mathcal{S}(\pi,f), \psi \in \mathcal{S}(\pi,g)} |\langle \varphi, \psi\rangle|^2. \tag{3.1}$$

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

$$P_B(f,g) \leqslant P_A(f\lceil A, g\lceil A), \tag{3.2}$$

because the restriction of any $*$-representation of B is a $*$-representation of A.

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

$$|F(b^+a)|^2 \leqslant f(a^+a)g(b^+b) \quad \text{for } a, b \in A. \tag{3.3}$$

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

$$F_{\varphi,\psi}(a) := \langle \pi(a)\varphi, \psi\rangle, \quad a \in A, \tag{3.4}$$

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

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

which proves that $F_{\varphi,\psi} \in \mathcal{G}(f,g)$. By Theorem 3.2 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 φ and ψ 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 [19].

THEOREM 3.2. *Suppose that $f, g \in \mathcal{P}(A)$. Then*

$$P_A(f,g) = \sup_{F \in \mathcal{G}(f,g)} |F(1)|^2. \tag{3.5}$$

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

$$P_A(f,g) = |\langle \varphi, \psi\rangle|^2. \tag{3.6}$$

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 transition probabilities. Recall that π_f denotes the GNS representation of A associated with $f \in \mathcal{P}(A)$ and φ_f is the corresponding algebraically cyclic vector.

PROPOSITION 3.3. *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*

$$F(b^+a) = \langle T\pi_f(a)\varphi_f, \pi_g(b)\varphi_g\rangle \quad \text{for } a, b \in A, \tag{3.7}$$

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

$$|F(b^+a)|^2 \leqslant f(a^*a)g(b^*b) = \|\pi_f(a)\varphi_f\|^2 \|\pi_g(b)\varphi_g\|^2 \quad \text{for } a, b \in A.$$

Hence there exists a bounded linear operator T of $\mathcal{H}(\overline{\pi}_g)$ into $\mathcal{H}(\overline{\pi}_f)$ such that $\|T\| \leqslant 1$ and (3.7) holds. Let $a, b, c \in A$. Using (3.7) we obtain

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

Hence $T\pi_f(b)\varphi_f \in \mathcal{D}(\pi_g(c)^*)$ 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, $T\pi_f(a)\varphi_f \in \mathcal{D}((\pi_g)^*)$. Then

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

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

Conversely, let $T \in I(\pi_f, (\pi_g)^*)$ and $\|T\| \leqslant 1$. Define $F(a) = \langle T\pi_f(a)\varphi_f, \varphi_g\rangle$ for $a \in A$. It is straightforward to check that (3.7) holds and hence (3.3), that is, $F \in \mathcal{G}(f,g)$.

Clearly, by (3.7), $F = 0$ is equivalent to $T = 0$. Thus we have a one-to-one correspondence between functionals F and operators T. ∎

Combining Theorem 3.2 and Proposition 3.3 and using the formula $F(1) = \langle T\varphi_f, \varphi_g\rangle$ we obtain

COROLLARY 3.4. *For any $f, g \in \mathcal{P}(A)$ we have*

$$P_A(f,g) = \sup_{T\in I(\pi_f,(\pi_g)^*),\|T\|\leqslant 1} |\langle T\varphi_f, \varphi_g\rangle|^2. \tag{3.8}$$

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

THEOREM 3.5. *Suppose that f and g are positive linear functionals on A such that their* GNS *representations π_f and π_g are essentially self-adjoint. Let π be a biclosed $*$-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*

$$P(f,g) = \sup_{T\in\pi(A)'_{ss},\|T\|\leqslant 1} |\langle T\varphi, \psi\rangle|^2. \tag{3.9}$$

Proof. Let $T \in \pi(A)'_{ss}$ and $\|T\| \leqslant 1$. Similarly, as in the proof of Proposition 3.3, we define $F(a) = \langle T\pi(a)\varphi, \psi\rangle$, $a \in A$. Since $\pi(A)'_{ss} \subseteq \pi(A)'_s$, we obtain

$$\begin{aligned}|F(b^+a)|^2 &= |\langle T\pi(b^+a)\varphi, \psi\rangle|^2 = |\langle \pi(b^+)T\pi(a)\varphi, \psi\rangle|^2 \\ &= |\langle T\pi(a)\varphi, \pi(b)\psi\rangle|^2 \leqslant \|\pi(a)\varphi\|^2\|\pi(b)\psi\|^2 = f(a^+a)g(b^+b)\end{aligned}$$

for $a, b \in A$, that is, $F \in \mathcal{G}(f,g)$. Clearly, we have $\langle T\varphi, \psi\rangle = F(1)$. Let ρ_f and ρ_g denote the restrictions $\pi\lceil\pi(A)\varphi$ and $\pi\lceil\pi(A)\psi$, respectively. Since $\rho_f \subseteq \pi$ and $\rho_g \subseteq \pi$ and π is biclosed, it follows from Proposition 2.2(iii) that $(\rho_f)^{**} \subseteq \pi^{**} = \pi$ and $(\rho_g)^{**} \subseteq \pi^{**} = \pi$. Since $\varphi \in S(\pi, f)$ and $\psi \in S(\pi, g)$, the representations ρ_f and ρ_g are unitarily equivalent to the GNS representations π_f and π_g, respectively. For notational simplicity we identify ρ_f with π_f and ρ_g with π_g. Since ρ_f and ρ_g are essentially self-adjoint by assumption, $(\rho_f)^{**}$ and $(\rho_g)^{**}$ are self-adjoint. Therefore, by Proposition 2.5, there are subrepresentations ρ_1 and ρ_2 of π 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 3.3, there is an intertwiner $T_0 \in I(\rho_f, (\rho_g)^*) \cong I(\pi_f, (\pi_g)^*))$ such that $\|T_0\| \leqslant 1$ and (3.7) holds with T replaced by T_0. Define $T : \mathcal{H}(\rho_f) \oplus \mathcal{H}(\rho_1) \to \mathcal{H}(\rho_g) \oplus \mathcal{H}(\rho_2)$ by $T(\xi_f, \xi_1) = (T_0\xi_f, 0)$. Clearly, T^* acts by $T^*(\eta_g, \eta_2) = (T_0^*\eta_g, 0)$. Since $(\rho_g)^{**} = (\rho_g)^*$ and

$(\rho_f)^{**} = (\rho_f)^*$ by assumption and $T_0 \in I(\rho_f, (\rho_g)^*)$, it follows from Proposition 8.2.3(iii) and (iv), in [16] 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 $T \in \pi(A)'_{ss}$ by (2.5). Then we have $\|T\| = \|T_0\| \leqslant 1$ and $F(1) = \langle T_0\varphi, \psi\rangle = \langle T\varphi, \psi\rangle$. Together with the first paragraph of this proof we have shown that the supremum over the operators $T \in \pi(A)'_{ss}$, $\|T\| \leqslant 1$, 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 3.2, this proves (3.9). ∎

REMARK 3.6. A slight modification of the preceding proof shows the following: If we assume that the closures $\overline{\pi}_f$ and $\overline{\pi}_g$ of the GNS representations π_f and π_g are self-adjoint, then the assertion of Theorem 3.5 remains valid if it is only assumed that π is *closed* rather than biclosed. A similar remark applies also for the subsequent applications of Theorem 3.5 given below.

Theorem 3.5 says that (in the case of essentially self-adjoint GNS representations π_f and π_g) the transition probability $P(f,g)$ is given by formula (3.9) in *any* fixed biclosed $*$-representation π for which the sets $S(\pi,f)$ and $S(\pi,g)$ are not empty and for *arbitrary* fixed vectors $\varphi \in S(\pi,f)$ and $\psi \in S(\pi,g)$. In particular, we may take $\pi := (\pi_f)^{**} \oplus (\pi_g)^{**}$, $\varphi := \varphi_f$, and $\psi := \varphi_g$.

THEOREM 3.7. *Suppose that $f,g \in \mathcal{P}(A)$ and the* GNS *representations π_f and π_g are essentially self-adjoint. Suppose that π is a biclosed $*$-representation of A and there exist vectors $\varphi \in S(\pi,f)$ and $\psi \in S(\pi,g)$. Let F_φ and F_ψ denote the vector functionals on the von Neumann algebra $\mathcal{M} := (\pi(A)'_{ss})'$ given by $F_\varphi(x) = \langle x\varphi, \varphi\rangle$ and $F_\psi(x) = \langle x\psi, \psi\rangle$, $x \in \mathcal{M}$. Then we have*

$$P_A(f,g) = P_{\mathcal{M}}(F_\varphi, F_\psi). \tag{3.10}$$

Further, there exist vectors $\varphi' \in S(\pi,f)$ and $\psi' \in S(\pi,g)$ such that $\langle x\varphi', \varphi'\rangle = \langle x\varphi, \varphi\rangle$ and $\langle x\psi', \psi'\rangle = \langle x\psi, \psi\rangle$ for $x \in \mathcal{M}$ and

$$P_A(f,g) = |\langle \varphi', \psi'\rangle|^2. \tag{3.11}$$

Proof. Since $\pi(A)'_{ss}$ is a von Neumann algebra, we have $T \in \pi(A)'_{ss}$ if and only if $T \in (\pi(A)'_{ss})'' = \mathcal{M}'$. Therefore, applying formula (3.9) to the $*$-representation π of A and to the identity representation of the von Neumann algebra $\mathcal{M}$, it follows that the supremum of $|\langle T\varphi, \psi\rangle|^2$ over all operators $T \in \pi(A)'_{ss} = \mathcal{M}'$, $\|T\| \leqslant 1$, is equal to $P_A(f,g)$ and also to $P_{\mathcal{M}}(F_\varphi, F_\psi)$. This yields the equality (3.10).

Now we prove the existence of vectors φ' and ψ' having the desired properties. In order to do so we go into the details of the proof of Appendix 7 in [2]. Besides we use some facts from von Neumann algebra theory [12]. We define a normal linear functional on the von Neumann algebra $\mathcal{M}'$ by $h(\cdot) = \langle \cdot\varphi, \psi\rangle$. Let $h = R_u|h|$ be the polar decomposition of h, where u is a partial isometry from $\mathcal{M}'$. Then we have $|h| = R_{u^*}h$ and hence $\|h\| = \||h|\| = |h|(1) = h(u^*) = \langle u^*\varphi, \psi\rangle$. Therefore, we obtain

$$P_{\mathcal{M}}(F_\varphi, F_\psi) = \sup_{T\in\mathcal{M}', \|T\|\leqslant 1} |\langle T\varphi, \psi\rangle|^2 = \|h\|^2 = \langle u^*\varphi, \psi\rangle^2, \tag{3.12}$$

where the first equality follows formula (3.9) applied to the von Neumann algebra $\mathcal{M}$. In the proof of Appendix 7 in [2] it was shown that there exist partial isometries $v, w \in \mathcal{M}'$ satisfying

$$\langle u^*\varphi, \psi\rangle = \langle v^*w\varphi, \psi\rangle, \tag{3.13}$$

$$w^*w \geqslant p(\varphi), v^*v \geqslant p(\psi), \tag{3.14}$$

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 (3.13) with (3.12) and (3.10) we obtain (3.11).

From (3.14) 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 π is closed, we have $w, w^* \in \pi(a)'_s$ by (2.5). 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

$$\begin{aligned}\langle \pi(a)\varphi', \varphi'\rangle &= \langle \pi(a)x\varphi, w\varphi\rangle = \langle w^*\pi(a)w\varphi, \varphi\rangle \\ &= \langle \pi(a)w^*w\varphi, \varphi\rangle = \langle \pi(a)\varphi, \varphi\rangle = f(a).\end{aligned}$$

That is, $\varphi' \in S(\pi, f)$. Similarly, $\psi' \in S(\pi, g)$. ∎

Theorem 3.10 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_φ and F_ψ 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 [18] to the unbounded case.

THEOREM 3.8. *Let $f, g \in \mathcal{P}(A)$ be such that the* GNS *representations π_f and π_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 π_h is the GNS representation of h with algebraically cyclic vector φ_h. By the assumptions $f(\cdot) = h(b^+ \cdot b)$ and $g(\cdot) = h(c^+ \cdot c)$ we have $\pi_h(b)\varphi_h \in S(\pi_h, f)$ and $\pi_h(c)\varphi_h \in S(\pi_h, g)$. Therefore,

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

To prove the converse inequality we want to apply Theorem 3.5 to the biclosed representation $\pi := (\pi_h)^{**}$. Suppose that $T \in \pi(A)'_{ss}$ and $\|T\| \leqslant 1$. 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

$$\begin{aligned}
|\langle T\pi_h(b)\varphi_h, \pi_h(c)\varphi_h\rangle|^2 &= |\langle T\pi(b)\varphi_h, \pi(c)\varphi_h\rangle|^2 = |\langle \pi(b)T\varphi_h, \pi(c)\varphi_h\rangle|^2 \\
&= |\langle RT\varphi_h, \varphi_h\rangle|^2 \leqslant \langle RT\varphi_h, T\varphi_h\rangle\langle R\varphi_h, \varphi_h\rangle \\
&= \langle RT\varphi_h, T\varphi_h\rangle h(c^+b). \qquad (3.15)
\end{aligned}$$

Since $T \in \pi(A)'_{ss}$, we have $TR \subseteq RT$. There exists a positive self-adjoint extension $\widetilde{R}$ of R on $\mathcal{H}(\pi)$ such that $T\widetilde{R} \subseteq \widetilde{R}T$ ([17], Exercise 14.14). The latter implies that $T\widetilde{R}^{1/2} \subseteq \widetilde{R}^{1/2}T$ and hence

$$\begin{aligned}
\langle RT\varphi_h, T\varphi_h\rangle &= \langle \widetilde{R}T\varphi_h, T\varphi_h\rangle = \langle \widetilde{R}^{1/2}T\varphi_h, \widetilde{R}^{1/2}T\varphi_h\rangle \\
&= \langle T\widetilde{R}^{1/2}\varphi_h, T\widetilde{R}^{1/2}\varphi_h\rangle \leqslant \langle \widetilde{R}^{1/2}\varphi_h, \widetilde{R}^{1/2}\varphi_h\rangle \\
&= \langle \widetilde{R}\varphi_h, \varphi_h\rangle = \langle R\varphi_h, \varphi_h\rangle = \langle \pi_h(c^+b)\varphi_h, \varphi_h\rangle = h(c^+b). \qquad (3.16)
\end{aligned}$$

Inserting (3.16) into (3.15) we get

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

Hence $P_A(f,g) \leqslant h(c^+b)$ by Theorem 3.5. ∎

REMARK 3.9. (i) 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 $F(c^+b) \geqslant 0$ for all positive linear functionals F on A.

(ii) If the closures of the GNS representations π_f and π_g are self-adjoint, we can set $\pi := \overline{\pi}_h$ in the preceding proof and it suffices to assume that $h(a^+c^+ba) \geqslant 0$ 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 ρ be a closed $*$-representation of A. We denote by $\mathbf{B}_1(\rho(A))_+$ the set of positive trace class operators on $\mathcal{H}(\rho)$ such that $t\mathcal{H}(\rho) \subseteq \mathcal{D}(\rho)$ and the closure of $\rho(a)t\rho(b)$ is trace class for all $a, b \in A$.

Now let $t \in \mathbf{B}_1(\rho(A))_+$. We define a positive linear functional f_t by

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

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

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 [15]. Recall that a *Frechet–Montel space* is a complete metrizable locally convex space such that each bounded sequence has a convergent subsequence.

THEOREM 4.1. *Let f be a linear functional on A and let ρ be a closed $*$-representation of A. Suppose that the locally convex space $\mathcal{D}(\rho)[\mathrm{t}_{\rho(A)}]$ is a Frechet–Montel space and $f(a) \geqslant 0$ whenever $\rho(a) \geqslant 0$ for $a \in A$. Then there exists an operator $t \in \mathbf{B}_1(\rho(A))_+$ such that $f = f_t$, that is, $f(a) = \operatorname{Tr} \rho(a) t$ for $a \in \mathcal{A}$.*

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

$$F_t(x) \equiv \operatorname{Tr} xt = \mathrm{tr}_{\mathcal{M}} x\widehat{t} \quad \text{for } x \in \mathcal{M}. \tag{4.1}$$

The element $\widehat{t}$ can be obtained as follows. Since $\mathcal{M}$ is a type I factor, there exist Hilbert spaces $\mathcal{H}_0$ and $\mathcal{H}_1$ such that, up to unitary equivalence, $\mathcal{H}(\pi) = \mathcal{H}_0 \otimes \mathcal{H}_1$ and $\mathcal{M} = \mathbf{B}(\mathcal{H}_0) \otimes \mathbb{C} \cdot I_{\mathcal{H}_1}$. The canonical trace of $\mathcal{M}$ is then given by $\mathrm{tr}_{\mathcal{M}}(y \otimes \lambda \cdot I_{\mathcal{H}_1}) := \operatorname{Tr}_1 \lambda y$, where Tr_1 denotes the trace on the Hilbert space $\mathcal{H}_1$. Now $\widetilde{F}_t(y) := F_t(y \otimes I_{\mathcal{H}_1})$, $y \in \mathbf{B}(\mathcal{H}_0)$, defines a positive normal linear functional $\widetilde{F}_t$ on $\mathbf{B}(\mathcal{H}_0)$. Hence there exists a unique positive trace class operator $\widetilde{t}$ on the Hilbert space $\mathcal{H}_0$ such $\widetilde{F}_t(y) = \operatorname{Tr} y\widetilde{t}$ for $y \in \mathbf{B}(\mathcal{H}_0)$. Set $\widehat{t} := \widetilde{t} \otimes I_{\mathcal{H}_1}$. Then we have $\mathrm{tr}_{\mathcal{M}}\widehat{t} = \operatorname{Tr}_1 t < \infty$ and (4.1) holds by construction.

Note that $\mathrm{tr}_{\mathcal{M}} = \operatorname{Tr}$ and $t = \widehat{t}$ if $\mathcal{M} = \mathbf{B}(\mathcal{H}(\rho))$.

THEOREM 4.2. *Let ρ be a closed $*$-representation of A such that the von Neumann algebra $\mathcal{M} := (\rho(A)'_{ss})'$ is a type* I *factor. For $s, t \in \mathbf{B}_1(\rho(A))_+$, let f_s, f_t denote the positive linear functionals on $\mathcal{A}$ defined by*

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

Suppose that the GNS *representations π_{f_s} and π_{f_t} are essentially self-adjoint. Then*

$$P_A(f_s, f_t) = (\mathrm{tr}_{\mathcal{M}} |\widehat{t}^{1/2} \widehat{s}^{1/2}|)^2 = (\mathrm{tr}_{\mathcal{M}} (\widehat{s}^{1/2} \widehat{t} \widehat{s}^{1/2})^{1/2})^2. \tag{4.2}$$

Proof. Let ρ_∞ be the orthogonal sum $\bigoplus_{n=0}^{\infty} \rho$ on $\mathcal{H}_\infty = \bigoplus_{n=0}^{\infty} \mathcal{H}(\rho)$. Since ρ is biclosed, so is the $*$-representation ρ_∞ of A. We want to apply Theorem 3.7. First we will describe the GNS representations π_{f_s} and π_{f_t} as $*$-subrepresentations of ρ_∞.

The result is well-known if $\mathcal{H}(\rho)$ is finite dimensional [18], so we can assume that $\mathcal{H}(\rho)$ is infinite dimensional. Since $s \in \mathbf{B}_1(\rho(A))_+$, 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 $n \in \mathbb{N}$,

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

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

$$f_s(a) = \sum_{n=1}^{\infty} \langle \rho(a)\varphi_n, \lambda_n\varphi_n\rangle. \tag{4.3}$$

All these facts are contained in Propositions 5.1.9 and 5.1.12 in [16]. Hence

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

defines a $*$-representation ρ_Φ of $\mathcal{A}$ on the domain

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

with algebraically cyclic vector $\Phi := (\lambda_n^{1/2}\varphi_n)_{n\in\mathbb{N}}$. From (4.3) 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_Φ in the representaton ρ_Φ. Therefore, by the uniqueness of the GNS representation, π_{f_s} is unitarily equivalent to ρ_Φ. Likewise, the GNS representation π_{f_t} is unitarily equivalent to the corresponding $*$-representation ρ_Ψ, 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 $\rho_\Phi \subseteq \rho_\infty$ and $\rho_\Psi \subseteq \rho_\infty$, we have $\Phi \in S(\rho_\infty, f_s)$ and $\Psi \in S(\rho_\infty, f_t)$.

Let $\mathcal{M}_\infty$ denote the von Neumann algebra $(\rho_\infty(A)'_{ss})'$. Then, by Theorem 3.7, we have

$$P_A(f_s, f_t) \equiv P_A(f_\Phi, f_\Psi) = P_{\mathcal{M}_\infty}(F_\Phi, F_\Psi). \tag{4.4}$$

Let $x \in \mathbf{B}(\mathcal{H}_\infty)$. We write x as a matrix $(x_{jk})_{j,k\in\mathbb{N}}$ with entries $x_{jk} \in \mathbf{B}(\mathcal{H}(\rho))$. Clearly, x belongs to $\rho_\infty(\mathcal{A})'_{ss}$ if and only if each entry x_{jk} is in $\rho(A)'_{ss}$. Further, it is easily verified that x is in $(\rho_\infty(\mathcal{A})'_{ss})'$ 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 $\mathcal{M}_\infty = (\rho_\infty(\mathcal{A})'_{ss})'$, that is, π is a $*$-representation of $\mathcal{M}$.

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

$$P_A(f_s, f_t) = P_{\mathcal{M}}(F_s, F_t) \tag{4.5}$$

by (4.4). It is proved in Corollary 1 of [3] (see also [18]) that

$$P_{\mathcal{M}}(F_s, F_t) = (\operatorname{tr}_{\mathcal{M}} |\widehat{t}^{1/2}\widehat{s}^{1/2}|)^2.$$

Combined with (4.5) this yields (4.8) and completes the proof. ∎

Let us keep the assumptions and the notation of Theorem 4.2. In general, $P_A(f_s, f_t)$ is different from $(\mathrm{Tr}\,(s^{1/2}ts^{1/2})^{1/2})^2$ as simple examples show. However, if in addition ρ is *irreducible* (that is, $\rho(A)'_{ss} = \mathbb{C}\cdot I$), then $s = \widehat{s}$ and $t = \widehat{t}$ as noted above and therefore by (4.2),

$$P_A(f_s, f_t) = (\mathrm{Tr}\,(s^{1/2}ts^{1/2})^{1/2})^2. \tag{4.6}$$

We now apply the preceding theorem to an interesting example.

EXAMPLE 4.3 (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

$$pq - qp = -\mathrm{i}1,$$

and let ρ be the Schrödinger representation of A, that is,

$$(\rho(q)\varphi)(x) = x\varphi(x), (\rho(p)\varphi)(x) = -\mathrm{i}\varphi'(x), \quad \varphi \in \mathcal{D}(\rho) := \mathcal{S}(\mathbb{R}), \tag{4.7}$$

on $L^2(\mathbb{R})$. Since ρ is irreducible, $\rho_\infty(A)'_{ss} = \mathbb{C}\cdot I$. Hence $\mathcal{M} = \mathbf{B}(\mathcal{H}(\rho))$ and $\mathrm{tr}_{\mathcal{M}} = \mathrm{Tr}$. Therefore, if $s, t \in \mathbf{B}_1(\pi(A))_+$ and if the GNS representations π_{f_s} and π_{f_t} are essentially self-adjoint, it follows from Theorem 4.2 and formula (4.6) that

$$P_A(f_s, f_t) = (\mathrm{Tr}\,|t^{1/2}s^{1/2}|)^2 = (\mathrm{Tr}\,(s^{1/2}ts^{1/2})^{1/2})^2. \tag{4.8}$$

Let us specialize this to the rank one case, that is, let $s = \varphi\otimes\varphi$ and $t = \psi\otimes\psi$ with $\varphi, \psi \in \mathcal{D}(\rho)$, 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 (4.8) yields

$$P_A(f_s, f_t) = |\langle \varphi, \psi\rangle|^2. \tag{4.9}$$

Recall that (4.9) holds if the GNS representations π_{f_s} and π_{f_t} are essentially self-adjoint. We shall see in Section 5 below that (4.9) is no longer true if this assumption is omitted.

Now we turn to the second main application.

THEOREM 4.4. *Let X be a locally compact topological Hausdorff space. Suppose that A is a $*$-subalgebra of $C(X)$ which contains the constant function* 1 *and separates the points of X. Let μ 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 nonnegative functions. Define positive linear functionals f_η and f_ξ on A by*

$$f_\eta(a) = \int_X a(x)\eta(x)\mathrm{d}\mu(x), \quad f_\xi(a) = \int_X a(x)\xi(x)\mathrm{d}\mu(x), \quad a \in A. \tag{4.10}$$

Suppose that the GNS *representations π_{f_η} and π_{f_ξ} are essentially self-adjoint. Then*

$$P_A(f_\eta, f_\xi) = \Big(\int_X \eta(x)^{1/2}\xi(x)^{1/2}\mathrm{d}\mu(x)\Big)^2. \tag{4.11}$$

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

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

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 $*$-subalgebra of $L^\infty(X,\mu)$ generated by the functions $(a\pm \mathrm{i})^{-1}$, 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 $(\overline{\pi(a)} \pm \mathrm{i}I)^{-1} = (a\pm\mathrm{i})^{-1}$, 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 ([10], 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_η and F_ξ denote the positive linear functionals on $\mathcal{M}$ defined by (4.10) 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 $P_{\mathcal{M}}(F_\eta,F_\xi) = \Big(\int_X \eta(x)^{1/2}\xi(x)^{1/2}\mathrm{d}\mu(x)\Big)^2$. Since $P_A(f_\eta,f_\xi) = P_{\mathcal{M}}(F_\eta,F_\xi)$ by Theorem 3.7, we obtain (4.11). ∎

In the following two examples we reconsider the one dimensional Hamburger moment problem (see Example 2.7) and we specialize the preceding theorem to the case where $X = \mathbb{R}$ and $A = \mathbb{C}[x]$.

EXAMPLE 4.5 (Determinate Hamburger moment problems). Let μ_η and μ_ξ be the positive Borel measures on $\mathbb{R}$ defined by $\mathrm{d}\mu_\eta = \eta\mathrm{d}\mu$ and $\mathrm{d}\mu_\xi = \xi\mathrm{d}\mu$. Since $\mathbb{C}[x] \subseteq L^1(\mathbb{R},\mu)$ and $\eta,\xi \in L^\infty(\mathbb{R},\mu)$ by the assumptions of Theorem 4.4, μ_η and μ_ξ are in $M(\mathbb{R})$. If both measures μ_η and μ_ξ are determinate, then the GNS representations $\pi_{f_{\mu_\eta}}$ and $\pi_{f_{\mu_\xi}}$ are essentially self-adjoint (as shown in Example 2.7) and hence formula (4.11) holds by Theorem 4.4.

EXAMPLE 4.6 (Indeterminate Hamburger moment problems). Suppose $\nu \in M(\mathbb{R})$ is an indeterminate measure such that $\nu(\mathbb{R}) = 1$.

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

satisfying

$$(4.12) \quad \eta(x)+\xi(x)=2, \quad \|\xi\|_\infty \leqslant 2, \quad \|\eta\|_\infty \leqslant 2, \quad \mathrm{d}\mu_1=\eta \mathrm{d}\mu, \quad \mathrm{d}\mu_2=\xi \mathrm{d}\mu.$$

Define $f(p)=\int p(x)\mathrm{d}\mu(x)$ for $p\in\mathbb{C}[x]$. Since $\mu_1,\mu_2,\mu\in V_\nu$, the functionals f_η and f_ξ defined by (4.10) 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 $J:=\Big(\int_X \eta(x)^{1/2}\xi(x)^{1/2}\mathrm{d}\mu(x)\Big)^2$. From (4.12) we obtain $\eta(x)\xi(x)=\eta(x)(2-\eta(x))\leqslant 1$ and hence $J\leqslant 1$, since $\mu(\mathbb{R})=1$. If J would be equal to 1, then $\eta(x)(2-\eta(x))=1$ μ-a.e. on $\mathbb{R}$ which implies that $\eta(x)=1$ μ-a.e. on $\mathbb{R}$ by (4.12). But then $\mu_1=\mu_2=\mu$ which contradicts the choice of measures μ_1 and μ_2. Thus we have proved that $J\neq 1=P_A(f_\eta,f_\xi)$, that is, formula (4.11) 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 μ on $\mathbb{R}^d$ such that all polynomials $p\in\mathbb{C}[x_1,\dots,x_d]$ are μ-integrable. For $\mu\in M(\mathbb{R}^d)$ we define a positive linear functional g_μ on the $*$-algebra $A:=\mathbb{C}[x_1,\dots,x_d]$ by

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

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 4.5 contains some answer under the assumption that both measures μ_η and μ_ξ are determinate. This suggests the following questions:

Problem 2. *What about the case when the measures μ_η and/or μ_ξ in Example* 4.5 *are not determinate?*

Problem 3. *Is formula* (4.11) *still valid in the multi-dimensional case $d>1$ if μ_η and μ_ξ are determinate ?*

It can be shown that the answer to Problem 3 is affirmative if all multiplication operators $\pi_\mu(x_j)$, $j=1,\dots,d$, are essentially self-adjoint. The latter assumption is sufficient, but not neccessary for μ being determinate [14]. In the multi-dimensional case determinacy turns out to be much more difficult than in the one-dimensional case, see e.g. [14].

5. VECTOR FUNCTIONALS OF THE SCHRÖDINGER REPRESENTATION

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

In this section A denotes the Weyl algebra (see Example 4.3) and π is the Schrödinger representation of A given by (4.7). For $\eta \in \mathcal{D}(\pi) = \mathcal{S}(\mathbb{R})$ let f_η denote the positive linear functional f_η on A given by

$$f_\eta(x) = \langle \pi(x)\eta, \eta \rangle, \quad x \in A.$$

Consider the following condition on the function η:

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

The main result of this section is the following theorem.

THEOREM 5.1. *Suppose that φ and ψ are functions of $C_0^\infty(\mathbb{R})$ satisfying condition ($*$). Then*

$$P_A(f_\varphi, f_\psi) = \Big(\sum_{k,l} \Big| \int_{\mathcal{J}_k(\varphi)\cap\mathcal{J}_l(\psi)} \varphi(x)\overline{\psi(x)}\mathrm{d}x \Big| \Big)^2. \tag{5.1}$$

(If $\mathcal{J}_k(\varphi) \cap \mathcal{J}_l(\psi)$ is empty, the corresponding integral is set zero.)

Before we turn to the proof of the theorem let us discuss formula (5.1) in two simple cases.

Case 1. If both sets $\mathcal{J}(\varphi)$ and $\mathcal{J}(\psi)$ consist of a single interval, then

$$P_A(f_\varphi, f_\psi) = \Big| \int_{\mathbb{R}} \varphi(x)\overline{\psi(x)}\mathrm{d}x \Big|^2 = |\langle \varphi, \psi \rangle|^2,$$

that is, in this case formula (4.9) holds.

Case 2. Let $\varphi, \psi \in C_0^\infty(\mathbb{R})$ be such that $\mathcal{J}(\varphi) = \mathcal{J}(\psi)$, $\mathcal{J}_k(\varphi) = \mathcal{J}_k(\psi)$ and $\varphi(x) = \epsilon_k \psi(x)$ on $\mathcal{J}_k(\varphi)$ for $k = 1, \ldots, r$, where $\epsilon_k \in \{1, -1\}$. Then formula (5.1) yields $P_A(f_\varphi, f_\psi) = \|\varphi\|^4$. It is easy to choose $\varphi \neq 0$ and the numbers ϵ_k such that $\langle \varphi, \psi \rangle = 0$, so formula (4.9) does not hold in this case.

The proof of Theorem 5.1 requires a number of technical preparations. The first aim is to desribe the closure $\overline{\pi}_{f_\eta}$ of the GNS representation π_{f_η} for a function $\eta \in C_0^\infty(\mathbb{R})$ satisfying condition ($*$).

Let ρ_η denote the restriction of π to the dense domain

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

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

LEMMA 5.2. *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 $\overline{\tau}_\eta = U\overline{\pi}_{f_\eta}U^*$, where τ_η denotes the restriction of π to $\mathcal{D}(\rho_\eta) = \pi(A)\eta$. Clearly, $\tau_\eta \subseteq \rho_\eta$ and hence $\overline{\tau}_\eta \subseteq \rho_\eta$, 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, $\pi(A)\eta$ is dense in $\mathcal{D}(\rho_\eta)$ in the graph topology of $\rho_\eta(A)$. For this the auxiliary Lemmas 5.3 and 5.4 proved below are essentially used.

Each element $a \in A$ is of a finite sum of terms $f(q)p^n$, where $n \in \mathbb{N}_0$ and $f \in \mathbb{C}[q]$. Since $\eta \in C_0^\infty(\mathbb{R})$, the set $\mathcal{J}(\eta)$ and hence the operators $\pi_0(f(q))$ are bounded. Therefore, the graph topology $\mathfrak{t}_{\rho_\eta(A)}$ is generated by the seminorms $\|\rho_\eta(p)^n \cdot\|$, $n \in \mathbb{N}_0$, on $\mathcal{D}(\rho_\eta)$. Let $\psi \in \mathcal{D}(\rho_\eta)$.

First assume that ψ vanishes in some neighbourhoods of the end points α_l, β_l. Then, by Lemma 5.4, for any $m \in \mathbb{N}$ there is sequence $(f_n)_{n\in\mathbb{N}}$ of polynomials such that

$$\lim_n \rho_\eta((\mathrm{i}p)^k)(\rho_\eta(f(q))\eta - \psi) = \lim_n((f_n\eta)^{(k)} - \psi^{(k)}) = 0$$

in $L^2(\mathcal{J}(\eta))$ for $k = 0, \ldots, m$. This shows that ψ is in the closure of $\rho_\eta(A)\eta$ with respect to the graph topology of $\rho_\eta(A)$.

The case of a general function ψ is reduced to the preceding case as follows. Suppose that $\varepsilon > 0$ and $2\varepsilon < \min_l |\beta_l - \alpha_l|$. We define

$$\psi_\varepsilon(x) = \psi(x - \varepsilon + 2\varepsilon(x - \alpha_l - \varepsilon)(\beta_l - \alpha_l - 2\varepsilon)^{-1}) \quad \text{for } x \in (\alpha_l, \beta_l)$$

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

$$\lim_{\varepsilon\to+0} \rho_\eta((\mathrm{i}p)^k)(\psi_\varepsilon - \psi) = \lim_{\varepsilon\to+0}(\psi_\varepsilon^{(k)} - \psi^{(k)}) = 0$$

in $L^2(\mathcal{J}(\eta))$ for $k \in \mathbb{N}_0$. Therefore, since ψ_ε is in the closure of $\rho_\eta(A)\eta$, so is ψ. ∎

LEMMA 5.3. *Suppose that $g \in C^{(k)}([\alpha, \beta])$, where $\alpha, \beta \in \mathbb{R}$ and $k \in \mathbb{N}$. Then there exists a sequence $(f_n)_{n\in\mathbb{N}}$ of polynomials such that $f_n^{(j)}(x) \Longrightarrow g^{(j)}(x)$ uniformly on $[\alpha, \beta]$ for $j = 0, \ldots, k$ as $n \to \infty$.*

Proof. By the Weierstrass theorem there is a sequence $(h_n)_{n\in\mathbb{N}}$ of polynomials such that $h_n(x) \Longrightarrow g^{(k)}(x)$ uniformly on $[\alpha, \beta]$. Fix $\gamma \in [\alpha, \beta]$ and set

$h_{n,k} := h_n$. Then

$$h_{n,k-1}(x) := g^{(k)}(\gamma) + \int_\gamma^x h_{n,k}(s)\mathrm{d}s \Longrightarrow g^{(k-1)}(x) = g^{(k)}(\gamma) + \int_\gamma^x g^{(k)}(s)\mathrm{d}s.$$

Clearly, $(h_{n,k-1})_{n\in\mathbb{N}}$ is a sequence of polynomials and we have $h'_{n,k-1}(x) = h_{n,k}(x)$ on $[\alpha,\beta]$. Proceeding by induction we obtain sequences $(h_{n,k-j})_{n\in\mathbb{N}}$, $j = 0,\ldots,k$, of polynomials such that $h_{n,k-j}(x) \Longrightarrow g^{(k-j)}(x)$ and $h'_{n,k-j}(x) = h_{n,k+1-j}(x)$ on $[\alpha,\beta]$. Setting $f_n := h_{n,0}$ the sequence $(f_n)_{n\in\mathbb{N}}$ has the desired properties. ∎

LEMMA 5.4. *Suppose that $\eta \in C_0^\infty(\mathbb{R})$ satisfies condition $(*)$. Let $\psi \in \bigoplus_{l=1}^r C_0^{(m)}((\alpha_l,\beta_l))$, where $m \in \mathbb{N}$. Then there exists a sequence $(f_n)_{n\in\mathbb{N}}$ of polynomials such that $\lim_{n\to\infty}(f_n\eta)^{(k)} = \psi^{(k)}$ in $L^2(\mathcal{J}(\eta))$ for $k = 0,\ldots,m$.*

Proof. By the assumption ψ vanishes in some neighbourhoods of the end points α_l and β_l. Set $\psi(x) = 0$ on $\mathbb{R}/\mathcal{J}(\eta)$. 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 5.3, there exists a sequence $(f_n)_{n\in\mathbb{N}}$ of polynomials such that $f_n^{(j)}(x) \Longrightarrow (\psi\eta^{-1})^{(j)}(x)$ for $j = 0,\ldots,m$ uniformly on $[\alpha,\beta]$. Then

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

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

Now we are able to give the

Proof of Theorem 5.1. Let us abbreviate $\pi_\varphi = \overline{\pi}_{f_\varphi}$ and $\pi_\psi = \overline{\pi}_{f_\psi}$. By Lemma 5.2 the closure $\pi_\psi = \overline{\pi}_{f_\psi}$ of the GNS representation π_{f_ψ} is unitarily equivalent to the representation ρ_ψ. For notational simplicy we shall identify the representations π_ψ and ρ_ψ via the unitary U defined in Lemma 5.2. 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 $C^\infty(\overline{\mathcal{J}_l(\psi)})$ and $g(t) = 0$ on $\mathbb{R}/\overline{\mathcal{J}(\psi)}$. Further, we have $(\pi_\psi)^*(f(q))g = f\cdot g$ and $(\pi_\psi)^*(p)g = -\mathrm{i}g'$ for $g \in \mathcal{D}((\pi_\psi)^*)$ and $f \in \mathbb{C}[q]$.

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

$$T(f\cdot\varphi) = T\pi_\varphi(f(q))\varphi = (\pi_\psi)^*(f(q))T\varphi = (\pi_\psi)^*(f(q))\xi = f\cdot\xi. \tag{5.2}$$

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

$$\int_\alpha^\beta |f(x)|^2|\xi(x)|^2\mathrm{d}x = \int_\alpha^\beta |T(f\cdot\varphi)(x)|^2\mathrm{d}x \leqslant \int_\alpha^\beta |f(x)|^2|\varphi(x)|^2\mathrm{d}x \tag{5.3}$$

for all polynomials f and hence for all functions $f \in C[\alpha, \beta]$ by the Weierstrass theorem. Hence (5.3) implies that

$$|\xi(x)| \leqslant |\varphi(x)| \quad \text{on } [\alpha, \beta]. \tag{5.4}$$

Therefore, $\xi(x) = 0$ if $x \in \mathbb{R}/\mathcal{J}(\varphi)$. Clearly, $\xi(x) = 0$ if $x \in \mathbb{R}/\overline{\mathcal{J}(\psi)}$, since $\xi \in \mathcal{D}((\pi_\psi)^*)$. Since φ satisfies condition $(*)$, 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 (5.2) that T is equal to the multiplication operator by the bounded function $\xi\varphi^{-1}$. (Note that $\xi\varphi^{-1}$ is bounded by (5.4).) In particular, we obtain

$$\varphi' \cdot \xi\varphi^{-1} = T\varphi' = T\pi_\varphi(\mathrm{i}p)\varphi = (\pi_\psi)^*(\mathrm{i}p)T\varphi = (\pi_\psi)^*(\mathrm{i}p)\xi = \xi'.$$

Thus, $\varphi'(x)\xi(x) = \varphi(x)\xi'(x)$ which in turn implies that $(\frac{\xi}{\varphi})'(x) = 0$ for all $x \in \mathcal{J}(\varphi) \cap \mathcal{J}(\psi)$. Hence $\frac{\xi}{\varphi}$ is constant, say $\xi(x) = \lambda\varphi(x)$ for some constant $\lambda \in \mathbb{C}$ on each connected component of $\mathcal{J}(\varphi) \cap \mathcal{J}(\psi)$. By (5.4), $|\lambda| \leqslant 1$. 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 $|\lambda_{k,l}| \leqslant 1$, is given. Set $\xi(x) = \lambda_{kl}\varphi(x)$ for $x \in \mathcal{J}_l(\varphi) \cap \mathcal{J}_k(\psi)$ and $\xi(x) = 0$ otherwise. From the description of the domain $\mathcal{D}((\pi_\psi)^*)$ given in the first paragraph of this proof it follows that $\xi \in \mathcal{D}((\pi_\psi)^*)$. Define $T(\pi_\varphi(a)\varphi) := (\pi_\psi)^*(a)\xi$, $a \in A$. 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 $\|T\| \leqslant 1$. Since $T\varphi = \xi$, we have

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

Therefore, the supremum of expressions $|\langle T\varphi, \psi\rangle|$ is obtained if we choose $\lambda_{k,l}$ such that the number $\lambda_{k,l} \int\limits_{\mathcal{J}_k(\varphi)\cap\mathcal{J}_l(\psi)} \varphi\overline{\psi}\mathrm{d}x$ is equal to its modulus $\Big| \int\limits_{\mathcal{J}_k(\varphi)\cap\mathcal{J}_k(\psi)} \varphi\overline{\psi}\mathrm{d}x \Big|$. This implies formula (5.1). ∎

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