The notion of observable and the moment problem for $*$-algebras and their GNS representations

Nicolò Drago[a], **Valter Moretti**[b]

Department of Mathematics, University of Trento, and INFN-TIFPA
via Sommarive 14, I-38123 Povo (Trento), Italy.
[a]nicolo.drago@unitn.it, [b]valter.moretti@unitn.it

February, 17, 2020

Abstract

We address some usually overlooked issues concerning the use of $*$-algebras in quantum theory and their physical interpretation. If $\mathfrak{A}$ is a $*$-algebra describing a quantum system and $\omega : \mathfrak{A} \to \mathbb{C}$ a state, we focus in particular on the interpretation of $\omega(a)$ as expectation value for an algebraic observable $a = a^* \in \mathfrak{A}$, studying the problem of finding a probability measure reproducing the moments $\{\omega(a^n)\}_{n\in\mathbb{N}}$. This problem enjoys a close relation with the selfadjointness of the (in general only symmetric) operator $\pi_\omega(a)$ in the GNS representation of ω and thus it has important consequences for the interpretation of a as an observable. We provide physical examples (also from QFT) where the moment problem for $\{\omega(a^n)\}_{n\in\mathbb{N}}$ does not admit a unique solution. To reduce this ambiguity, we consider the moment problem for the sequences $\{\omega_b(a^n)\}_{n\in\mathbb{N}}$, being $b \in \mathfrak{A}$ and $\omega_b(\cdot) := \omega(b^* \cdot b)$. Letting $\mu^{(a)}_{\omega_b}$ be a solution of the moment problem for the sequence $\{\omega_b(a^n)\}_{n\in\mathbb{N}}$, we introduce a consistency relation on the family $\{\mu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$. We prove a 1-1 correspondence between consistent families $\{\mu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ and positive operator-valued measures (POVM) associated with the symmetric operator $\pi_\omega(a)$. In particular there exists a unique consistent family of $\{\mu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ if and only if $\pi_\omega(a)$ is maximally symmetric. This result suggests that a better physical understanding of the notion of observable for general $*$-algebras should be based on POVMs rather than projection-valued measure (PVM).

Contents

1 Introduction

Physical observables in *quantum theory* – namely the physical properties of the system under investigation – can be conveniently described in the algebraic framework by a suitable C^*-algebra $\mathfrak{A}$. (The standard Hilbert space formulation is included referring to the von Neumann algebra $\mathfrak{A} = \mathfrak{B}(\mathsf{H})$.) There is however a technically less rigid formulation where the algebra $\mathfrak{A}$ is no longer a C^*-algebra but it is a less tamed $*$-*algebra*. This second approach seems to be strictly necessary in *quantum field theory* (QFT) both in constructive [22] and perturbative [12] approaches, also in curved spacetime and especially in presence of self interaction. The C^*-algebraic setting is not at disposal there, since almost all relevant operators are no longer bounded in any reasonable C^*- norm (see however [6] as a recent new viewpoint on the subject). In particular, locally-covariant renormalization procedures are performed within the $*$-algebraic formulation (see [4] for a recent review).

When dealing with unital $*$-algebras for describing quantum systems, the notion of (quantum) *observable* has a more delicate status than in the C^*-algebra formulation which, in our view, has not yet received sufficient attention in the literature.

First of all, contrarily to the standard requirements of quantum theory, it is generally false that every Hermitian element $a = a^* \in \mathfrak{A}$ – to which we shall refer to as an *algebraic* observable – is represented by an (essentially) selfadjoint operator $\pi_\omega(a)$ – henceforth called *quantum* observable – in a given GNS representation induced by an algebraic state $\omega : \mathfrak{A} \to \mathbb{C}$. In general, $\pi_\omega(a)$ results to be symmetric admitting many or none selfadjoint extensions – *cf.* example 3.

This problem is actually entangled with another issue concerning the standard physical interpretation of $\omega(a)$ as *expectation value* of the algebraic observable a in the state ω. This interpretation is usually considered folklore without a critical discussion as it should instead deserve. To be operationally effective, that interpretation would need a *probability distribution* $\mu^{(a)}_\omega$ over $\mathbb{R}$ – which may be provided by the spectral measure of $\overline{\pi_\omega(a)}$ if the latter is selfadjoint, *i.e.* when the *algebraic* observable a defines a *quantum* observable in the GNS representation of an algebraic state.

Independently of the existence of a spectral measure, the problem of finding $\mu^{(a)}_\omega$ can be tackled in the framework of the more general *Hamburger moment problem*, looking for a probability measure whose moments coincide to the known values $\{\omega(a^n)\}_{n\in\mathbb{N}}$. However, in the general case, there are many such measures for a given pair (a, ω), independently of the fact that $\pi_\omega(a)$ admits one, many or none selfadjoint extensions – *cf.* example 11. Therefore a discussion on the possible physical meaning of these measures seems to be necessary.

We stress that all these problems are proper of the $*$-algebra approach whereas they are almost automatically solved when the structure is enriched to a C^*-algebra. For instance the above-mentioned spectral measure always exists when $\mathfrak{A}$ is a C^*-algebra, since $\pi_\omega(a)$ is always selfadjoint if $a = a^*$ in that case. Stated differently, the notion of algebraic and quantum observables always agree in the C^*-algebraic setting. However as already said, $*$-algebras are more useful in real applications especially in QFT and, in that sense, they are more close to physics than C^*-algebras.

The goal of this work is to analyze the above mentioned issues also producing some examples and counterexampled arising from elementary formalism of *quantum mechanics* (QM) and QFT. Even if these problems cannot be avoided, we present some partially positive results.

The technical objects of our discussion will consist of a $*$-algebra $\mathfrak{A}$, an Hermitian element a, the class of deformed states $\mathfrak{A} \ni c \mapsto \omega_b(c) := \omega(b^*cb)/\omega(b^*b)$, with $b \in \mathfrak{A}$, constructed out of a given initial state ω. We also consider families of measures $\{\mu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ over $\mathbb{R}$ such that $\mu^{(a)}_{\omega_b}$ solve the corresponding Hamburger moment problem for the moments $\{\omega_b(a^n)\}_{n\in\mathbb{N}}$.

As a first result, we establish that if the measures $\mu^{(a)}_{\omega_b}$ are uniquely determined for every b and a fixed pair (a, ω), then $\overline{\pi_\omega(a)}$ and every $\overline{\pi_{\omega_b}(a)}$ are selfadjoint. This provides a sufficient condition for which an algebraic observable defines quantum observables referring to a certain class of algebraic states. The converse statement is however false – *cf.* example 11 – as it follows from elementary models in QM and QFT.

As a second, more elaborated, result we prove that for fixed $a^* = a \in \mathfrak{A}$ and ω, when assuming some physically natural coherence constraints on the measures $\mu^{(a)}_{\omega_b}$ varying $b \in \mathfrak{A}$, the admitted families of constrained measures $\{\mu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ are one-to-one with all possible positive operator-valued measures (POVMs) associated to the symmetric operator $\pi_\omega(a)$ through Naimark's decomposition procedure for symmetric operators. We shall refer to each of these POVM as a *generalized* observable. Therefore, $\overline{\pi_\omega(a)}$ is maximally symmetric if and only if there is only one such measure for every fixed b – that is, there is a unique generalized observable associated with the given algebraic observable through the GNS representation of ω. These unique measures are those induced by the unique POVM of $\overline{\pi_\omega(a)}$, which is a projection-valued measure, if the operator is selfadjoint.

Structure of this work. This paper is organized as follows. Section 2 discuss in detail the issues arising in the interpretation of algebraic observables $a = a^* \in \mathfrak{A}$ of a $*$-algebra $\mathfrak{A}$ as quantum observables in their GNS representations. Section 3 contains a first result concerning essential selfadjointness of $\pi_\omega(a)$ when the measures solving the moment problem for every deformed state are unique. Section 4 contains a recap of the basic theory of POVMs and the theory of generalized selfadjoint extensions of symmetric operators – some complements appear also in appendix A. Section 5 is the core of the work where are established the main theorems arising from the two issues discussed in the introduction. Section 6 offers a summary of the results established in the paper and some open issue. Appendix A includes some complements about reducing subspaces, generalized selfadjoint extensions of symmetric operators and present the proofs of some technical propositions.

Notation and conventions. We adopt throughout the paper the standard definition of **complex measure** [25]: a map $\mu : \Sigma \to \mathbb{C}$ which is *unconditionally* σ*-additive* over the σ-algebra Σ. With this definition the *total variation* $||\mu|| := |\mu|(\Sigma)$ turns out to be finite.
We adopt standard notation and definitions and, barring the symbol of the adjoint operator and that of scalar product, they are the same as in [15]. In particular, an operator in a Hilbert space H is indicated by $A : D(A) \to \mathsf{H}$, or simply A, where the domain $D(A)$ is always supposed to be a linear subspace of H. The scalar product $\langle x|y\rangle$ of a Hilbert space is supposed to be antilinear in the *left* entry. $\mathfrak{B}(\mathsf{H})$ denotes the C^*-algebra of bounded operators A in Hilbert space H with $D(A) = \mathsf{H}$. $\mathscr{L}(\mathsf{H})$ indicates the lattice of orthogonal projectors over the Hilbert space H. The adjoint of an operator A in a Hilbert space is always denoted by $A^\dagger$, while the symbol a^* indicates the adjoint of an element a of a $*$-algebra. A representation of unital $*$-algebras is supposed to preserve the identity.

The closure of a closable operator $A : D(A) \to \mathsf{H}$ is indicated by $\overline{A}$. If $A : D(A) \to \mathsf{H}$ and $B : D(B) \to \mathsf{H}$ we assume the usual convention concerning standard domains, in particular: (i) $D(BA) := \{\psi \in D(A) \mid A\psi \in D(B)\}$; (ii) $D(A + B) := D(A) \cap D(B)$; (iii) $D(aA) := D(A)$ for $a \in \mathbb{C} \setminus \{0\}$ and $D(0A) := \mathsf{H}$. The symbol $A \subset B$ permits the case $A = B$. If A and B are operators $A \subset B$ means that $D(A) \subset D(B)$ and $B\restriction_{D(A)}= A$. An operator A in a Hilbert space H is said to be **Hermitian** if $\langle Ax|y\rangle = \langle x|Ay\rangle$ for every $x, y \in D(A)$. A Hermitian operator A is **symmetric** if $D(A)$ is dense in H (equivalently, $A \subset A^\dagger$). A symmetric operator is **selfadjoint** if $A = A^\dagger$, **essentially selfadjoint** if it admits a unique selfadjoint extension (equivalently, if $\overline{A}$ is selfadjoint), in this case $\overline{A}$ is the unique selfadjoint extension of A. A **conjugation** in the Hilbert space H is an *antilinear* isometric map $C : \mathsf{H} \to \mathsf{H}$ such that $CC = I$, where I always denotes the **identity operator** $I : \mathsf{H} \ni x \mapsto x \in \mathsf{H}$.

2 Issues in the interpretation of $a = a^* \in \mathfrak{A}$ as an observable

This section has the twofold goal of presenting the problems discussed within this work and introducing part of the mathematical machinery used in the rest of the paper. For the generally used notation and conventions not directly explained in the text[1], see Section 1.

2.1 $*$-algebras, states, GNS construction

There are at least two approaches to quantum theories. The most known is the Hilbert-space formulation where the physical observables of a quantum system are represented by **quantum observables**, namely (essentially) selfadjoint operators in the Hilbert space of the system. There, (normal) states are given by positive trace-class unit-trace operators and pure states are unit vectors up to phases.

The second approach instead relies upon the structure of unital **$*$-algebra** $\mathfrak{A}$, i.e., an associative complex algebra equipped with an identity element $\mathbb{I}$ and an antilinear involution *. This is the most elementary mathematical machinery to describe and handle the set of observables of a quantum system in the algebraic formalism. **Algebraic observables** are here the elements

[1] When a new term is introduced and defined, its name appears in **boldface** style.

$a \in \mathfrak{A}$ which are **Hermitian** $a = a^*$. This approach is in particular suitable when dealing with the algebra of *quantum fields* (see, e.g., [14, 27, 13, 12, 22]).

Example 1:
(1) If (M, g) is a given *globally hyperbolic spacetime* [4], a complex unital $*$-algebra $\mathfrak{A}(M, g)$ is associated to a free *Klein-Gordon* real scalar field Φ. It is uniquely defined [14] by requiring the elements of $\mathfrak{A}(M, g)$ are finite complex linear combinations of the identity $\mathbb{I}$ and finite products of elements $\Phi(f)$, called (abstract) **quantum field operators**, where $f \in C_c^\infty(M; \mathbb{R})$ are real-valued *smearing functions* and the following requirements are true for $a, b \in \mathbb{R}$, $f, h \in C_c^\infty(M; \mathbb{R})$.

(i) ($\mathbb{R}$-linearity) $\Phi(af + bh) = a\Phi(f) + b\Phi(h)$;

(ii) (Hermiticity) $\Phi(f)^* = \Phi(f)$;

(iii) (field equations) $\Phi(Pf) = 0$;

(iv) (bosonic commutation relations) $[\Phi(f), \Phi(g)] = iE(f, g)\mathbb{I}$.

Above $P : C^\infty(M) \to C^\infty(M)$ is the *Klein-Gordon operator* for a given squared mass $m^2 \geq 0$, and referred to the metric g and $E \in \mathcal{D}'(M \times M)$ is the *causal propagator* of P. It turns out that $\Phi(f) = \Phi(f')$ if and only if $E(f - f') = 0$ – where $(Ef)(x) := E(x, f)$ [13, 27, 14] – which, in turn, means $f - f' = Pg$ for some $g \in C_c^\infty(M)$.
Field operators $\Phi(f)$ are in particular *algebraic observables*. When introducing a self-interaction – different from the classical gravitational field, which is already encompassed in the formalism – the $*$-algebra $\mathfrak{A}(M, g)$ has to be suitably enlarged in order to implement perturbative treatements of the dynamics and *renormalization* procedures [4].
(2) Still assuming that (M, g) is a (time-oriented) globally hyperbolic spacetime, an alternative but equivalent construction, especially exploited in Minkowski spacetime, is the **symplectic formulation**, where the quantum fields are viewed as formal field operators $\Phi[\varphi]$ smeared against real smooth *solutions of the KG equation* φ with compact Cauchy data on every spacelike Cauchy surface Σ of (M, g). The real linear space of these solutions will be denoted by $Sol[M, g]$. The *algebraic observables* $\Phi[\varphi]$ are generators of a complex unital $*$-algebra $\mathfrak{A}[M, g]$ and are supposed to satisfy, for $a, b \in \mathbb{R}$ and $\varphi, \tilde{\varphi} \in Sol[M, g]$,

(i) ($\mathbb{R}$-linearity) $\Phi[a\varphi + b\tilde{\varphi}] = a\Phi[\varphi] + b\Phi[\tilde{\varphi}]$;

(ii) (Hermiticity) $\Phi[\varphi]^* = \Phi[\varphi]$;

(iii) (bosonic commutation relations) $[\Phi[\varphi], \Phi[\tilde{\varphi}]] = -i\sigma(\varphi, \tilde{\varphi})\mathbb{I}$,

where we have introduced the *symplectic form* on $Sol[M, g]$

$$\sigma(\varphi, \tilde{\varphi}) := \int_\Sigma (\varphi \nabla_n \tilde{\varphi} - \tilde{\varphi} \nabla_n \varphi) d\mu_\Sigma \,, \tag{1}$$

where Σ is any spacelike Cauchy surface of (M, g), ∇_n denotes the derivative along the future-oriented orthogonal direction with respect to Σ, and μ_Σ is the natural measure induced by g on Σ. The integral does not depend on the choice of Σ. It turns out that $E : C_c^\infty(M) \to Sol[M, g]$

is surjective and, from that abd the other prperties of E, it is not difficult to prove that [13, 27] there is a unique unital $*$-algebra isomorphism $\alpha : \mathfrak{A}(M,g) \to \mathfrak{A}[M,g]$ defined by

$$\alpha(\Phi(h)) = \Phi[Eh]\,, \quad \text{for every } h \in C_c^\infty(M). \tag{2}$$

In this sense the formulation relying on $\mathfrak{A}(M,g)$ and that referring to $\mathfrak{A}[M,g]$ are equivalent.
If (M,g) is the $(d+1)$-dimensional Minkowski spacetime, the symplectic formulation can be reformulated by enlarging $Sol[M,g]$ to the space of real smooth solutions of KG equation with Cauchy data which are real $\mathbb{R}^d$-Schwartz functions on every $x^0 =$ constant 3-space, where $(x^0, x^1, \dots, x^n) \in \mathbb{R}^{d+1}$ deniting any system of Minkowskian coordinates on M. ■

As is well known, an (algebraic) **state** on a unital $*$-algebra $\mathfrak{A}$ is a linear map $\phi : \mathfrak{A} \to \mathbb{C}$ which is **positive** ($\phi(a^*a) \geq 0$ for $a \in \mathfrak{A}$), and **normalized** ($\phi(\mathbb{I}) = 1$). Per definition a **non-normalized state** is a linear, positive functional $\omega\colon \mathfrak{A} \to \mathbb{C}$ such that $\omega(\mathbb{I}) \neq 0$. Notice that $\omega(\mathbb{I}) = \omega(\mathbb{I}\mathbb{I}) = \omega(\mathbb{I}^*\mathbb{I}) > 0$ therefore a non-normalized state defines a unique state $\widehat{\omega}(a) := \omega(\mathbb{I})^{-1}\omega(a)$ for $a \in \mathfrak{A}$. A state is said to be **pure** if it is an extremal element of the convex body of states. For an algebraic observable $a = a^* \in \mathfrak{A}$, the physical interpretation of $\phi(a)$ is the *expectation value* of a in the state ϕ.

In the following, we shall address the discussion about the possible interpretation of an algebraic observable $a \in \mathfrak{A}$ as a *quantum observable* in some Hilbert space formulation. Later, we shall discuss the interpretation of $\phi(a)$ as an expectation value with respect to some probability measure and the interplay with the former issue. To this end, we list a few fundamental technical notions and results we shall exploit througout the work.

The basic link between the algebraic formalism and the Hilbert space formulation of quantum theories is provided by a celebrated construction developed by Gelfand, Naimark, and Segal and known as *GNS construction* (see, e.g., [14, 16]). It is valid for every algebraic state over a unital $*$-algebra and trivially extends to non-normalized states. The construction admits a more sophisticated topological version for C^*-algebras – *cf.* section 2.2.

Theorem 2 (GNS construction)**:** *Let $\mathfrak{A}$ be a unital $*$-algebra and $\omega : \mathfrak{A} \to \mathbb{C}$ a (non-normalized) algebraic state. There exists a quadruple $(\mathsf{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \psi_\omega)$ called* **GNS quadruple** *of $(\mathfrak{A}, \omega)$, where*

(1) H_ω is a Hilbert space whose scalar product is denoted by $\langle\,|\,\rangle$,

(2) $\mathcal{D}_\omega \subset \mathsf{H}_\omega$ is a dense subspace,

(3) $\pi_\omega : \mathfrak{A} \ni a \mapsto \pi_\omega(a)$ – with $\pi_\omega(a) : \mathcal{D}_\omega \to \mathcal{D}_\omega$ – is a unital algebra representation with the property that $\pi_\omega(a^*) \subset \pi_\omega(a)^\dagger$, where † denotes the adjoint in H_ω,

(4) $\psi_\omega \in \mathsf{H}_\omega$ is a vector such that

(i) $\mathcal{D}_\omega = \pi_\omega(\mathfrak{A})\psi_\omega$,

(ii) $\omega(a) = \langle \psi_\omega | \pi_\omega(a)\psi_\omega\rangle$ for every $a \in \mathfrak{A}$, in particular $||\psi_\omega||^2 = \omega(\mathbb{I})$.

If $(\mathsf{H}, \mathcal{D}, \pi, \psi)$ satisfies (1)-(4), then there is a surjective isometric map $U : \mathsf{H}_\omega \to \mathsf{H}$ such that $U(\mathcal{D}_\omega) = \mathcal{D}$, $\pi(a) = U\pi_\omega(a)U^{-1}$ for $a \in \mathfrak{A}$, and $\psi = U\psi_\omega$.

If $\mathfrak{A}$ is a unital $*$-algebra and ω a (non-normalized) state on it, the set

$$G_{(\mathfrak{A},\omega)} := \{a \in \mathfrak{A} \mid \omega(a^*a) = 0\} \tag{3}$$

is a **left-ideal** of $\mathfrak{A}$ (a linear subspace such that $ba \in G_{(\mathfrak{A},\omega)}$ if $a \in G_{(\mathfrak{A},\omega)}$ and $b \in \mathfrak{A}$) as elementary consequence of Cauchy-Schwarz inequality and positivity of ω. $G_{(\mathfrak{A},\omega)}$ is called **Gelfand ideal**. For later convenience we recall that the proof of the GNS theorem leads to

$$\mathfrak{A}/G_{(\mathfrak{A},\omega)} = \mathcal{D}_\omega\,, \quad \pi_\omega(a)[b] = [ab] \quad \text{if } a \in \mathfrak{A}\,, [b] \in \mathfrak{A}/G_{(\mathfrak{A},\omega)}\,, \quad \text{and } \psi_\omega = [\mathbb{I}]. \tag{4}$$

In particular, $\ker(\pi_\omega) \subset G_{(\mathfrak{A},\omega)}$ and π_ω is faithful when $G_{(\mathfrak{A},\omega)} = \{0\}$[2].

2.2 Issue A: interpretation of $\pi_\omega(a)$ as a quantum observable

When the unital *-algebra $\mathfrak{A}$ is a **unital C^*-algebra** (i.e., a Banach space with respect to a norm satisfying $||ab|| \leq ||a||||b||$ and $||a^*a|| = ||a||^2$), then the GNS representation $\pi_\omega(a)$ continuously extends to a $*$-algebra representation of $\mathfrak{A}$ to $\mathfrak{B}(\mathsf{H}_\omega)$ (see, e.g., [15]). The extended representation denoted by the same symbol π_ω satisfies $\|\pi_\omega(a)\| \leq \|a\|$ if $a \in \mathfrak{A}$, where equality holds for all a if and only if π_ω is injective. In particular, for C^*-algebras, it holds $\pi_\omega(a^*) = \pi_\omega(a)^\dagger$ if $a \in \mathfrak{A}$. Therefore, Hermitian elements of $\mathfrak{A}$ are always represented by (bounded) selfadjoint operators independently of ω, as it happens in the standard Hilbert space formulation of quantum theories. Here, the two notions of observable always agree.

If $\mathfrak{A}$ is only a $*$-algebra, the picture becomes more complex. Every operator $\pi_\omega(a)$ has the common dense invariant domain $\mathcal{D}_\omega$ by definition and it is closable, since its adjoint operator $\pi_\omega(a)^\dagger$ extends $\pi_\omega(a^*)$ which has again the dense domain $\mathcal{D}_\omega$. As a consequence, $\pi_\omega(a)$ is a *symmetric operator* provided that $a = a^*$. If $\pi_\omega(a)$ is *essentially selfadjoint* for *every* ω, then no issue pops out and we can conclude that the *algebraic* observable a has a definite meaning as a *quantum* observable also in the Hilbert space formalism.[3]. However, we cannot *a priori* exclude the possibility that for some (possibly unnormalized) state ω and some $a = a^* \in \mathfrak{A}$, $\pi_\omega(a)$ may admit *different* selfadjoint extensions. Or, worse, that $\pi_\omega(a)$ admits *no* selfadjoint extensions at all (its deficiency indices are different). In these situations, an algebraic observable a may fail to be interpretable as a quantum observable, and therefore we are lead to the question whether a should be though as a physical observablein any sense. As shown by the following examples, there are concrete cases where $\pi_\omega(a)$ has either none or more than one self-adjoint extension.

Example 3:
(1) Let us define the space $\mathscr{S}$ of complex-valued smooth functions with domain $[0,1]$ which vanish at 0 and 1 with all of their derivatives. Consider the unital $*$-algebra $\mathfrak{A}$ of differential operators acting on the function of the invariant space $\mathscr{S}$, made of all finite complex linear combinations of finite compositions in arbitrary order of (i) the operator $P := -i\frac{d}{dx}$ representing the *momentum* algebraic observable for a particle confined in the box $[0,1]$, (ii) *smoothed position* algebraic observables represented by multiplicative operators $f\cdot$ induced by real-valued functions $f \in \mathscr{S}$, and (iii) the constantly 1 function again acting multiplicatively and also defining the unit of the algebra. The involution is $A^* := A^\dagger\restriction_{\mathscr{S}}$ ($\dagger$ being the adjoint in $L^2([0,1],dx) \supset \mathscr{S}$)

[2]The converse does not hold, since $\ker(\pi_\omega)$ is a two-sided $*$-ideal and thus $\ker(\pi_\omega) \subsetneq G_{(\mathfrak{A},\omega)}$ in the general case.

[3] A sufficient condition (by no means necessary!) assuring essential selfadjointeness of $\pi_\omega(a)$ for a fixed Hermitian element $a \in \mathfrak{A}$ and *every* non-normalized state ω is that [19] there exist $b_\pm \in \mathfrak{A}$ such that $(a \pm i\mathbb{I})b_\pm = \mathbb{I}$ (equivalently $b'_\pm(a \pm i\mathbb{I}) = \mathbb{I}$, where $b'_\pm = b^*_\mp$). This is because the written condition trivially implies that $\mathrm{Ran}(\pi_\omega(a) \pm iI) \supset \mathcal{D}_\omega$ and thus $\mathrm{Ran}(\pi_\omega(a) \pm iI)$ is dense, so that the symmetric operator $\pi_\omega(a)$ is essentially selfadjoint (see, e.g. [15, Thm. 5.18]).

so that $P^* = P$. We stress that we are here considering $\mathfrak{A}$ as an abstract algebra (i.e., up to isomorphisms of unital $*$-algebras) independently of the concrete realization in terms of operators we described above. Now consider the non-normalized state $\omega : \mathfrak{A} \to \mathbb{C}$ defined as, where dx is the Lebesgue measure on $\mathbb{R}$,

$$\omega(A) := \int_0^1 \psi(x)(A\psi)(x)dx \quad A \in \mathfrak{A}\,.$$

Above, $\psi \in \mathscr{S}$ is a fixed non-negative function vanishing *only* at 0 and 1. The GNS structure is easy to be constructed taking advantage of the uniqueness part of GNS theorem,

$$\mathsf{H}_\omega = L^2([0,1], dx)\,, \quad \pi_\omega(A) = A\restriction_{\mathcal{D}_\omega}\,, \quad \psi_\omega := \psi\,,$$

and $\mathcal{D}_\omega$ is a suitable subspace of $\mathscr{S}$ which however includes $C_c^\infty(0,1)$, the space of smooth complex maps $f : [0,1] \to \mathbb{C}$ supported in $(0,1)$, so that $\mathcal{D}_\omega$ is dense in $L^2([0,1], dx)$ as is due. The deficiency spaces $N_\pm := \ker(\pi_\omega(P)^* \mp i) = \mathrm{Ran}(\pi_\omega(P) \pm i)^\perp$ of $\pi_\omega(P) = P\restriction_{\mathcal{D}_\omega}$ are

$$\begin{aligned} N_\pm &:= \left\{ g_\pm \in L^2([0,1], dx) \;\middle|\; \int_0^1 \overline{g_\pm}(f' \mp f)dx = 0 \quad \forall f \in \mathcal{D}_\omega \right\} \\ &= \left\{ g_\pm \in L^2([0,1], dx) \;\middle|\; \int_0^1 \overline{g_\pm(x)e^{\pm x}} \left(f(x)e^{\mp x}\right)' dx = 0 \quad \forall f \in \mathcal{D}_\omega \right\} \end{aligned} \qquad (5)$$

If $\mathcal{D}_\omega$ were replaced by $C_c^\infty(0,1)$ in (5), [15, Lemma 5.30] would imply $g_\pm(x) = ce^{\mp x}$ for $c \in \mathbb{C}$. However these functions would also satisfy (5) if $f \in \mathscr{S}$, as one immediately proves per direct inspection. Since $C_c^\infty(0,1) \subset \mathcal{D}_\omega \subset \mathscr{S}$, we conclude that $N_\pm = \mathrm{span}\{e^{\mp x}\}$. Therefore the symmetric operator $\pi_\omega(P)$ is *not* essentially selfadjoint on its GNS domain $\mathcal{D}_\omega$, but it admits a one-parameter class of different selfadjoint extensions according to *von Neumann's extension theorem* (see, e.g. [15, Thm. 5.37]). Stated differently, P is an algebraic observable which does not admit a quantum-observable interpretation in the considered GNS Hilbert space.

(2) Let us define the space $\mathscr{E}$ of complex-valued smooth functions with domain $[0, +\infty)$ which vanish at 0 with all of their derivatives and tend to 0 with all of their derivatives for $x \to +\infty$ faster than every negative power of x. Consider the unital $*$-algebra $\mathfrak{B}$ of differential operators acting on the functions of the invariant space $\mathscr{E}$, made of all finite complex linear combinations of finite compositions in arbitrary order of (i) the operator $P := -i\frac{d}{dx}$ which again we would like to interpret as the algebraic momentum observable for a particle confined to stay in the half line, (ii) smoothed position algebraic observables represented by multiplicative operators $f\cdot$ induced by real-valued functions $f \in \mathscr{E}$, and (iii) the constantly 1 function again acting multiplicatively and also defining the unit of the algebra. The involution is $A^* := A^\dagger\restriction_{\mathscr{E}}$ ($\dagger$ being the adjoint in $L^2([0, +\infty), dx) \supset \mathscr{E}$) so that $P^* = P$. As before, we are here considering $\mathfrak{B}$ as an abstract algebra (i.e., up to isomorphisms of unital $*$-algebras) independently of the concrete realization we presented above. Next consider the non-normalized state $\phi : \mathfrak{B} \to \mathbb{C}$ defined as

$$\phi(A) := \int_0^{+\infty} \chi(x)(A\chi)(x)dx \quad A \in \mathfrak{B}\,. \qquad (6)$$

Above, $\chi \in \mathscr{E}$ is a fixed non-negative function vanishing *only* at 0. Uniqueness part of the GNS theorem proves that the GNS structure is

$$\mathsf{H}_\phi = L^2([0, +\infty), dx)\,, \quad \pi_\phi(A) = A\restriction_{\mathcal{D}_\phi}\,, \quad \psi_\phi := \chi\,,$$

and $\mathcal{D}_\phi$ is a suitable subspace of $\mathscr{E}$ which however includes $C_c^\infty(0,+\infty)$, the space of smooth complex maps $f:[0,+\infty)\to\mathbb{C}$ whose supports are included in $(0,+\infty)$. Hence $\mathcal{D}_\phi$ is dense in $L^2([0,+\infty),dx)$ as is due. The deficiency spaces $N_\pm$ of $\pi_\phi(P)=P\restriction_{\mathcal{D}_\phi}$ can be computed easily

$$N_\pm := \left\{ g_\pm \in L^2([0,+\infty),dx) \;\middle|\; \int_0^{+\infty} \overline{g_\pm}(f'\mp f)dx = 0 \quad \forall f\in\mathcal{D}_\phi \right\}$$
$$= \left\{ g_\pm \in L^2([0,+\infty),dx) \;\middle|\; \int_0^{+\infty} \overline{g_\pm(x)e^{\pm x}}\left(f(x)e^{\mp x}\right)' dx = 0 \quad \forall f\in\mathcal{D}_\phi \right\} \tag{7}$$

If $\mathcal{D}_\phi$ were replaced by $C_c^\infty(0,+\infty)$ in (7), [15, Lemma 5.30] would imply $g_\pm(x)=ce^{\mp x}$ for $c\in\mathbb{C}$. Evidently ce^x cannot be accepted as an element of $L^2([0,+\infty),dx)$ unless $c=0$, so that, since $C_c^\infty(0,+\infty)\subset\mathcal{D}_\phi$, we conclude that $N_-=\{0\}$. The functions ce^{-x} would fulfill (7) even if $\mathcal{D}_\phi$ were replaced by $\mathscr{E}$, as one immediately proves per direct inspection. Since $C_c^\infty(0,+\infty)\subset\mathcal{D}_\phi\subset\mathscr{E}$, we conclude that $N_+=\mathrm{span}\{e^{-x}\}$ whereas $N_-=\{0\}$. Therefore the symmetric operator $\pi_\phi(P)$ is *not* essentially selfadjoint on its GNS domain $\mathcal{D}_\phi$ and it does *not* admit selfadjoint extensions. More strongly, as $N_+=\{0\}$ but $N_-\neq\{0\}$, we have that $\overline{\pi_\phi(P)}$ is *maximally symmetric*: it does not admit proper symmetric extensions [1, Thm. 3, p.97]. *Once again, the algebraic observable P does not admit a quantum-observable interpretation in the considered GNS Hilbert space.* ∎

In summary, it seems that, dealing with $*$-algebras which are not C^*-algebras, there is not a perfect match between the notion of algebraic observable (Hermitian element of $\mathfrak{A}$) and that of quantum observable (selfadjoint operator in the (GNS) Hilbert space formulation). In particular, Hermitian elements of $*$-algebras are usually represented by merely symmetric operators in the GNS representations with many or none selfadjoint extensions. This issue is relevant when dealing with the problem of measurement, see in particular [10, 11] where the problem of measurement is discussed for the algebra of quantum fields in a locally covariant framework.

2.3 Issue B: interpretation of $\omega(a)$ as expectation value and the moment problem

Let us pass to discuss the interpretation of $\omega(a)$ as *expectation value* for $a=a^*\in\mathfrak{A}$, where ω is a (possibly non-normalized) state[4]. To rigorously accept this folk physical interpretation, we should assume that the pair (a,ω) admits a physically meaningful uniquely associated positive σ-additive measure $\mu_\omega^{(a)}$ over $\mathbb{R}$ such that

$$\omega(a) = \int_{\mathbb{R}} \lambda d\mu_\omega^{(a)}(\lambda)\,. \tag{8}$$

It is natural to also suppose that μ is defined on the Borel σ-algebra $\mathscr{B}(\mathbb{R})$, since this is the case for measures arising from the spectral theory as it is standard in quantum theories. Identity (8) is far from being able to determine $\mu_\omega^{(a)}$. However, the structure of $*$-algebra permits us to define real polynomials of algebraic observables and ω does assign values to all those algebraic observables.

[4]In the non-normalized case, the meaning of expectation value would be actually reserved to $\widehat{\omega}(a)=\omega(\mathbb{I})^{-1}\omega(a)$, though, for shortness, we improperly also call $\omega(a)$ expectation value in the rest of the work.

In particular, for $a = a^* \in \mathfrak{A}$ and $n \in \mathbb{N}$, it is natural to interpret a^n as the algebraic observable whose values are λ^n if λ is a value attained by a. For this reason we shall strengthen (8) by requiring that

$$\omega(a^n) = \int_{\mathbb{R}} \lambda^n d\mu_\omega^{(a)}(\lambda) \quad \text{for every } n \in \mathbb{N} . \tag{9}$$

In this way, $\omega(a^n)$ is interpreted as the n-th *moment* of the unknown measure $\mu_\omega^{(a)}$. Finding a finite *positive Radon measure* over $\mathbb{R}$ when its moments are fixed is a quite famous problem named *Hamburger moment problem*, extensively treated in the pure mathematical literature (see [21] for a modern textbook on the subject).

Remark 4: A **positive Radon measure** is a positive σ-additive measure defined on the Borel sets of a Hausdorff locally-compact space (here $\mathbb{R}$ equipped with the Euclidean topology) which is both outer and inner regular and assigns a finite value to every compact set. All measures considered above are necessarily finite because $\omega(a^0) = \omega(\mathbb{I})$ exists in $[0, +\infty)$ by hypothesis. In $\mathbb{R}^n$, all finite positive σ-additive Borel measures are automatically Radon in view of [25, Thm. 2.18]. Therefore, "positive Radon measure" can be equivalently replaced by "positive σ-additive Borel measure" in the rest of the discussion related to the moment problem. ■

At this juncture, for a given Hermitian $a \in \mathfrak{A}$ and a given non-normalized state $\omega : \mathfrak{A} \to \mathbb{C}$, we should tackle two problems if we want to insist with the standard interpretation of $\omega(a)$ as expectation value.

(M1) Does a positive σ-additive Borel measure $\mu_\omega^{(a)}$ over $\mathbb{R}$ satisfying (9) exist?

(M2) Is it unique?

Issues A and B are related in several ways. Here is a first example of that interplay arising when facing (M1) and (M2). If $\pi_\omega(a)$ is essentially selfadjoint, a measure as in (M1) directly arises form the GNS construction. It is simply constructed out of the projection-valued measure (PVM) $P^{(\overline{\pi_\omega(a)})} : \mathscr{B}(\mathbb{R}) \to \mathfrak{B}(\mathsf{H}_\omega)$ of the selfadjoint operator $\overline{\pi_\omega(a)}$ over H_ω:

$$\mu_\omega^{(a)}(E) := \langle \psi_\omega | P^{(\overline{\pi_\omega(a)})}(E) \psi_\omega \rangle , \quad E \in \mathscr{B}(\mathbb{R}) . \tag{10}$$

This opportunity is always present if $\mathfrak{A}$ is a unital C^*-algebra, since $\pi_\omega(a) \in \mathfrak{B}(\mathsf{H}_\omega)$ is selfadjoint in that case. Concerning (M2), it is possible to prove that the measure defined in (10) is also *unique* when $\mathfrak{A}$ is a C^*-algebra.

Proposition 5: *Let $\mathfrak{A}$ be a unital $*$-algebra, $a = a^* \in \mathfrak{A}$, and $\omega : \mathfrak{A} \to \mathbb{C}$ is a non-normalized state. The following facts hold.*

(a) *If $\pi_\omega(a)$ is essentially selfadjoint, then there exists a (necessarily finite) positive σ-additive Borel measure $\mu_\omega^{(a)} : \mathscr{B}(\mathbb{R}) \to [0, +\infty)$ satisfying (9).*

(b) *If furthermore $\mathfrak{A}$ is a C^*-algebra, then the measure $\mu_\omega^{(a)}$ is unique.*

Proof. (a) The measure (10) is a finite positive σ-additive Borel measure over $\mathbb{R}$ due to standard properties of spectral measures, it also satisfies (9). Indeed, since $D([\overline{\pi_\omega(a)}]^n) \supset D(\pi_\omega(a)^n) \supset D(\pi_\omega(a^n)) = \mathcal{D}_\omega \ni \psi_\omega$, from spectral theory (see. e.g. [15]) we have

$$\int_{\mathbb{R}} \lambda^n d\mu_\omega^{(a)} = \langle \psi_\omega | [\overline{\pi_\omega(a)}]^n \psi_\omega \rangle = \langle \psi_\omega | \pi_\omega(a^n) \psi_\omega \rangle = \omega(a^n) \ .$$

(b) Let us suppose that $\mathfrak{A}$ is also a C^*-algebra. Since $|\omega(a^n)| \leq \omega(\mathbb{I})\|a\|^n$, *Carleman's condition* [21, Corollary 4.10] assures that there exists at most one positive Radon measure satisfying (9). Observe that $\mu_\omega^{(a)}$ is a positive Radon measure in view of Remark 4. □

There are cases of unital $*$-algebras $\mathfrak{A}$ and (possibly unnormalized) states $\omega : \mathfrak{A} \to \mathbb{C}$ such that Hermitian elements $a \in \mathfrak{A}$ exist whose associated GNS operator $\pi_\omega(a)$ is not essentially selfadjoint – see Example 3. In this situation Proposition 5 cannot be directly exploited. If $\pi_\omega(a)$ admits selfadjoint extensions (it is sufficient that it commutes with a *conjugation*) each of these selfadjoint extensions induces a measure $\mu_\omega^{(a)}$ as above. However, measures satisfying (M1) for the pair (a, ω) do exist, and they are not necessarily unique, even if $\pi_\omega(a)$ does *not* admit any selfadjoint extension – *cf.* Examples 3-11 – making the situation even more intricate.

The following proposition can be proved noticing that positivity of ω and its linearity implies that the set of candidate moments $m_n := \omega(a^n)$ satisfies the hypotheses of [24, Thm. X.4]. However, we intend to provide a direct construction (which is nothing but the proof of the quoted theorem written with a different language).

Proposition 6: *Let $\mathfrak{A}$ be a unital $*$-algebra, $a = a^* \in \mathfrak{A}$, and $\omega : \mathfrak{A} \to \mathbb{C}$ a non-normalized state. Then there exists a positive σ-additive Borel measure $\mu_\omega^{(a)} : \mathscr{B}(\mathbb{R}) \to [0, +\infty)$ satisfying (9).*

Proof. Define a subspace $\mathcal{D}_\omega^{(a)}$ of $\mathcal{D}_\omega$ as follows $\mathcal{D}_\omega^{(a)} := \{\pi_\omega(p(a))\psi_\omega \,|\, p : \mathbb{R} \to \mathbb{C} \text{ polynomial}\}$ and define the closed subspace $\mathsf{H}_\omega^{(a)}$ of H_ω as the closure of $\mathcal{D}_\omega^{(a)}$. By construction, $\pi_\omega(a)$ leaves $\mathcal{D}_\omega^{(a)}$ invariant and $\pi_\omega(a)\restriction_{\mathcal{D}_\omega^{(a)}}$ is symmetric in $\mathsf{H}_\omega^{(a)}$. Finally, $\pi_\omega\restriction_{\mathcal{D}_\omega^{(a)}}$ commutes with the *conjugation* $C : \mathsf{H}_\omega^{(a)} \to \mathsf{H}_\omega^{(a)}$ obtained as the unique continuous extension of the antilinear isometric involutive map $\pi_\omega(p(a))\psi_\omega \mapsto \pi_\omega(p(a))^\dagger\psi_\omega$ over $\mathcal{D}_\omega^{(a)}$ (use the fact that $a = a^*$). In view of the von Neumann criterion (see, e.g. [15, Thm. 5.43]), $\pi_\omega\restriction_{\mathcal{D}_\omega^{(a)}}$ admits selfadjoint extensions $\widehat{a}_\omega$ on $\mathsf{H}_\omega^{(a)}$. The same argument exploited to prove (a) in Proposition 5 restricted to $\mathsf{H}_\omega^{(a)}$ concludes the proof because

$$\mu_\omega^{(a)}(E) := \langle \psi_\omega | P^{(\widehat{a}_\omega)}(E)\psi_\omega \rangle \ , \quad E \in \mathscr{B}(\mathbb{R}) \tag{11}$$

satisfies all requirements for every such selfadjoint extension $\widehat{a}_\omega$. □

In turn, the proof of the Proposition 6 raises another issue. Are all measures $\mu_\omega^{(a)}$ associated with a pair (a, ω) spectrally constructed from selfadjoint extensions over $\mathsf{H}_\omega^{(a)}$ of $\pi_\omega(a)\restriction_{\mathcal{D}_\omega^{(a)}}$ when this operator admits such extensions? The answer is once again negative as it can be grasped from the detailed discussion about the moment problem in the operatorial approach appearing in Ch.6 of [21]. All measures satisfying (M1) are in fact spectrally obtained by *enlarging* the Hilbert space $\mathsf{H}_\omega^{(a)}$ *without reference to the original common GNS Hilbert space* H_ω.

This fact eventually suggests that, in principle, there could be a plethora of measures associated with (a, ω) as solutions of the moment problem with dubious physical meaning, because they are vaguely related with the underpinning physical theory described by $\mathfrak{A}$ and ω. Our feeling is that focusing on the *whole* class of the measures satisfying (M1) for a given pair (a, ω) is probably a wrong approach to tackle the problem of the interpretation of $\omega(a)$ as expectation value. Further physical meaningful information has to be added in order to reduce the number of elements of the family of measures.

There are some relevant papers in the literature on related topics, in particular [8, 9] where a *non commutative* version of the moment problem (both existence and uniqueness) is addressed, carefully analyzed and solved for $*$-algebras, and finally also applied to the $*$-algebra of quantum fields. There, the unknown is the non-normalized state on the $*$-algebra. Conversely, the state is *a priori* known here and we focus on the standard moment problem referred to a measure associated to the state for fixed Hermitian element of the algebra. Another important difference is that in [8, 9] natural separating C^*-seminorms on $\mathfrak{A}$ are exploited. Here we instead stick to the minimal purely algebraic structure of $\mathfrak{A}$.

3 Selfadjointness of $\overline{\pi_\omega(a)}$ and uniqueness of moment problems

In the discussion developed in section 2, when presenting the issues A and B, we completely overlooked the physically meaningful fact that other elements $b \in \mathfrak{A}$ than a exist. These elements can be used to generate new non-normalized states ω_b out of ω defined by $\omega_b(a) := \omega(b^*ab)$: ω_b is viewed as a deformation of ω. When we are given the triple $\mathfrak{A}, a, \omega$ (with $a = a^*$) we also know the formal expectation values $\omega_b(a)$. We expect that these deformed states and the associated measures $\mu^{(a)}_{\omega_b}$ solving the moment problem with respect to ω_b should enter the game. Theorem 9 below shows that it is the case.

3.1 Deformations of a non-normalized state

Definition 7: If ω is a non-normalized state (or a state) over $\mathfrak{A}$, we will denote by ω_b the non-normalized state, called b-**deformation** of ω

$$\omega_b(a) := \omega(b^*ab) \quad \forall a \in \mathfrak{A}\,, \tag{12}$$

where $b \in \mathfrak{A}$. The limit case of the zero functional ω_b obtained from b with $\omega(b^*b) = 0$ is included, and we call that ω_b **singular deformation**. ■

From the final uniqueness part of Theorem 2, the GNS structure of a non-singular deformation ω_b is evidently

$$(\mathsf{H}_{\omega_b}, \mathcal{D}_{\omega_b}, \pi_{\omega_b}, \psi_{\omega_b}) = \left(\overline{\pi_\omega(\mathfrak{A})\psi_{\omega_b}}, \pi_\omega(\mathfrak{A})\psi_{\omega_b}, \pi_\omega\restriction_{\mathcal{D}_{\omega_b}}, \pi_\omega(b)\psi_\omega\right)\,. \tag{13}$$

If ω_b is singular we *define*,

$$(\mathsf{H}_{\omega_b}, \mathcal{D}_{\omega_b}, \pi_{\omega_b}, \psi_{\omega_b}) := (\{0\}, \{0\}, 0, 0)\,. \tag{14}$$

Remark 8: Observe that $\omega_b = \omega_{b'}$ if $[b] = [b']$ referring to the Gelfand-ideal quotient. Therefore the non-normalized states ω_b would be better labelled by the vectors in $\mathcal{D}_\omega = \mathfrak{A}/G_{(\mathfrak{A},\omega)}$. ■

3.2 Selfadjointness of $\overline{\pi_\omega(a)}$ and uniqueness of moment problems for deformed non-normalized states

The fact that focusing on the deformations ω_b goes towards the correct direction in order to clarify issues A and B is evident from the following result, the first main result of the paper, which connects uniqueness of the measures $\mu^{(a)}_{\omega_b}$ with selfadjointness of $\overline{\pi_\omega(a)}$.

Theorem 9: *Let $\mathfrak{A}$ be a unital $*$-algebra, $a^* = a \in \mathfrak{A}$, and $\omega : \mathfrak{A} \to \mathbb{C}$ a non-normalized state. Assume that the finite positive σ-additive Borel measure $\mu^{(a)}_{\omega_b} : \mathscr{B}(\mathbb{R}) \to [0, +\infty)$ solving the moment problem for every non-singular deformation ω_b*

$$\omega_b(a^n) = \int_{\mathbb{R}} \lambda^n d\mu^{(a)}_{\omega_b}(\lambda) \quad \textit{for every } n \in \mathbb{N}. \tag{15}$$

is unique[5]*. The following facts hold for every deformation ω_b.*

- **(a)** *$\pi_\omega(a)$ is essentially selfadjoint in H_ω and, more generally, all operators $\pi_{\omega_b}(a)$ are essentially selfadjoint in the respective H_{ω_b}.*
- **(b)** *All measures $\mu^{(a)}_{\omega_b}$ are induced by the single PVM $P^{(\overline{\pi_\omega(a)})}$ in the sense that*

$$\mu^{(a)}_{\omega_b}(E) = \langle \psi_{\omega_b} | P^{(\overline{\pi_{\omega_b}(a)})}(E)\psi_{\omega_b}\rangle\,, \quad E \in \mathscr{B}(\mathbb{R})\,, \tag{16}$$

$$P^{(\overline{\pi_{\omega_b}(a)})}(E) = P^{(\overline{\pi_\omega(a)})}(E)\restriction_{\mathsf{H}_{\omega_b}}\,, \quad E \in \mathscr{B}(\mathbb{R})\,. \tag{17}$$

Proof. (a) *Carleman's condition* [21, Corollary 4.10] assures that, if ω_b is singular, only the zero measure $\mu^{(a)}_{\omega_b} = 0$ solves the moment problem.We can therefore assume that there is a unique measure solving the moment problem for every $b \in \mathfrak{A}$. From [21, Thm. 6.10] translated into our GNS-like formulation as in the proof of Proposition 6 and using the notation introduced therein, we have that $\mu^{(a)}_{\omega_b}$ is unique if and only if $\pi_{\omega_b}(a)\restriction_{\pi_{\omega_b}(\mathfrak{A}_a)\psi_b}$ is essentially selfadjoint in $\overline{\pi_{\omega_b}(\mathfrak{A}_a)\psi_b}$ – where $\mathfrak{A}_a$ denotes the $*$-algebra generated by a. Now observe that the set of all vectors $\psi_{\omega_b} = \pi_\omega(b)\psi_\omega$, for $b \in \mathfrak{A}$, is dense in H_ω since it coincides with $\mathcal{D}_\omega$, so that it is a dense set of uniqueness vectors for the symmetric operator $\pi_\omega(a)$ in H_ω, which is therefore essentially selfadjoint in view of *Nussbaum's lemma* (Lemma on p. 201 of [24]). Essential selfadjointness of $\pi_{\omega_b}(a)$ can be established similarly, taking (13) and (14) into account. By hypothesis, fixing $b \in \mathfrak{A}$, also the measures $\mu^{(a)}_{\omega_{cb}}$ are uniquely determined by the deformations ω_{cb} with $c \in \mathfrak{A}$. The set of all vectors $\psi_{\omega_{cb}} = \pi_\omega(cb)\psi_\omega = \pi_\omega(c)\psi_{\omega_b}$, for $c \in \mathfrak{A}$, is dense in H_{ω_b} since it coincides to $\mathcal{D}_{\omega_b}$, so that it is a dense set uniqueness vectors for the symmetric operator $\pi_{\omega_b}(a)$ in H_{ω_b} which is essentially selfadjoint due to Nussbaum's lemma again.
(b) Assuming (17), then (16) is a trivial consequence of the uniqueness hypothesis and (a) of Proposition 5 applied to the non-normalized state ω_b. Let us prove (17) to conclude. We know that $\overline{\pi_\omega(a)}$ admits $\mathcal{D}_{\omega_b}$ as invariant subspace from (13) and (14), furthermore $\pi_\omega(a)\restriction_{\mathcal{D}_{\omega_b}} = \pi_{\omega_b}(a)$ is essentially selfadjoint in the Hilbert space H_{ω_b}, which is a closed subspace of H_ω, and H_{ω_b} is the closure of $\mathcal{D}_{\omega_b}$. Proposition 40 implies that H_{ω_b} reduces $\overline{\pi_\omega(a)}$ (see Appendix A.1) so that $\overline{\pi_{\omega_b}(a)}$ is the part of $\overline{\pi_\omega(a)}$ on H_{ω_b}. Using the properties of the PVMs, it is easy to prove that if a

[5] If ω_b is not singular, some $\mu^{(a)}_{\omega_b}$ exists due to Proposition 6. If it is singular, the zero measure solves the moment problem.

closed subspace H_0 reduces a selfadjoint operator T, then the PVM of the part of T on H_0 (which is selfadjoint in view of Proposition 39) is the restriction to H_0 of the PVM of T. Applying this result to $\overline{\pi_\omega(a)}$ and $\overline{\pi_{\omega_b}(a)}$, uniqueness of the PVM of a selfadjoint operator implies that the PVM of $\overline{\pi_{\omega_b}(a)}$ is nothing but the restriction to H_{ω_b} of the PVM of $\overline{\pi_\omega(a)}$. This is just (17). □

Example 10: A simple example of application of Theorem 9 is the following. (It is not physically interesting, but it just provides evidence that the very strong hypotheses of Theorem 9 are fulfilled in some case.) Consider the unital Abelian $*$-algebra $\mathbb{C}_{[0,1]}[x]$ made of all complex polynomials $p : [0,1] \to \mathbb{C}$ in the variable x with the involution defined as the standard point-wise complex conjugation, and the unit given by the constantly 1 polynomial. Define the state

$$\omega(p) = \int_0^1 p(x)dx \quad p \in \mathbb{C}_{[0,1]}[x] \, .$$

Using in particular the Stone-Weierstrass theorem and the uniqueness part of the GNS theorem, it is easy to prove that a GNS representation is

$$\mathsf{H}_\omega := L^2([0,1], dx) \, , \quad \pi_\omega(p) = p\cdot \, , \quad \mathcal{D}_\omega = \mathbb{C}_{[0,1]}[x] \, , \quad \psi_\omega = 1$$

where $p\cdot$ denotes the polynomial p acting as multiplicative operator on $\mathbb{C}_{[0,1]}[x]$. Evidently $\omega_q(p) = \int_0^1 |q(x)|^2 p(x)\, dx$. Hence $|\omega_q(x^n)| \leq \frac{C_q}{n+1}$ where $C_q = \max_{[0,1]} |q|^2$. *Carleman's condition* [21, Corollary 4.10] assures that there exists at most one positive Radon measure satisfying (15) for $b = p$ and $a = x$. Hence we can apply Theorem 9 and this means in particular that $\pi_\omega(x)$, i.e. the symmetric multiplicative operator x with domain consisting of the complex polynomials on $[0,1]$, is essentially selfadjoint in $L^2([0,1], dx)$. ■

At this point, it may seem plausible that the statement (a) of Proposition 5 can be reversed proving that, if $a^* = a \in \mathfrak{A}$, essential selfadjointness of all $\pi_{\omega_b}(a)$ is equivalent to uniqueness of all the measures $\mu^{(a)}_{\omega_b}$. Unfortunately life is not so easy as a consequence of the last item of the pair of examples below. The former example concerns again QM whereas the latter concerns elementary QFT as in Example 1.

Example 11: (1) Let $\mathfrak{A}_{\mathrm{CCR},1}$ be the $*$-algebra generated by I, Q, P defined as follows. $Q, P, I : \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R})$ are respectively the operators

$$(Q\psi)(x) = x\psi(x) \, , \quad (P\psi)(x) = -i\frac{d}{dx}\psi(x) \, , \quad (I\psi)(x) = \psi(x) \, , \quad x \in \mathbb{R} \, .$$

The finite linear combinations of finite compositions of these operators with arbitrary order form a unital $*$-algebra with unit I, provided the involution is defined as $A^* := A^\dagger\restriction_{\mathscr{S}(\mathbb{R})}$ where here † is the adjoint in $L^2(\mathbb{R}, dx)$, so that $P^* = P$ and $Q^* = Q$. It is important to stress that we are here considering $\mathfrak{A}_{\mathrm{CCR},1}$ as an abstract algebra (i.e., up to isomorphisms of unital $*$-algebras) independently of the above concrete realization. Consider the state ω

$$\omega(A) = \int_{\mathbb{R}} \overline{\psi_0(x)}(A\psi_0)(x)\, dx \quad A \in \mathfrak{A}_{\mathrm{CCR},1} \, , \quad \psi_0(x) = \pi^{-\frac{1}{4}} e^{-\frac{x^2}{2}} \, .$$

The choice of ω is evidently related with the ground state of the harmonic oscillator. Exploiting the uniqueness part of the GNS theorem, it is not difficult to prove that the GNS construction generated by ω leads to

$$\mathsf{H}_\omega = L^2(\mathbb{R}, dx) \ , \ \ \pi_\omega(A) = A\restriction_{\mathcal{D}_\omega} \ , \ \ \psi_\omega = \psi_0 \ .$$

The crucial point which differentiates the found representation of $\mathfrak{A}_{\text{CCR},1}$ from the concrete initial realization, is that now $\mathcal{D}_\omega \subsetneq \mathscr{S}(\mathbb{R})$. Indeed, $\mathcal{D}_\omega$ results to be the dense subspace of $L^2(\mathbb{R}, dx)$ made of all finite linear combinations of *Hermite functions* $\{\psi_n\}_{n\in\mathbb{N}}$ (the eigenstates of the harmonic oscillator Hamiltonian). $\mathcal{D}_\omega$ is dense just because $\{\psi_n\}_{n\in\mathbb{N}}$ is a Hilbert basis of $L^2(\mathbb{R}, dx)$.

Let us pass to consider the deformations ω_B, $B \in \mathfrak{A}_{\text{CCR},1}$. Using as equivalent generators I and $A := \frac{1}{\sqrt{2}}(X + iP)$, $A^* = \frac{1}{\sqrt{2}}(X - iP)$ – the elements of $\mathfrak{A}_{\text{CCR},1}$ corresponding to the annihilation and creation operators – instead of I, Q, P to define $\mathfrak{A}_{\text{CCR},1}$, one easily sees that

$$\mathcal{D}_\omega = \mathcal{D}_{\omega_B} \ , \quad \mathsf{H}_\omega = \mathsf{H}_{\omega_B} \ , \quad \text{and} \quad \pi_{\omega_B} = \pi_\omega \quad \text{for every choice of } B \in \mathfrak{A}_{\text{CCR},1} \ .$$

The first identity holds because $\psi_\omega \in \mathcal{D}_{\omega_B}$ as established in lemma 43 in appendix and $\pi_{\omega_B}(\cdot) = \pi_\omega(\cdot)\restriction_{\mathcal{D}_{\omega_B}}$, for every $B \in \mathfrak{A}_{\text{CCR},1}$ such that $\omega(B^*B) > 0$ according to (13). The remaining identities are trivial consequences of the first ones. Regarding the problem of essentially selfadjointness, we have that

(a) $\pi_{\omega_B}(Q^k)$ (and $\pi_{\omega_B}(P^k)$) are essentially selfadjoint for $k = 1, 2$ because of *Nelson's theorem* [24, Thm. X39] as the ψ_ns are a set of *analytic vectors* for $\pi_{\omega_B}(Q)$ and $\pi_{\omega_B}(Q^2)$. This is consequence of the estimate, arising form

$$X = \frac{1}{\sqrt{2}}\left(A + A^*\right) \ , \tag{18}$$

$$||\pi_\omega(Q^k)\psi_n|| \leq 2^{k/2}\sqrt{(n+k)!} \ , \qquad n = 0, 1, \dots \ , \ k = 1, 2, \dots \ , \tag{19}$$

arising from [24, Example 2 p.204] which implies

$$||\pi_\omega(Q^k)^m\psi_n|| \leq 2^{mk/2}\sqrt{(n+mk)!} \ , \qquad m, n = 0, 1, \dots \ , \ k = 1, 2, \dots \ ; \tag{20}$$

and of the fact that the span $\mathcal{D}_{\omega_B} = \mathcal{D}_\omega$ of the ψ_ns is furthermore dense in $\mathsf{H}_{\omega_B} = \mathsf{H}_\omega$.

(b) $\pi_\omega(Q^4) = \pi_{\omega_B}(Q^4)$ is essentially selfadjoint. In fact, it is symmetric, *bounded from below* and a direct computation based on (20) proves that the ψ_n are *semianalytic vectors* for it, hence we can apply [24, Thm. X40] which guarantees that $\pi_{\omega_B}(Q^4)$ is essentially selfadjoint.

Let us focus on the moment problem relative to (Q^k, ω). Observe that, if a and $a^+ \subset a^\dagger$ are the standard *annihilation* and *creation operators* defined on $\mathcal{D}_\omega$ such that

$$[a, a^+] = I, \ \ [a, a] = [a^+, a^+] = 0, \quad \text{and } a\psi_0 = 0, \tag{21}$$

then it holds

$$\pi_\omega(Q) = \frac{1}{\sqrt{2}}\left(\pi_\omega(A) + \pi_\omega(A^*)\right) = \frac{1}{\sqrt{2}}\left(a + a^+\right) \ . \tag{22}$$

Therefore, if $s_n^{(k)}$ denotes the n-th moment of Q^k in the state ω ,we have

$$s_n^{(k)} := \omega(Q^{kn}) = \frac{1}{2^{kn/2}} \left\langle \psi_0 \left| (a+a^+)^{kn} \ \psi_0 \right. \right\rangle = \pi^{-\frac{1}{2}} \int_{\mathbb{R}} x^{kn} e^{-x^2} dx \,. \tag{23}$$

The moment problem relative to (Q^k, ω) admits at least a solution $\mu_\omega^{(Q^k)}$ due to Proposition 6 because Q^k is Hermitian in the algebra. Let us examine uniqueness of this measure, i.e, in the jargon of moment problem theory, we go to check if the moment problem is *determinate* taking advantage of the results discussed in [21].

$k=1$ We may directly compute $s_{2n+1}^{(1)} = 0$ and $s_{2n}^{(1)} = 2^{-2n}(2n-1)!!$, which satisfies the hypothesis of *Carleman's condition* [21, Cor. 4.10]: the moment problem for $\{s_n^{(1)}\}_{n\in\mathbb{N}}$ is thus *determinate.*

$k=2$ We may apply *Cramer's condition* [21, Cor.4.11] to conclude that the moment problem for $\{s_n^{(2)}\}_{n\in\mathbb{N}}$ is again *determinate.*

$k=3$ We have

$$s_n^{(3)} := \pi^{-\frac{1}{2}} \int_{\mathbb{R}} x^{3n} e^{-x^2} dx = \frac{1}{3\sqrt{\pi}} \int_{\mathbb{R}} y^n \frac{e^{-y^{\frac{2}{3}}}}{y^{\frac{2}{3}}} dy =: \int_{\mathbb{R}} y^n f(y) dy \,. \tag{24}$$

We now apply *Krein's condition* for indeterminacy [21, Thm. 4.14]: since

$$\int_{\mathbb{R}} \frac{\log f(x)}{1+x^2} dx = -\int \frac{\log(3\sqrt{\pi})}{1+x^2} dx - \int_{\mathbb{R}} \frac{x^{\frac{2}{3}}}{1+x^2} dx - \frac{2}{3} \int_{\mathbb{R}} \frac{\log|x|}{1+x^2} dx > -\infty \,,$$

the moment problem for $\{s_n^{(3)}\}_{n\in\mathbb{N}}$ is *not determinate.*

$k=4$ We have

$$s_n^{(4)} = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} x^{4n} e^{-x^2} dx = \frac{2}{\sqrt{\pi}} \int_0^{+\infty} x^{4n} e^{-x^2} dx = \frac{1}{2\sqrt{\pi}} \int_0^{+\infty} y^n \frac{e^{-y^{\frac{1}{2}}}}{y^{\frac{3}{4}}} dy =: \int_{\mathbb{R}} y^n f(y) dy \,.$$

Once again Krein's condition is satisfied:

$$\int_{\mathbb{R}} \frac{\log f(x)}{1+x^2} dx = -\int_0^{+\infty} \frac{\log(2\sqrt{\pi})}{1+x^2} dx - \int_0^{+\infty} \frac{x^{\frac{1}{2}}}{1+x^2} dx - \frac{3}{4} \int_0^{+\infty} \frac{\log x}{1+x^2} dx > -\infty \,.$$

The moment problem associated with $\{s_n^{(4)}\}_{n\in\mathbb{N}}$ is therefore *not determinate.*

The case $k=4$ provides a counter-example to the converse of Theorem 9 in elementary QM. In fact, there are many measures $\mu_\omega^{(Q^4)}$ associated to the pair $(\pi_\omega(Q^4), \omega)$ because the moment problem is indeterminate, but every $\pi_{\omega_B}(Q^4) = \pi_\omega(Q^4)$ is essentially selfadjoint.
All the found results can be recast for P^n by exploiting the unitary map (Fourier transform) that transforms $\pi_\omega(Q)$ to $\pi_\omega(P)$ and $\pi_\omega(P)$ to $-\pi_\omega(Q)$ leaving ψ_0 invariant.

(2) Taking advantage of the results presented in [27], let us consider again the $*$-algebra of bosonic fields as in item (2) of example 1 whose $*$-algebra is $\mathfrak{A}[M,g]$ and the generators (field operators smeared with real smooth solutions of the KG equation with compactly supported Cauchy data) are denoted by $\Phi[\varphi]$. A particularly relevant class of states $\omega : \mathfrak{A}[M,g] \to \mathbb{C}$ is the one of *Gaussian* ones (also known as *quasifree*, see e.g., [13, 27, 4]). If ω is Gaussian [14], then there is a $\mathbb{R}$-linear map $K\colon Sol[M,g] \to \mathsf{H}_\omega^{(1)}$, where $\mathsf{H}_\omega^{(1)}$ is a Hilbert space called *one-particle space*, with the following properties:

(a) $K(Sol[M,g]) + iK(Sol[M,g])$ is dense in $\mathsf{H}_\omega^{(1)}$;

(b) for all $\varphi, \tilde\varphi \in Sol[M,g]$ it holds $\langle K\varphi, K\tilde\varphi\rangle = \omega(\Phi[\varphi]\Phi[\tilde\varphi])$;

(c) for all $\varphi, \tilde\varphi \in Sol[M,g]$ it holds $Im\langle K\varphi, K\tilde\varphi\rangle = -\frac{1}{2}\sigma(\varphi,\tilde\varphi)$.

Moreover the pair $(K, \mathsf{H}_\omega^{(1)})$ is unique up to unitary transformations and it determines the GNS structure of ω as we are going to illustrate. From now on, $\mathcal{F}_+(\mathsf{H}_\omega^{(1)})$ is the *bosonic Fock space* relying upon the *one-particle subspace* $\mathsf{H}_\omega^{(1)}$ and $\mathsf{H}_\omega^{(n)} \subset \mathcal{F}_+(\mathsf{H}_\omega^{(1)})$ is the subspace made of all symmetrized products of $n = 1, 2, \ldots$ factors in $\mathsf{H}_\omega^{(1)}$. Furthermore a_x and $a_x^+ \subset (a_x^+)^\dagger$, with $x \in \mathsf{H}_\omega^{(1)}$, are standard *bosonic annihilation* and *creation operators* defined on the dense invariant subspace $\mathcal{N}_\omega$ given by the finite span of ψ_ω and all spaces $\mathsf{H}_\omega^{(n)}$. They satisfy,

$$[a_x, a_y^+] = \langle x|y\rangle I, \quad [a_x, a_y] = [a_x^+, a_y^+] = 0, \quad \text{and } a_x\psi_\omega = 0, \tag{25}$$

where $\langle\cdot|\cdot\rangle$ is the inner product in $\mathsf{H}_\omega^{(1)}$. The GNS structure of ω is as follows.

(i) $\mathsf{H}_\omega = \mathcal{F}_+(\mathsf{H}_\omega^{(1)})$.

(ii) The representation π_ω has the explicit form[6] (to compare with (18))

$$\pi_\omega(\Phi[\varphi]) = \left(a_{K\varphi} + a_{K\varphi}^+\right)|_{\mathcal{D}_\omega}\,, \tag{26}$$

where $\mathcal{D}_\omega$ is defined below.

(iii) $\mathcal{D}_\omega \subset \mathcal{N}_\omega$ is the span of the vectors constructed by applying the operators $a_{K\varphi}^+$, with $\varphi \in Sol[M,g]$, to the GNS cyclic vector ψ_ω a finite but arbitrarily large number of times.

(iv) ψ_ω coincides with the vacuum state vector of $\mathcal{F}_+(\mathsf{H}_\omega^{(1)})$.

An estimate similar to (19) holds true [24, Proof of Theorem X.41, p.210][7]

$$||a_x\psi||\,, ||a_x^+\psi|| \le \sqrt{(n+1)}||x||||\psi||\,, \qquad x \in \mathsf{H}_\omega^{(1)}\,, \psi \in \mathsf{H}_\omega^{(n)}\,, n = 0, 1, \ldots\,, \tag{27}$$

and also, for $\varphi \in Sol[M,g]$ and $n = 0, 1, \ldots\,,\ k = 1, 2, \ldots$,

$$||\pi_\omega((2^{-1/2}\Phi[\varphi])^k)\psi|| \le ||K\varphi||^k 2^{k/2}\sqrt{(n+k)!}||\psi||\,, \qquad \psi \in \mathsf{H}_\omega^{(n)} \cap \mathcal{D}_\omega, \tag{28}$$

[6] The creation and annihilation operators $a, a^\dagger$ appearing in Eq.(3.2.28) in [27] are our $-ia_{K\varphi}$ and $ia_{K\varphi}^+$.

[7] The field operators $\Phi_S(f)$ used there correspond to our $2^{-1/2}\pi_\omega(\Phi[\varphi])$.

as a consequence of (26).
Let us pass to discuss the GNS quadruple of deformations ω_b with the hypothesis that ω is pure. It turns out that ω is *pure if and only if* $K(Sol[M,g])$ alone is dense in $\mathsf{H}^{(1)}$ [13]. In that case, if $\varphi \in Sol[M,g]$, there must be a sequence $\varphi_n \in Sol[M,g]$ such that $K\varphi_n \to iK\varphi$ for $n \to +\infty$. Since a_x and a_x^+ are respectively antilinear and linear in their arguments $x \in \mathsf{H}_\omega^{(1)}$, we have from (26) and (27),

$$a_{K\varphi}\psi = \lim_{n\to+\infty} \frac{1}{2}\left(\pi_\omega(\Phi[\varphi]) + i\pi_\omega(\Phi[\varphi_n])\right)\psi \quad \text{and} \quad a^+_{K\varphi}\psi = \lim_{n\to+\infty} \frac{1}{2}\left(\Phi[\varphi]) - i\pi_\omega(\Phi[\varphi_n])\right)\psi$$

for every given $\psi \in \mathcal{D}_\omega$. Using these identities and taking estimates (27) into account for passing from iterated limits in n to single limits in n, one sees that $\pi_\omega(\mathfrak{A}[M,g])\pi_\omega(b)\psi_\omega$ is dense in H_ω for every given $b \in \mathfrak{A}[M,g]$ such that $\omega(b^*b) \neq 0$. We conclude that, if ω is pure, the GNS structure of the (non-singular) deformation ω_b is

$$\mathcal{D}_{\omega_b} = \pi_\omega(\mathfrak{A}(M,g))\pi_\omega(b)\psi_\omega\,, \quad \mathsf{H}_{\omega_b} = \mathsf{H}_\omega = \mathcal{F}_+(\mathsf{H}_\omega^{(1)})\,, \quad \pi_{\omega_b} = \pi_\omega|_{\mathcal{D}_{\omega_b}}\,, \quad \psi_{\omega_b} = \pi_\omega(b)\psi_\omega.$$

In particular $\mathcal{D}_{\omega_b} \subset \mathcal{D}_\omega$. There are however special physically important cases where $\mathcal{D}_{\omega_b} = \mathcal{D}_\omega$ so that all the discussion about the CCR algebra of X and P in the previous example, including the counterexamples, can be completely recast in this QFT context. The form above of the GNS quadruple of ω_b implies that $\mathcal{D}_{\omega_b} = \mathcal{D}_\omega$ is equivalent to $\psi_\omega \in \mathcal{D}_{\omega_b}$. A sufficient condition for $\psi_\omega \in \mathcal{D}_{\omega_b}$ is that,

$$\text{for every } \varphi \in Sol[M,g] \text{ there is } \varphi' \in Sol[M,g] \text{ such that } K\varphi' = iK\varphi\,. \tag{29}$$

This requirement implies in particular that the state ω is pure and also promotes $a_{K\varphi}$ and $a^+_{K\varphi}$ to elements and generators of the algebra $\mathfrak{A}[M,g]$ as in the case of the CCR of X and P. Everything is established in lemma 44 in appendix A.3. When (29) is valid, the GNS structure of the (non-singular) deformation ω_b is therefore again

$$\mathcal{D}_{\omega_b} = \mathcal{D}_\omega\,, \quad \mathsf{H}_{\omega_b} = \mathsf{H}_\omega = \mathcal{F}_+(\mathsf{H}_\omega^{(1)})\,, \quad \pi_{\omega_b} = \pi_\omega\,, \quad \psi_{\omega_b} = \pi_\omega(b)\psi_\omega. \tag{30}$$

The validity of (29) is in particular guaranteed if (M,g) is the standard *four dimensional Minkowski spacetime* and ω is the (pure) *Poincaré invariant Gaussian vacuum state* for the Klein-Gordon quantum field with *strictly positive* mass $m > 0$. Here, the Klein-Gordon operator reads $P = -\frac{\partial^2}{\partial t^2} + \Delta - m^2$ where Δ is the standard spatial Laplacian in $\mathbb{R}^3$ and we are using a given Minkowskian coordinate system $(t,\mathbf{x}) \in \mathbb{R}\times\mathbb{R}^3$ whose $t = 0$ surface is the preferred Cauchy surface Σ we will henceforth use. In this case, the general Fock-space structure of the GNS representation of ω declared in (a)-(c), (i)-(iv) is valid also redefining the space $Sol[M,g]$ as the space of real smooth solutions of KG equation with Cauchy data (in particular on Σ) which belongs to $\mathscr{S}(\mathbb{R}^3)_\mathbb{R}$ (the real space of real-valued Schwartz functions on $\mathbb{R}^3$). It turns out that $\mathsf{H}_\omega^{(1)} = L^2(\mathbb{R}^3, d\mathbf{k})$ and

$$(K\varphi)(\mathbf{k}) = \frac{1}{\sqrt{2}(\mathbf{k}^2+m^2)^{1/4}} \int_{\mathbb{R}^3} \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} \left(\sqrt{-\Delta+m^2}\varphi(0,\mathbf{x}) + i\partial_t\varphi(0,\mathbf{x})\right) d\mathbf{x}\,, \quad \varphi \in Sol[M,g]\,.$$

The crucial observation is that, if $\varphi(0,\cdot), \partial_t\varphi(0,\cdot) \in \mathscr{S}(\mathbb{R}^3)_\mathbb{R}$ then

$$f := -(-\Delta+m^2)^{-1/2}\partial_t\varphi(0,\cdot)\,, \quad p := (-\Delta+m^2)^{1/2}\varphi(0,\cdot)$$

still satisfy $f, p \in \mathscr{S}(\mathbb{R}^3)_{\mathbb{R}}$ so that there is a unique $\varphi' \in Sol[M,g]$ with Cauchy conditions $\varphi'(0,\cdot) = f$ and $\partial_t\varphi'(0,\cdot) = p$ and due to the above expression for K, φ' satisfies (29).

In summary, for a state $\omega : \mathfrak{A}[M,g] \to \mathbb{C}$, we finally have the following results analogous to the ones in the quantum mechanical case of (1) example 11 and established with an essentially identical procedure [8].

(a) $\pi_\omega(\Phi[\varphi]^k)$ are essentially selfadjoint for $k = 1,2$ since the vectors in $\mathsf{H}_\omega^{(n)} \cap \mathcal{D}_\omega$ for all n, whose span is dense in H_ω, are analytic vectors for $k = 1,2$ for those symmetric operators. This is consequence of the inequality arising from (28), for $n = 0, 1, \dots, m, k = 1, 2, \dots$

$$||\pi_\omega(((2^{-1/2}\Phi[\varphi])^k)^m\psi|| \leq (2||K\varphi||^2)^{mk/2}\sqrt{(n+mk)!}||\psi||\,, \quad \psi \in \mathsf{H}_\omega^{(n)} \cap \mathcal{D}_\omega, \tag{31}$$

(a1) When assuming (29), the result in (a) extends to $\pi_{\omega_b}(\Phi[\varphi]^k)$, for every $b \in \mathfrak{A}[M,g]$, just in view of the the GNS structure (30), by noticing that $\pi_{\omega_b}(\Phi[\varphi]^k) = \pi_\omega(\Phi[\varphi]^k)$, $\mathsf{H}_{\omega_b} = \mathsf{H}_\omega$ and $\mathsf{H}_\omega^{(n)} \cap \mathcal{D}_\omega = \mathsf{H}_\omega^{(n)} \cap \mathcal{D}_{\omega_b}$.

(b) $\pi_\omega(\Phi[\varphi]^4)$ is essentially selfadjoint because $\pi_\omega(\Phi[\varphi]^4)$ is bounded below – still using (31) – while the vectors in $\cup_n(\mathsf{H}_\omega^{(n)} \cap \mathcal{D}_\omega) = \cup_n(\mathsf{H}_\omega^{(n)} \cap \mathcal{D}_{\omega_b})$ are semi-analytic vectors for $\pi_\omega(\Phi[\varphi]^4)$ and their span is dense in H_ω.

(b1) When assuming (29), the result in (b) extends to $\pi_{\omega_b}(\Phi[\varphi]^4)$,for every $b \in \mathfrak{A}[M,g]$, just in view of the the GNS structure (30), by noticing that $\pi_{\omega_b}(\Phi[\varphi]^4) = \pi_\omega(\Phi[\varphi]^4)$, $\mathsf{H}_{\omega_b} = \mathsf{H}_\omega$ and $\mathsf{H}_\omega^{(n)} \cap \mathcal{D}_\omega = \mathsf{H}_\omega^{(n)} \cap \mathcal{D}_{\omega_b}$.

Concerning the moment problem of $\pi_\omega(\Phi[\varphi]^k)$ with $K\varphi \neq 0$, the sequence of moments

$$s_n^{(k)} := \omega((2^{-1/2}\Phi[\varphi])^{kn}) = \frac{1}{2^{kn/2}}\left\langle \psi_\omega \left| (a_{K\varphi} + a_{K\varphi}^+)^{kn}\, \psi_\omega \right.\right\rangle\,, \tag{32}$$

is identical to the analogous sequence (23) of $\pi_\omega(Q^k)$ discussed in the previous example just because (21) and (25) are formally identical (for $||K\varphi|| = 1$ otherwise it is sufficient to normalize φ accordingly) and the moments are just computed using only them as is evident if comparing (23) and (32). Therefore, for $k = 1,2$ the problem is determinate, whereas it is not determinate for $k = 3,4$.
Assuming (29), thus in Minkowski spacetime in particular, $k = 4$ provides counter-examples to the converse of Theorem 9 in elementary QFT: there are many measures $\mu_\omega^{(\Phi[\varphi]^4)}$ associated to the pair $(\Phi[\varphi]^4, \omega)$ because the moment problem is indeterminate, but every $\pi_{\omega_b}(\Phi[\varphi]^4) = \pi_\omega(\Phi[\varphi]^4)$ is essentially selfadjoint. ■

[8] Condition (29) has been verified for the algebra $\mathfrak{A}[M,g]$ when (M,g) is 4D Minkowski spacetime and the generators $\Phi[\varphi]$ are smeared with real test Schwartz functions serving as Cauchy data. This is a very special case which is suitable in Minkowski spacetime especially because therein the Cauchy surfaces can be chosen as submanifolds isometrically isomorphic to $\mathbb{R}^3$. However, we expect that the conclusions (a1), (b1) hold true also for the algebra $\mathfrak{A}(M,g)$ (i.e., field operators smeared with Cauchy data in $C_c^\infty(\mathbb{R}^3)$) as the closure of the π_ω-representation of the generators $\Phi(f) \in \mathfrak{A}(M,g)$ and $\Phi[Ef] \in \mathfrak{A}[M,g]$ coincides, though a rigorous proof of this fact is not presented here. Some standard spacetime-deformation argument would probably allow to prove similar conclusions for a number of pure quasifree states in curved spacetimes too, though we refrain to specify the precise set of states. We are grateful to an anonymous referee for drawing our attention on these issues.

Remark 12: Since $\pi_\omega(Q^4) \geq 0$, we can try to restrict our analysis of existence and uniqueness problem for measures solving the moment problem for the sequence $\{s_n^{(4)}\}_{n\in\mathbb{N}}$ when they are supported in $[0, +\infty)$ rather than in the whole $\mathbb{R}$. This alternate formulation is called *Stieltjes moment problem*. However, if this problem were determinate with unique measure μ, the standard Hamburger problem would be determine as well (but we know that it is not) unless $\mu(\{0\}) \neq 0$ on account of [20, Corollary 8.9]. Since $\overline{\pi_\omega(Q^4)}$ is selfadjoint, that unique μ would also with the measure (10) obtained from the PVM of $\overline{\pi_\omega(Q^4)}$ with $\mathbb{R}$ replaced for $[0, +\infty)$ since also this spectral measure is a solution of the same moment problem over $[0, +\infty)$. On the other hand, $\overline{\pi_\omega(Q^4)}$ has empty point spectrum (it is the multiplicative operator x^4 in $L^2(\mathbb{R}, dx)$), against the assumption $\mu(\{0\}) \neq 0$. Therefore also Stieltjes problem is *not determinate*. A similar comment can be ascribed to $\Phi[\varphi]^4$. ■

Remark 13: Example 11 shows that powers of a quantum field $\Phi(h)^k$ may lead to algebraic observables with a possibly non-determinated moment problem. It would be interesting to see whether a similar result holds for the Wick powers $:\Phi^k:(h)$ of a quantum field and in particular for the stress-energy tensor. Results on the self-adjointness of these observables are already present in the literature [23, 26]. We postpone the discussion of this example to a future investigation. ■

Corollary 35 below can be in a sense interpreted as a weak converse of Theorem 9. However, to see it, a suitable mathematical technology must be introduced.

4 The notion of POVM and its relation with symmetric operators

A *Positive Operator Valued Measure* (POVM for short) is an extension of the notion of *Projection Valued Measure* (PVM). Since PVMs are one-to-one with selfadjoint operators and have the physical meaning of a quantum observable (see, e.g., [15] for a thorough discussion on the subject), POVMs provide a generalization of the notion of quantum observable. Similarly to the fact that PVMs are related with selfadjoint operators, it results that POVMs are connected to merely *symmetric* operators, even if this interplay is more complicated. Since GNS operators $\pi_\omega(a)$ representing Hermitian elements are in general only symmetric, the notion of POVM seems to be relevant in our discussion on Issue A.

We briefly collect below some material on POVMs and generalized extension of symmetric operator – see [1, 5, 7] for a complete discussion.

Remark 14: The complete equivalence between the notion of POVM used in [5, 7] and the older notion of *spectral function* adopted in [1] is discussed and established in Section 4.9 of [5], especially Theorem 4.3 therein. In [5], spectral functions are called *semispectral functions* while normalized POVMs are named *semispectral measures*. ■

4.1 POVM as a generalized observable in a Hilbert space

(Ω, Σ) will henceforth denote a measurable space, where Σ is a σ-algebra on the set Ω. $\mathfrak{B}(\mathsf{H})$ will denote the space of bounded linear operators on the Hilbert space H and $\mathscr{L}(\mathsf{H}) \subset \mathfrak{B}(\mathsf{H})$ is the space of orthogonal projections over H. We start from the following general definition which admits some other equivalent formulations [7] (see Remark 4.4 of [5] in particular, where the second requirement below is alternatively and equivalently stated).

Definition 15: *An operator-valued map $Q\colon \Sigma \to \mathfrak{B}(\mathsf{H})$ is called* **positive-operator valued measure** *(POVM) if it satisfies the following two conditions:*

1. *for all $E \in \Sigma$, $Q(E) \geq 0$;*
2. *for all $\psi, \varphi \in \mathsf{H}$ the map $Q_{\psi,\varphi}\colon \Sigma \ni E \mapsto \langle\psi|Q(E)\varphi\rangle \in \mathbb{C}$ defines a* complex σ-additive measure *according to [25]* [9].

A POVM Q is said to be **normalized** *if $Q(\Omega) = I$.* ■

Remark 16: A normalized POVM is a standard PVM (e.g. see [15, 20]) if and only if $Q(E)Q(F) = Q(E \cap F)$ for $E, F \in \Sigma$, so that $Q(E) \in \mathscr{L}(\mathsf{H})$. ■

Normalized POVMs are physically intepreted and called **generalized observables**, in the Hilbert-space formulation of quantum theory and we henceforth adopt this interpretation and apply it to our context. Since $Q(E) \geq 0$ for every POVM, the map $Q_{\psi,\psi}\colon \Sigma \ni E \mapsto \langle\psi|Q(E)\psi\rangle$ always defines a *finite positive* σ-additive measure for every fixed $\psi \in \mathsf{H}$ which is also a *probability measure* on (Ω, Σ) if Q is normalized and $||\psi|| = 1$. Similarly to what happens for a PVM, the physical interpretation of $\langle\psi|Q(E)\psi\rangle$ is the probability that, measuring the *generalized observable* associated to the normalized POVM when the state is represented by the normalized vector ψ, the outcome belongs to the Borel set $E \subset \mathbb{R}$.

What is lost within this more general framework in comparison with the physical interpretation of PVMs is (a) the logical interpretation of $Q(E)$ as an elementary *YES-NO observable* also known as *test*, (b) the possibility to describe the *post-measurement* state with the standard Lüders-von Neumann reduction postulate exploiting only the POVM (more information must be supplied), (c) the fact that observables $Q(E)$ and $Q(F)$ are necessarily compatible.

There exists an extended literature on these topics and we refer the reader to [5] for a modern also physically minded treatise on the subject. Another difference concerns the one-to-one correspondence between PVM over $\mathbb{R}$ and selfadjoint operators which, in the standard spectral theory, permits to identify PVMs (quantum observables) with selfadjoint operators.

Switching to POVMs, it turns out that there is a more complicated correspondence between normalized POVMs and *symmetric operators* which we will describe shortly. The typical generalized observable which can be described in terms of a POVM is the (arrival) *time observable* of a particle [5]. That observable cannot be described in terms of selfadjoint operators (PVMs) if one insists on the validity of CCR with respect to the energy observable and these no-go results are popularly known as *Pauli's theorem* (see, e.g. [16]).

A celebrated result due to Naimark establishes that POVMs are connected to PVMs through the famous *Naimark's dilation theorem*, which we state for the case of a normalized POVM [1, Thm. Vol II, p.124] (see [7] for the general case).

[9] With reference to [25, Ch. 6] this implies that for all $E \in \mathscr{B}(\Sigma)$ and for all countable partitions $E = \cup_{n\in\mathbb{N}} E_n$, with $E_n \in \mathscr{B}(\Sigma)$ and $E_n \cap E_m = \varnothing$ if $n \neq m$, it holds $Q_{\psi,\varphi}(E) = \sum_{n\in\mathbb{N}} Q_{\psi,\varphi}(E_n)$, where the series is absolutely convergent. In particular, the *total variation* of this measure $|Q_{\psi,\varphi}|$ is a *finite* positive σ-additive measure. Notice that $Q_{\psi,\psi}$ is a finite positive measure.

Theorem 17: [Naimark's dilation theorem] *Let* $Q\colon \Sigma \to \mathfrak{B}(\mathsf{H})$ *be a normalized POVM. Then there exists a Hilbert space* K *which includes* H *as a closed subspace, i.e.* $\mathsf{K} = \mathsf{H} \oplus \mathsf{H}^\perp$*, and a PVM* $P\colon \Sigma \to \mathscr{L}(\mathsf{K})$ *such that*

$$Q(E) = P_{\mathsf{H}} P(E)\restriction_{\mathsf{H}} \qquad \forall E \in \Sigma\,, \tag{33}$$

where $P_{\mathsf{H}} \in \mathscr{L}(\mathsf{K})$ *is the orthogonal projector onto* H*. The triple* $(\mathsf{K}, P_{\mathsf{H}}, P)$ *is called* **Naimark's dilation triple**.

Remark 18: A slightly more general way to state the theorem above, is stating that, for a normalized POVM $Q\colon \Sigma \to \mathfrak{B}(\mathsf{H})$, there exist a Hilbert space K_0 and an isometry $V : \mathsf{K}_0 \to \mathsf{K}$ such that

$$Q(E) = V^\dagger P(E) V \qquad \forall E \in \Sigma\,. \tag{34}$$

In this way, $V^\dagger V = I_{\mathsf{K}_0}$ and $VV^\dagger \in \mathscr{L}(\mathsf{K})$ is the orthogonal projector onto the closed subspace $V(\mathsf{K}_0) \subset \mathsf{K}$. Within this formulation, *Naimark's dilation triple* is defined as (K, V, P). In (33), $\mathsf{K}_0 = \mathsf{H}$ and V is the inclusion map $\mathsf{H} \hookrightarrow \mathsf{K}$, so that $P_{\mathsf{H}} = VV^\dagger$. ■

4.2 Generalized selfadjoint extensions of symmetric operators

POVMs arise naturally when dealing with generalized extensions of *symmetric operators*. As is well known, a selfadjoint operator A in a Hilbert space H does not admit proper symmetric extensions in H. This is just a case of a more general class of symmetric operators.

Definition 19: A symmetric operator A on a Hilbert space H is said to be **maximally symmetric** if there is no symmetric operator B on H such that $B \supsetneq A$. ■

Remark 20:
(1) A maximally symmetric operator is necessarily closed, since the closure of a symmetric operator is symmetric as well.
(2) It turns out that [1, Thm. 3, p.97] *a closed symmetric operator is maximally symmetric (and not selfadjoint) iff one of its deficiency indices is* 0 *(and the other does not vanish).*
(3) An elementary useful result (immediately arising from, e.g. [15, Thm. 5.43]) is that, *if a maximally symmetric operator* A *on* H *satisfies* $CA \subset AC$ *for a conjugation* $C : \mathsf{H} \to \mathsf{H}$*, then* A *is selfadjoint.* ■

Symmetric operators can also admit extensions in a more general fashion and these extensions play a crucial rôle in the connection between symmetric operators and POVMs.

Definition 21: Let A be a symmetric operator on a Hilbert space H. A **generalized symmetric** (resp. **selfadjoint**) **extension** of A is a symmetric (resp. selfadjoint) operator B on a Hilbert space K such that

(i) K contains H as a closed subspace (possibly $\mathsf{K} = \mathsf{H}$),

(ii) $A \subset B$ in K,

(iii) every closed subspace $\mathsf{K}_0 \subset \mathsf{K}$ such that $\{0\} \neq \mathsf{K}_0 \subset \mathsf{H}^\perp$ does not *reduce* B (see Appendix A.1).

■

Every non-selfadjoint symmetric operator (possibly maximally symmetric) always admits generalized selfadjoint extensions as established in Theorem 42. Selfadjoint operators are instead maximal also in respect of this more general sort of extension.

Proposition 22: *A selfadjoint operator does not admit proper generalized symmetric extensions.*

Proof. See Appendix A.3. □

4.3 Decomposition of symmetric operators in terms of POVMs

Naimark extended part of the spectral theory usually formulated in terms of PVMs for normal closed operators (selfadjoint in particular) to the more general case of a symmetric operator [17, 18] where POVMs replace PVMs. A difference with the standard theory is that, unless the symmetric operator is *maximally symmetric*, the POVM which decomposes it is not unique.

Theorem 23: *For a symmetric operator A in the Hilbert space H the following facts hold.*

(a) *There exists a normalized POVM $Q^{(A)}\colon \mathscr{B}(\mathbb{R}) \to \mathfrak{B}(\mathsf{H})$ satisfying*

$$\langle\psi|A\varphi\rangle = \int_{\mathbb{R}} \lambda dQ^{(A)}_{\psi,\varphi}(\lambda)\,, \quad \|A\varphi\|^2 = \int_{\mathbb{R}} \lambda^2 dQ^{(A)}_{\varphi,\varphi}(\lambda)\,, \quad \forall\psi\in\mathsf{H}, \varphi\in D(A)\,, \tag{35}$$

(b) *Every normalized POVM $Q^{(A)}\colon \mathscr{B}(\mathbb{R}) \to \mathfrak{B}(\mathsf{H})$ satisfying (35) is of the form*

$$Q^{(A)}(E) := P_{\mathsf{H}}P(E)\restriction_{\mathsf{H}} \qquad \forall E\in\mathscr{B}(\mathbb{R})\,.$$

for some Naimark's dilation triple $(\mathsf{K}, P_{\mathsf{H}}, P)$ of $Q^{(A)}$ arising from a generalized selfadjoint extension $B = \int_{\mathbb{R}} \lambda dP(\lambda)$ of A in K,

$$A = B\restriction_{D(A)} \quad \text{and} \quad D(A) \subset \{\psi\in\mathsf{H} |\ \lambda \in L^2(\mathbb{R}, Q^{(A)}_{\psi,\psi})\}\,. \tag{36}$$

(c) *A normalized POVM $Q^{(A)}$ satisfying (35) is a PVM if and only if the selfadjoint operator B constructed out of Naimark's dilation triple of $Q^{(A)}$ as in (b) can be chosen as a standard selfadjoint extension of A.*

(d) *If A is closed, a normalized POVM $Q^{(A)}$ as in (35) exists that, referring to (b), also satisfies*

$$A = B\restriction_{D(B)\cap\mathsf{H}} \quad \text{and} \quad D(A) = \{\psi\in\mathsf{H} |\ \lambda \in L^2(\mathbb{R}, Q^{(A)}_{\psi,\psi})\}\,. \tag{37}$$

(e) *If A is closed, then A is maximally symmetric if and only if there is a unique normalized POVM $Q^{(A)}$ as in (35). In this case, (37) is valid for all choices of $(\mathsf{K}, P_{\mathsf{H}}, P)$ generating $Q^{(A)}$ as in (b).*

(f) *If A is selfadjoint, there is a unique normalized POVM $Q^{(A)}$ satisfying (35), and it is a PVM. In this case $\mathsf{K} = \mathsf{H}$, $Q^{(A)} = P$, and $A = B$ for all choices of $(\mathsf{K}, P_{\mathsf{H}}, P)$ generating $Q^{(A)}$ as in (b).*

Proof. See Appendix A.3. □

Corollary 24: *Let A be a symmetric operator in H. Then*

(a) *A and $\overline{A}$ admits the same class of POVMs satisfying (a) of Theorem 23 for A and $\overline{A}$ respectively.*

(b) *A admits a unique normalized POVM as in (a) of Theorem 23 if and only $\overline{A}$ is maximally symmetric. In this case*

$$D(\overline{A}) = \{\psi \in \mathsf{H} |\ \lambda \in L^2(\mathbb{R}, Q^{(A)}_{\psi,\psi})\} .$$

(c) *The unique normalized POVM as in (b) is a PVM if A is also essentially selfadjoint.*

Proof. Every generalized selfadjoint extension of $\overline{A}$ is a generalized extension of A, since $A \subset \overline{A}$. Every generalized selfadjoint extension of A is closed (because selfadjoint) so that it is also a generalized selfadjoint extension of $\overline{A}$. In view of (b) of Theorem 23, A and $\overline{A}$ have the same class of associated POVMs satisfying (a) of that theorem. Therefore A admits a unique POVM if and only if $\overline{A}$ is maximally symmetric as a consequence of (e) and the identity regarding $D(\overline{A})$ is valid in view of (d) of Theorem 23. Finally, this POVM is a PVM if A is also essentially selfadjoint due to (f) Theorem 23. □

Definition 25: If A is a symmetric operator in the Hilbert space H, a normalized POVM $Q^{(A)}$ over the Borel σ-algebra over $\mathbb{R}$ which satisfies (a) of Theorem 23, i.e.

$$\langle\psi|A\varphi\rangle = \int_{\mathbb{R}} \lambda dQ^{(A)}_{\psi,\varphi}(\lambda) , \qquad \|A\varphi\|^2 = \int_{\mathbb{R}} \lambda^2 dQ^{(A)}_{\varphi,\varphi}(\lambda) , \qquad \forall \psi \in \mathsf{H}, \varphi \in D(A) ,$$

is said to be **associated** to A or, equivalently, to **decompose** A. ■

4.4 Hermitian operators as integrals of POVMs

While a symmetric operator admits at least one normalized POVM which decomposes it according to Definition 25, not all normalized POVMs decompose symmetric operators. The main obstruction comes from the second equation in (35) as well as from the difficulty to identify a convenient notion of operator integral with respect to a POVM. This aspect of POVMs has been investigated in [7] (see also [5] for further physical comments) in wide generality. We only state and prove an elementary result which, though it is not explicitly stated in [7], it is however part of the results discussed therein. In particular, every POVM over $\mathbb{R}$ can be weakly integrated determining a *unique* Hermitian operator over a natural domain. It is worth stressing that the result strictly depends on the choice of this domain and different alternatives are possible in principle [5, 7] (see also (1) Remark 27 below).

Theorem 26: *If $Q \colon \mathscr{B}(\mathbb{R}) \to \mathfrak{B}(\mathsf{H})$ is a normalized POVM in the Hilbert space H, define the subset $D(A^{(Q)}) \subset \mathsf{H}$,*

$$D(A^{(Q)}) := \left\{ \psi \in \mathsf{H} \,\middle|\, \int_{\mathbb{R}} \lambda^2 dQ_{\psi,\psi}(\lambda) < +\infty \right\} . \qquad (38)$$

The following facts are valid.

(a) *$D(A^{(Q)})$ is a subspace of H (which is not necessarily dense or non-trivial).*

(b) *There exists a unique operator $A^{(Q)} : D(A^{(Q)}) \to \mathsf{H}$ such that*

$$\langle \varphi | A^{(Q)} \psi \rangle = \int_{\mathbb{R}} \lambda dQ_{\varphi,\psi}(\lambda) \,, \quad \forall \varphi \in \mathsf{H} \,, \forall \psi \in D(A^{(Q)}) \,. \tag{39}$$

(c) *$A^{(Q)}$ is Hermitian, so that $A^{(Q)}$ is symmetric if and only if $D(A^{(Q)})$ is dense.*

(d) *If $(\mathsf{K}, P_{\mathsf{H}}, P)$ is a Naimark's dilation triple of Q, then*

$$A^{(Q)}\psi = P_{\mathsf{H}} \int_{\mathbb{R}} \lambda dP(\lambda)\psi \,, \quad \forall \psi \in D(A^{(Q)}) \,. \tag{40}$$

(e) *If there exists a Naimark's dilation triple $(\mathsf{K}, P_{\mathsf{H}}, P)$ of Q such that*

$$\int_{\mathbb{R}} \lambda dP(\lambda)(D(A^{(Q)})) \subset \mathsf{H} \,, \tag{41}$$

then $A^{(Q)}$ is closed and

$$||A^{(Q)}\psi||^2 = \int_{\mathbb{R}} \lambda^2 dQ_{\psi,\psi}(\lambda) \,, \quad \forall \psi \in D(A^{(Q)}) \,. \tag{42}$$

Proof. See Appendix A.3. □

Remark 27:
(1) Even if $A^{(Q)}$ is symmetric, we cannot say that Q decomposes $A^{(Q)}$ according to Def. 25, because generally (42) fails. However, it is still possible that (42) holds when restricting $A^{(Q)}$ to a subspace $D \subset D(A^{(Q)})$. This is the case if (39) is true for $D(A^{(Q)})$ replaced for D. The operator $A^{(Q)}|_D$ is still Hermitian and satisfies (39) for $\psi \in D$. This is just the situation treated in (a) and (b) of Theorem 23 when identifying $A = A^{(Q^{(A)})}|_{D(A)}$ where $Q^{(A)}$ is a POVM decomposing the symmetric operator A according to (a) Theorem 23. Here $D(A) \subset D(A^{(Q^{(A)})})$ is dense and, in general, $A^{(Q^{(A)})} \supset A$ and (42) is valid on $D(A)$, but not on $D(A^{(Q^{(A)})})$. If A is maximally symmetric, $A = A^{(Q^{(A)})}$ necessarily.
(2) Theorems 23 and 26 can be used to define a function $f(A)$ of a symmetric operator A in H when A itself can be decomposed along the normalized POVM $Q^{(A)}$ according to Definition 25, and $f : \mathbb{R} \to \mathbb{R}$ is Borel measurable. It is simply sufficient to observe that $Q'(E) := Q^{(A)}(f^{-1}(E))$ is still a normalized POVM when E varies in $\mathscr{B}(\mathbb{R})$, so that $f(A)$ can be defined according to definitions (38) and (39) just by integrating Q'. Therefore, from the standard measure theory, it arises

$$\langle \varphi | f(A)\psi \rangle = \int_{\mathbb{R}} \mu \, dQ'_{\varphi,\psi}(\mu) = \int_{\mathbb{R}} f(\lambda) \, dQ^{(A)}_{\varphi,\psi}(\lambda) \quad \text{if } \varphi \in \mathsf{H} \text{ and } \psi \in D(f(A)) \,, \tag{43}$$

$$D(f(A)) = \left\{ \psi \in \mathsf{H} \,\middle|\, \int_{\mathbb{R}} \mu^2 dQ'_{\psi,\psi}(\mu) < +\infty \right\} = \left\{ \psi \in \mathsf{H} \,\middle|\, \int_{\mathbb{R}} |f(\lambda)|^2 dQ^{(A)}_{\psi,\psi}(\lambda) < +\infty \right\} . \tag{44}$$

When A is selfadjoint, so that we deal with a PVM, this definition of $f(A)$ coincides to the standard one. It is however necessary to stress that, when Q is properly a POVM,

(a) unless f is bounded (in that case $D(f(A)) = \mathsf{H}$), there is no guarantee that the Hermitian operator $f(A)$ has a dense domain nor that $||f(A)\psi||^2 = \int_{\mathbb{R}} |f(\lambda)|^2 dQ^{(A)}_{\psi,\psi}(\lambda)$ for $\psi \in D(f(A))$ as observed in Remark (1)[10],

(b) $f(A)$ does not satisfy the same properties as those of the standard functional calculus of selfadjoint operators , just because the fundamental property of PVMs $Q(E)Q(E') = Q(E \cap E')$ is false for POVMs,

(c) the notion of $f(A)$ also depends on the normalized POVM $Q^{(A)}$ exploited to decompose A, since $Q^{(A)}$ is unique if and only if A is maximally symmetric. ■

5 Observable interpretation of $\pi_\omega(a)$ in terms of POVMs and expectation-value interpretation of $\omega(a)$

We are in a position to apply the developed theory to tackle the initial problems stated in issues A and B establishing the main results of this work.

5.1 Interpretation of $\pi_\omega(a)$ in terms of POVMs

Coming back to symmetric operators arising from GNS representations, the summarized theory of POVMs and Corollary 24 in particular have some important consequences concerning a possible interpretation of $\pi_\omega(a)$ as a generalized observable when it is not essentially selfadjoint. Consider the symmetric operator $\pi_\omega(a)$ when $a^* = a \in \mathfrak{A}$ and $\omega : \mathfrak{A} \to \mathbb{C}$ is a non-normalized state on the unital $*$-algebra $\mathfrak{A}$. We have that

(1) $\pi_\omega(a)$ and $\overline{\pi_\omega(a)}$ share the same class of associated normalized POVMs $Q^{(a,\omega)}$ so that they support the same physical information when interpreting them as generalized observables. More precisely, each of these POVMs endows those symmetric operators with the physical meaning of generalized observable in the Hilbert space H_ω. This is particularly relevant when $\pi_\omega(a)$ does not admit selfadjoint extensions;

(2) the above class of normalized POVMs however includes also all possible PVMs of all possible selfadjoint extensions of $\pi_\omega(a)$ provided they exist. Hence, the standard notion of quantum observable in Hilbert space is encompassed;

(3) $Q^{(a,\omega)}$ is unique if and only if $\overline{\pi_\omega(a)}$ is maximally symmetric but not necessarily selfadjoint;

(4) That unique POVM is a PVM if $\pi_\omega(a)$ is essentially selfadjoint.

Even if the symmetric operator $\pi_\omega(a)$ does *not* admit a selfadjoint extension, it can be considered a generalized observable with some precautions, since it admits decompositions in terms of POVMs which are *generalized observables* in their own right. However, in general, there are *many* POVMs associated with *one* given symmetric operator $\pi_\omega(a)$. Next section tackles the problem of reducing this number in relation with the expectation-value interpretation of $\omega_b(a)$.

[10] In particular, if $f : \mathbb{R} \ni \lambda \to \lambda \in \mathbb{R}$, we have $A = f(A)\restriction_{D(A)}$, but the domain of $f(A)$ according to (38) is in general larger than $D(A)$, and $||f(A)\psi||^2 = \int_{\mathbb{R}} |f(\lambda)|^2 dQ^{(A)}_{\psi,\psi}(\lambda)$ is valid for $\psi \in D(A)$.

5.2 *Expectation-value interpretation of $\omega_b(a)$ by means of consistent class of measures solving the moment problem*

Let us now come to the expectation-value interpretation of $\omega(a)$ extended to the deformations $\omega_b(a)$. This inteprentation relies upon the choice of a measure $\mu^{(a)}_\omega$ viewed as a particular case of the large class of measures $\mu^{(a)}_{\omega_b}$ associated to deformed states ω_b. All these measures are assumed to solve the moment problem (15) for (a, ω_b), where the case $n = 1$ is just the expectation-value interpretation of $\omega_b(a)$ and $\omega(a)$ in particular for $b = \mathbb{I}$.

The final discussion in (1) and (2) in Example 11 shows that, in physically relevant cases, there are many measures solving the moment problem relative to (a, ω_b) in general, even if the operator $\pi_\omega(a)$ is essentially selfadjoint. We need some physically meaningful strategy to reduce the number of those measures.

This section proves that, once we have imposed suitable physically meaningful requirements on the measures $\mu^{(a)}_{\omega_b}$, a new connection arises between the remaining classes of physically meaningful measures and POVMs decomposing the symmetric operators $\pi_{\omega_b}(a)$. These POVMs also generate the said measures $\mu^{(a)}_{\omega_b}$.

We start by noticing that when b is a function of the Hermitian element $a \in \mathfrak{A}$, the measures $\mu^{(a)}_{\omega_b}$ and $\mu^{(a)}_\omega$ are not independent, in particular it holds

$$\int_{\mathbb{R}} \lambda^{2k+1} d\mu^{(a)}_\omega(\lambda) = \omega(a^{2k+1}) = \omega_{a^k}(a) = \int_{\mathbb{R}} \lambda \, d\mu^{(a)}_{\omega_{a^k}}(\lambda) \,.$$

However, referring only to the subalgebra generated by a, we miss the information of the whole algebra $\mathfrak{A}$ which contains a. We therefore try to restrict the class of the measures $\mu^{(a)}_{\omega_b}$ by imposing some natural compatibility conditions among the measures $\mu^{(a)}_{\omega_b}$ associated with *completely general* elements $b \in \mathfrak{A}$. As a starting point, let us consider a family of measures $\{\mu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ each of which is a solution to the moment problem (15) relative to (a, ω_b), with $\mu^{(a)}_{\omega_b} = 0$ if ω_b is singular. Since for all $b, c \in \mathfrak{A}$, $z \in \mathbb{C}$, and every real polynomial p,

$$\begin{aligned} \omega_{b+c}(p(a)) + \omega_{b-c}(p(a)) &= 2[\omega_b(p(a)) + \omega_c(p(a))] \,. \\ \omega_{zb}(p(a)) &= |z|^2 \omega_b(p(a)) \,, \end{aligned} \tag{45}$$

we also have

$$\int_{\mathbb{R}} p(\lambda) d\mu^{(a)}_{\omega_{b+c}}(\lambda) + \int_{\mathbb{R}} p(\lambda) d\mu^{(a)}_{\omega_{b-c}}(\lambda) = 2\left[\int_{\mathbb{R}} p(\lambda) d\mu^{(a)}_{\omega_b}(\lambda) + \int_{\mathbb{R}} p(\lambda) d\mu^{(a)}_{\omega_c}(\lambda) \right] . \tag{46}$$

$$\int_{\mathbb{R}} p(\lambda) d\mu^{(a)}_{\omega_{zb}}(\lambda) = |z|^2 \int_{\mathbb{R}} p(\lambda) d\mu^{(a)}_{\omega_b}(\lambda) \,, \tag{47}$$

Finally observe that the following directional continuity property holds true for $b, c, a = a^* \in \mathfrak{A}$, and every real polynomial p,

$$\omega_{b+tc}(p(a)) \to \omega_b(p(a)) \quad \text{for } \mathbb{R} \ni t \to 0 \,,$$

that implies

$$\int_{\mathbb{R}} p(\lambda) d\mu^{(a)}_{\omega_{b+tc}}(\lambda) \to \int_{\mathbb{R}} p(\lambda) d\mu^{(a)}_{\omega_b}(\lambda) \quad \text{for } \mathbb{R} \ni t \to 0 \,. \tag{48}$$

Identities (46)-(48) are true for every choice of measures associated with the algebraic observable a and the deformations ω_b, so that they *cannot* be used as contraints to reduce the number of those measures.

We observe that the above relations actually regard *polynomials* $p(a)$ of a. From the physical side, dealing only with polynomials seems a limitation since we expect that, at the end of the game, after having introduced some technical information, one would be able to define more complicated functions of a (as it happens when dealing with C^*-algebras), because these observables are physically necessary and have a straightforward operational definition: $f(a)$ *heuristically represents the algebraic observable (if any) that attains the values* $f(\lambda)$*, where* λ *are the values attained by* a. If $\mu^{(a)}_{\omega_b}$ is physically meaningful and $f : \mathbb{R} \to \mathbb{R}$ is a bounded measurable function (we restrict ourselves to bounded functions to avoid subtleties with domains), we expect that the (unknown) algebraic observable $f(a)$ is however represented by the function $f(\lambda)$ in the space $L^2(\mathbb{R}, d\mu^{(a)}_{\omega_b})$ and, as far as expectation values are concerned, $\omega_b(f(a)) = \int_{\mathbb{R}} f(\lambda)\, d\mu^{(a)}_{\omega_b}(\lambda)$.

This viewpoint can be also heuristically supported from another side. If we deal with $\pi_{\omega_b}(a)$ instead of a itself and we decompose the symmetric operator $\pi_{\omega_b}(a)$ with a POVM, the function $f(\pi_{\omega_b}(a))$ can be defined according to (2) Remark 27. If we now assume that $\mu^{(a)}_{\omega_b} = Q^{(\pi_{\omega_b}(a))}_{\psi_{\omega_b},\psi_{\omega_b}}$ we just have that the algebraic observable $f(a)$ is represented by the function $f(\lambda)$ when we compute the expectation values: according to (43) for $\varphi = \psi = \psi_{\omega_b}$, we have $\omega_b(f(a)) = \langle\psi_{\omega_b}|\pi_{\omega_b}(f(a))\psi_{\omega_b}\rangle = \int_{\mathbb{R}} f(\lambda)\, d\mu^{(a)}_{\omega_b}(\lambda)$.

We therefore strengthen equations (46)-(48) *by requiring that the physically interesting measures are such that (46)-(48) are valid for arbitrary bounded measurable functions* $f : \mathbb{R} \to \mathbb{R}$ *in place of polynomials* p.

The resulting condition, just specializing to characteristic functions $f = \chi_E$ for every Borel measurable set E over the real line, leads to the following identities, which imply the previous ones (stated for general bounded measurable functions)

$$\mu^{(a)}_{\omega_{b+c}} + \mu^{(a)}_{\omega_{b-c}} = 2\left[\mu^{(a)}_{\omega_b} + \mu^{(a)}_{\omega_c}\right], \quad \mu^{(a)}_{\omega_{zb}} = |z|^2 \mu^{(a)}_{\omega_b} \tag{49}$$

$$\mu^{(a)}_{\omega_{b+tc}}(E) \to \mu^{(a)}_{\omega_b}(E) \quad \text{if } \mathbb{R} \ni t \to 0, \tag{50}$$

Remark 28: (1) We stress that (49) and (50) are *not* consequences of (46)-(48) in the general case, in particular because polynomials are not necessarily dense in the relevant L^1 spaces, since the considered Borel measures have non-compact support in general and we cannot directly apply Stone-Weierstass theorem. (49) and (50) are however necessarily satisfied when all considered measures $\mu^{(a)}_{\omega_b}$ are induced by a unique PVM as for instance in the strong hypotheses of Theorem 9: (16) immediately implies (49) and (50). This is also the case for a C^*-algebra, since the measures arise from PVMs due to Proposition 6.
(2) Identities (49) and (50) remain valid also when labeling the measures with the classes $[b] \in \mathfrak{A}/G(\mathfrak{A}, \omega) = \mathcal{D}_\omega$ since these only involve the linear structure of $\mathfrak{A}$ which survive the quotient operation. ■

We can state the following general definition, taking remark (2) into account in particular.

Definition 29: If $\mathcal{D}$ is a complex vector space, a family of positive σ-additive measures $\{\nu_\psi\}_{\psi\in\mathcal{D}}$

over the measurable space (Ω, Σ) such that

$$\nu_{\psi+\varphi} + \nu_{\psi-\varphi} = 2\big[\nu_\psi + \nu_\varphi\big]\,, \quad \nu_{z\psi} = |z|^2\nu_\psi \qquad \text{for all } \psi,\varphi \in \mathcal{D} \text{ and } z \in \mathbb{C} \tag{51}$$

$$\nu_{\psi+t\varphi}(E) \to \nu_\psi(E) \quad \text{if } \mathbb{R} \ni t \to 0, \quad \text{for every fixed triple } \psi,\varphi \in \mathcal{D} \text{ and } E \in \Sigma. \tag{52}$$

is said to be **consistent**. ■

Remark 30: From Definition 29, ν_0 is the zero measure ($\nu_0(E) = 0$ if $E \in \Sigma$). ■

5.3 Consistent classes of measures and POVMs

We now apply the summarized theory of POVMs to prove that the family of POVMs associated to $\pi_\omega(a)$ is one-to-one with the family of consistent classes of measures solving the moment problem for all ω_b. The proof consists of two steps. Here is the former.

If $Q^{(a,\omega)}$ is a POVM associated to $\pi_\omega(a)$ for $a^* = a \in \mathfrak{A}$ and for a non-normalized state $\omega : \mathfrak{A} \to \mathbb{C}$, let $\nu^{(a)}_{\omega_b}$ be the Borel measure defined by

$$\nu^{(a)}_{\omega_b}(E) := \langle \psi_{\omega_b} | Q^{(a,\omega)}(E) \psi_{\omega_b}\rangle \quad \text{if } E \in \mathscr{B}(\mathbb{R})\,, \tag{53}$$

for every deformation ω_b.

Theorem 31: *Consider the unital $*$-algebra $\mathfrak{A}$, a non-normalized state $\omega : \mathfrak{A} \to \mathbb{C}$, an element $a = a^* \in \mathfrak{A}$ and the family of measures $\{\nu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ defined in (53) with respect to a normalized POVM $Q^{(a,\omega)}$ associated to $\pi_\omega(a)$. Then*

(a) *$\{\nu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ is a consistent family over $\mathcal{D}_\omega = \mathfrak{A}/G(\mathfrak{A},\omega)$.*

(b) *Each $\nu^{(a)}_{\omega_b}$ is a solution of the moment problem (15) relative to (a, ω_b).*

Proof. Let us focus on Theorem 23 for $A := \pi_\omega(a)$ with $D(A) = \mathcal{D}_\omega$ and $\mathsf{H} = \mathsf{H}_\omega$. According to (b), the POVM $Q^{(A)} = Q^{(a,\omega)}$ can be written as $Q^{(A)} = P_{\mathsf{H}} P|_{\mathsf{H}}$ for a PVM P of a selfadjoint operator $B : D(B) \to \mathsf{K}$ defined on a larger Hilbert space K, including H as a closed subspace, such that $A = B{\restriction_{D(A)}}$. Observe that $\pi_\omega(b)\psi_\omega \in \mathcal{D}_\omega = D(\pi_\omega(a^n)) = D(\pi_\omega(a)^n) = D(A^n) \subset D(B^n)$ where, in the last inclusion, we have exploited $A = B{\restriction_{D(A)}}$ and $A(\mathcal{D}_\omega) \subset \mathcal{D}_\omega$. By the standard spectral theory of selfadjoint operators we therefore have ($\psi_{\omega_b} := \pi_\omega(b)\psi_\omega$)

$$\langle \pi_\omega(b)\psi_\omega | B^n \pi_\omega(b)\psi_\omega\rangle = \int_{\mathbb{R}} \lambda^n dP_{\psi_{\omega_b},\psi_{\omega_b}}(\lambda) = \int_{\mathbb{R}} \lambda^n dQ^{(A)}_{\psi_{\omega_b},\psi_{\omega_b}}(\lambda) = \int_{\mathbb{R}} \lambda^n d\nu^{(a)}_{\omega_b}(\lambda)\,,$$

where, in the last passage we have used $Q^{(A)} = P_{\mathsf{H}} P|_{\mathsf{H}}$, $P_{\mathsf{H}}\pi_\omega(b)\psi_\omega = \pi_\omega(b)\psi_\omega$, and (53). On the other hand, per construction, $A^n\pi_\omega(b)\psi_\omega = B^n\pi_\omega(b)\psi_\omega$ and eventually the GNS theorem yields $\omega_b(a^n) = \langle \pi_\omega(b)\psi_\omega | A^n\pi_\omega(b)\psi_\omega\rangle = \langle \pi_\omega(b)\psi_\omega | B^n\pi_\omega(b)\psi_\omega\rangle$. In summary, if $n = 0, 1, 2\ldots$ and $b \in \mathfrak{A}$,

$$\omega_b(a^n) = \int_{\mathbb{R}} \lambda^n dQ^{(A)}_{\psi_{\omega_b},\psi_{\omega_b}}(\lambda)\,.$$

We have established that each measure (53) is a solution of the moment problem relative to (a, ω_b). By direct inspection, one immediately sees that $\{\nu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ defined as in (53) satisfies Definition 29. □

The result is reversed with the help of the following abstract technical proposition.

Proposition 32: *Let X be a complex vector space and $p : X \to [0, +\infty)$ such that*

(i) $p(\lambda x) = |\lambda| p(x)$ *for every pair* $x \in X$ *and* $\lambda \in \mathbb{C}$,

(ii) $p(x+y)^2 + p(x-y)^2 = 2[p(x)^2 + p(y)^2]$ *for every pair* $x, y \in X$,

(iii) $p(x+ty) \to p(x)$ *for* $\mathbb{R} \ni t \to 0^+$ *and every fixed pair* $x, y \in X$.

Under these hypotheses,

(a) *p is a seminorm on X,*

(b) *there is a unique positive semi definite Hermitian scalar product $X \times X \ni (x, y) \mapsto (x|y)_p \in \mathbb{C}$ such that $p(x) = \sqrt{(x|x)_p}$ for all $x \in X$,*

(c) *the scalar product in (b) satisfies*

$$(x|y)_p = \frac{1}{4}\sum_{k=0}^{3}(-i)^k p(x + i^k y)^2 \qquad \text{for } x, y \in X. \tag{54}$$

Proof. See Appendix A.3 □

We can now establish another main result of the work, which is the converse of Theorem 31. Together with the afore-mentioned theorem, it proves that for $a^* = a \in \mathfrak{A}$ and a non-normalized state $\omega : \mathfrak{A} \to \mathbb{C}$, the family of normalized POVMs associated with the given symmetric operator $\pi_\omega(a)$ is one-to-one with the family of consistent classes of measures of all $\omega_b(a)$ which solve the moment problem for all deformations ω_b, when $b \in \mathfrak{A}$.

Theorem 33: *Consider the unital $*$-algebra $\mathfrak{A}$, a non-normalized state $\omega : \mathfrak{A} \to \mathbb{C}$, $a = a^* \in \mathfrak{A}$, and a consistent class of measures $\{\mu^{(a)}_{\omega_b}\}_{b \in \mathfrak{A}}$ solutions of the moment problem relative to the pairs (a, ω_b) for $b \in \mathfrak{A}$. Then*

(a) *There is a unique normalized POVM $Q^{(a,\omega)} : \mathscr{B}(\mathbb{R}) \to \mathcal{B}(\mathsf{H}_\omega)$ such that, if $b \in \mathfrak{A}$,*

$$\mu^{(a)}_{\omega_b}(E) = \langle \psi_{\omega_b} | Q^{(a,\omega)}(E) \psi_{\omega_b} \rangle \qquad \forall E \in \mathscr{B}(\mathbb{R}), \tag{55}$$

(b) *$Q^{(a,\omega)}$ decomposes $\pi_\omega(a)$ according to Definition 25 so that, in particular,*

$$\mathcal{D}_\omega = D(\pi_\omega(a)) \subset \left\{ \psi \in \mathsf{H}_\omega \;\middle|\; \int_{\mathbb{R}} \lambda^2 dQ^{(a,\omega)}_{\psi,\psi}(\lambda) < +\infty \right\}. \tag{56}$$

(c) *$Q^{(a,\omega)}$ decomposing $\pi_\omega(a)$ is unique if and only if $\overline{\pi_\omega(a)}$ is maximally symmetric. In this case*

$$D(\overline{\pi_\omega(a)}) = \left\{ \psi \in \mathsf{H}_\omega \;\middle|\; \int_{\mathbb{R}} \lambda^2 dQ^{(a,\omega)}_{\psi,\psi}(\lambda) < +\infty \right\} \tag{57}$$

and that unique $Q^{(a,\omega)}$ is a PVM if and only if $\overline{\pi_\omega(a)}$ is selfadjoint. In that case $Q^{(a,\omega)}$ coincides with the PVM of $\overline{\pi_\omega(a)}$.

(d) *Let us define*

$$Q^{(a,\omega_b)}(E) := P_{\omega_b} Q^{(a,\omega)}(E)\restriction_{\mathsf{H}_{\omega_b}}, \tag{58}$$

where $P_{\omega_b} : \mathsf{H}_\omega \to \mathsf{H}_\omega$ is the orthogonal projector onto H_{ω_b}. It turns out that, for $b \in \mathfrak{A}$, *(i)* $Q^{(a,\omega_b)}$ *is a normalized POVM in* H_{ω_b}.

(ii) It holds

$$\langle\psi_{\omega_b}|Q^{(a,\omega_b)}(E)\psi_{\omega_b}\rangle = \mu^{(a)}_{\omega_b}(E) \qquad \forall E\in\mathscr{B}(\mathbb{R})\,, \tag{59}$$

(iii) $Q^{(a,\omega_b)}$ *decomposes* $\pi_{\omega_b}(a)$ *in the sense of Definition 25.*

Proof. (a) It is clear that, if a normalized POVM exists satisfying (55) for all $b\in\mathfrak{A}$, then it is unique. Indeed, taking advantage of the polarization identity, another similar POVM Q would satisfy $\langle\psi_{\omega_b}|(Q(E)-Q^{(a,\omega)}(E))\psi_{\omega_c}\rangle = 0$ for every $\psi_{\omega_b},\psi_{\omega_c}\in\mathcal{D}_\omega$, which is a dense set. Therefore, $(Q(E)-Q^{(a,\omega)}(E))\psi_{\omega_c}=0$ for every $\psi_{\omega_c}\in\mathcal{D}_\omega$. Continuity of $Q(E)-Q^{(a,\omega)}(E)$ yields $Q(E)=Q^{(a,\omega)}(E)$.
Let us prove that a normalized POVM satisfying (55) for all $b\in\mathfrak{A}$ exists. Fix $E\in\mathscr{B}(\mathbb{R})$. Since the positive measures $\nu_{\psi_{\omega_b}} := \mu^{(a)}_{\omega_b}$ satisfy the identities (51) and (52), $\mathcal{D}_\omega\ni\psi\mapsto\sqrt{\nu_\psi(E)}$ fulfills the hypotheses of Proposition 32. Consequently, that function is a seminorm over $\mathcal{D}_\omega$ and there is a unique semidefinite Hermitian scalar product inducing it:

$$(\psi_{\omega_b}|\psi_{\omega_c})_E := \frac{1}{4}\sum_{k=0}^{3}(-i)^k\mu^{(a)}_{\omega_{b+i^kc}}(E)\,. \tag{60}$$

Applying Cauchy-Schwarz inequality, we have

$$|(\psi_{\omega_b}|\psi_{\omega_c})_E|^2 \le \|b\|_E^2\|c\|_E^2 = \mu^{(a)}_{\omega_b}(E)\mu^{(a)}_{\omega_c}(E) \le \mu^{(a)}_{\omega_b}(\mathbb{R})\mu^{(a)}_{\omega_c}(\mathbb{R}) = \omega_b(\mathbb{I})\omega_c(\mathbb{I}) = ||\psi_{\omega_b}||^2_{\mathsf{H}_\omega}\,||\psi_{\omega_c}||^2_{\mathsf{H}_\omega}\,.$$

Exploiting Riesz' theorem, it then follows that $(\,|\,)_E$ continuously extends to $\mathsf{H}_\omega\times\mathsf{H}_\omega$ and moreover there exists a unique selfadjoint positive operator $Q(E)\in\mathfrak{B}(\mathsf{H}_\omega)$ with $0\le Q(E)\le 1$ such that

$$(\psi|\varphi)_E = \langle\psi|Q(E)\varphi\rangle \qquad \forall\psi,\varphi\in\mathsf{H}_\omega\,. \tag{61}$$

The map $Q\colon\mathscr{B}(\mathbb{R})\ni E\mapsto Q(E)\in\mathfrak{B}(\mathsf{H}_\omega)$ is a normalized POVM according to Definition 15 as we go to prove. In fact, $Q(E)\ge 0$ as said above and, since

$$\langle\psi_{\omega_b}|Q(E)\psi_{\omega_c}\rangle = \frac{1}{4}\sum_{k=0}^{3}(-i)^k\mu^{(a)}_{\omega_{b+i^kc}}(E) \qquad \forall\psi_{\omega_b},\psi_{\omega_c}\in\mathcal{D}_\omega\,, \tag{62}$$

the left-hand side is a complex Borel measure over $\mathbb{R}$ since the right-hand side is a complex combination of such measures. Finally, $E=\mathbb{R}$ produces

$$\langle\psi_{\omega_b}|Q(\mathbb{R})\psi_{\omega_c}\rangle = \frac{1}{4}\sum_{k=0}^{3}(-i)^k||\psi_{\omega_b}+i^k\psi_{\omega_c}||^2 = \langle\psi_{\omega_b}|\psi_{\omega_c}\rangle \qquad \forall\psi_{\omega_b},\psi_{\omega_c}\in\mathcal{D}_\omega\,. \tag{63}$$

As $\mathcal{D}_\omega$ is dense in H_ω, it implies $Q(\mathbb{R})=I$ so that the candidate POVM Q is normalised. To conclude the proof of the fact that $Q^{(a,\omega)}:=Q$ is a POVM, it is sufficient to prove that $\mathscr{B}(\mathbb{R})\ni E\mapsto\langle\psi|Q(E)\varphi\rangle\in\mathbb{C}$ is a complex measure no matter we choose $\psi,\phi\in\mathsf{H}_\omega$ (and not only for $\psi,\phi\in\mathcal{D}_\omega$ as we already know). A continuity argument from the case of $\psi,\varphi\in\mathcal{D}_\omega$

proves that the said map is at least additive so that, in particular $\langle\psi|Q(\varnothing)\varphi\rangle = 0$, because $Q(\mathbb{R}) = I$. Let us pass to prove that the considered function is unconditionally σ-additive so that it is a complex measure as wanted. If the sets $E_n \in \mathscr{B}(\mathbb{R})$ when $n \in \mathbb{N}$ satisfy $E_k \cap E_h = \varnothing$ for $h \neq k$, consider the difference

$$\Delta_N := \sum_{n=0}^{N} \langle\psi|Q(E_n)\varphi\rangle - \langle\psi|Q(E)\varphi\rangle$$

where $E := \cup_{n\in\mathbb{N}} E_n$. We want to prove that $\Delta_N \to 0$ for $N \to +\infty$. Δ_N can be decomposed as follows

$$\begin{aligned}\Delta_N = &\sum_{n=0}^{N}\langle\psi - \psi_{\omega_b}|Q(E_n)(\varphi-\psi_{\omega_c})\rangle + \sum_{n=0}^{N}\langle\psi_{\omega_b}|Q(E_n)(\varphi-\psi_{\omega_c})\rangle + \sum_{n=0}^{N}\langle\psi - \psi_{\omega_b}|Q(E_n)\psi_{\omega_c}\rangle \\ &+ \sum_{n=0}^{N}\langle\psi_{\omega_b}|Q(E_n)\psi_{\omega_c}\rangle - \langle\psi_{\omega_b}|Q(E)\psi_{\omega_c}\rangle \\ &- \langle\psi-\psi_{\omega_b}|Q(E)(\varphi-\psi_{\omega_c})\rangle - \langle\psi_{\omega_b}|Q(E)(\varphi-\psi_{\omega_c})\rangle - \langle\psi-\psi_{\omega_b}|Q(E)\psi_{\omega_c}\rangle \,.\end{aligned}$$

Using additivity and defining $F_N := \cup_{n=0}^{N} E_n$, we can re-arrange the found expansion as

$$\begin{aligned}\Delta_N = &\langle\psi - \psi_{\omega_b}|Q(F_N)(\varphi-\psi_{\omega_c})\rangle + \ \langle\psi_{\omega_b}|Q(F_N)(\varphi-\psi_{\omega_c})\rangle + \langle\psi - \psi_{\omega_b}|Q(F_N)\psi_{\omega_c}\rangle \\ &+ \sum_{n=0}^{N}\langle\psi_{\omega_b}|Q(E_n)\psi_{\omega_c}\rangle - \langle\psi_{\omega_b}|Q(E)\psi_{\omega_c}\rangle \\ &- \langle\psi-\psi_{\omega_b}|Q(E)(\varphi-\psi_{\omega_c})\rangle - \langle\psi_{\omega_b}|Q(E)(\varphi-\psi_{\omega_c})\rangle - \langle\psi-\psi_{\omega_b}|Q(E)\psi_{\omega_c}\rangle \,.\end{aligned}$$

Since $||Q(E)||\,, ||Q(F_N)|| \leq ||Q(\mathbb{R})|| = 1$, we have the estimate

$$\begin{aligned}|\Delta_N| \leq\ &2||\psi - \psi_{\omega_b}||||\varphi - \psi_{\omega_c}|| + 2||\psi_{\omega_b}||||\varphi-\psi_{\omega_c}|| + 2||\psi-\psi_{\omega_b}||||\psi_{\omega_c}|| \\ &+ \left|\sum_{n=0}^{N}\langle\psi_{\omega_b}|Q(E_n)\psi_{\omega_c}\rangle - \langle\psi_{\omega_b}|Q(E)\psi_{\omega_c}\rangle\right| \,.\end{aligned}$$

This inequality concludes the proof: given $\psi, \varphi \in \mathsf{H}_\omega$, since $\mathcal{D}_\omega$ is dense, we can fix $\psi_{\omega_b}, \psi_{\omega_c} \in \mathcal{D}_\omega$ such that the sum of the first three addends is bounded by $\epsilon/2$. Finally, exploiting the fact that $\mathscr{B}(\mathbb{R}) \ni E \mapsto \langle\psi_{\omega_b}|Q^{(a)}(E)\psi_{\omega_c}\rangle$ is σ-additive, we can fix N sufficiently large that the last addend is bounded by $\epsilon/2$. So, if $\epsilon > 0$, there is N_ϵ such that $|\Delta_N| < \epsilon$ if $N > N_\epsilon$ as wanted. Notice that the series $\sum_{n=0}^{+\infty}\langle\psi|Q(E_n)\varphi\rangle$ can be re-ordered arbitrarily since we have proved that its sum is $\langle\psi|Q(E)\varphi\rangle$ which does not depend on the order used to label the sets E_n because $E := \cup_{n\in\mathbb{N}} E_n$. The function $\mathscr{B}(\mathbb{R}) \ni B \mapsto \langle\psi|Q(B)\varphi\rangle \in \mathbb{C}$ is *unconditionally* σ-additive as we wanted to prove.
(b) Since the measures $\mu^{(a)}_{\omega_b}$ are solutions of the moment problem for the pairs (a, ω_b), for $k = 0, 1, 2, \ldots$ and $\psi_{\omega_b} \in \mathcal{D}_\omega$, we have

$$\langle\psi_{\omega_b}|\pi_\omega(a)^k\psi_{\omega_b}\rangle = \omega_b(a^k) = \int_{\mathbb{R}} \lambda^k d\mu^{(a)}_{\omega_b}(\lambda) = \int_{\mathbb{R}} \lambda^k dQ^{(a,\omega)}_{\psi_{\omega_b},\psi_{\omega_b}}(\lambda)\,. \tag{64}$$

Choosing $k = 2$ we obtain

$$||\pi_\omega(a)\psi||^2 = \int_{\mathbb{R}} \lambda^2 dQ^{(a,\omega)}_{\psi,\psi}(\lambda) \quad \text{for every } \psi \in D(\pi_\omega(a)) = \mathcal{D}_\omega,$$

which, in particular, also implies (56). It remains to be established the identity

$$\langle \varphi | \pi_\omega(a)\psi \rangle = \int_{\mathbb{R}} \lambda dQ^{(a,\omega)}_{\varphi,\psi}(\lambda) \quad \text{for every } \varphi \in \mathsf{H}_\omega \text{ and } \psi \in D(\pi_\omega(a)) \,. \tag{65}$$

From (64) with $k = 1$ we conclude that, for every $\psi_{\omega_b} \in \mathcal{D}_\omega$,

$$\langle \psi_{\omega_b} | \pi_\omega(a)\psi_{\omega_b} \rangle = \int_{\mathbb{R}} \lambda dQ^{(a,\omega)}_{\psi_{\omega_b},\psi_{\omega_b}}(\lambda) = \langle \psi_{\omega_b} | A\psi_{\omega_b} \rangle \,,$$

where A is the Hermitian operator uniquely constructed out of the POVM $Q^{(a)}$ according to Theorem 26. Notice that the domain of A is $\left\{ \psi \in \mathsf{H}_\omega \;\middle|\; \int_{\mathbb{R}} \lambda^2 dQ^{(a,\omega)}_{\psi,\psi}(\lambda) < +\infty \right\}$ that includes $\mathcal{D}_\omega$ for (56) that we have already proved. Polarization identity applied to both sides of $\langle \psi_{\omega_b} | \pi_\omega(a)\psi_{\omega_b} \rangle = \langle \psi_{\omega_b} | A\psi_{\omega_b} \rangle$ immediately proves that $\langle \varphi | \pi_\omega(a)\psi \rangle = \langle \varphi | A\psi \rangle$ for every pair $\varphi, \psi \in \mathcal{D}_\omega$. Since this space is dense, we conclude that $\pi_\omega(a) = A\restriction_{\mathcal{D}_\omega}$. Identity (65) is therefore valid as an immediate consequence of (b) Theorem 26.
(c) Everything follows from (c), (d), (e), (f) of Theorem 23 and (a) of Corollary 24.
(d) (i) is true per direct inspection. (ii) is consequence of (55) using $\psi_{\omega_b} \in \mathsf{H}_{\omega_b} \subset \mathsf{H}_\omega$. (iii) arises from the fact that $Q^{(a,\omega)}$ decomposes $\pi_\omega(a)$, (58) and (13). □

Remark 34: Item (d) physically states that the POVMs $Q^{(a,\omega_b)}$ are consistent with both the expectation-value interpretation of each $\omega_b(a)$ and the interpretation of every $\overline{\pi_{\omega_b}(a)}$ as generalized observable. We stress that, if $Q^{(a,\omega)}$ is a PVM because, for example, $\overline{\pi_\omega(a)}$ is selfadjoint, it is still possible that $Q^{(a,\omega_b)}$ is merely a POVM and not a PVM. ■

The next result can be considered as a *weaker* version of both Theorem 9 and its converse (the proper converse of Theorem 9 does not exist as we have seen).

Corollary 35: *Let $\mathfrak{A}$ be a unital $*$-algebra, $\omega \colon \mathfrak{A} \to \mathbb{C}$ a non-normalized state and $a = a^* \in \mathfrak{A}$. $\overline{\pi_\omega(a)}$ is maximally symmetric if and only if there exists a unique family of consistent measures $\{\mu^{(a)}_{\omega_b}\}_{b\in\mathfrak{A}}$ solutions of the moment problem (15) relative to the pairs (a, ω_b) for $b \in \mathfrak{A}$.*

Proof. It immediately follows from (c) of Theorem 33, equation (55) and Theorem 23. □

Example 36: Let us come back to the algebra $\mathfrak{B}$ equipped with the non-normalized state ϕ (6) defined in (2) in Example 3. As already observed, the operator $\overline{\pi_\phi(P)}$ is not selfadjoint but it is maximally symmetric so that it admits only one POVM decomposing it and an associated unique consistent family of measures $\mu^{(P)}_{\phi_B}$ solving the moment problem for all deformations ϕ_B, $B \in \mathfrak{B}$. Making use of standard properties of Fourier transform, it is easy to prove that these measures are

$$\mu^{(P)}_{\phi_B}(E) := \int_E \left| \widehat{B\chi}(k) \right|^2 dk \,, \quad E \in \mathscr{B}(\mathbb{R}) \,,$$

where the functions $B\chi$ (for $B \in \mathfrak{B}$) are assumed to be extended to the whole $\mathbb{R}$ as the zero function for $x \leq 0$ determining Schwartz functions and

$$\widehat{f}(k) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ikx} f(x) dx \,,$$

for f in Schwartz space over $\mathbb{R}$, is the standard Fourier transform. At this point, it is easy to check that the unique POVM decomposing $\overline{\pi_\phi(P)}$ is

$$Q^{(\overline{\pi_\phi(P)},\phi)}(E) = P_+ P(E)\restriction_{L^2([0,+\infty),dx)} , \quad E \in \mathscr{B}(\mathbb{R})$$

where $P_+ : L^2(\mathbb{R}, dx) \to L^2(\mathbb{R}, dx)$ is the orthogonal projector onto $L^2([0, +\infty), dx)$ viewed as closed subspace of $L^2(\mathbb{R}, dx)$, and P is the PVM of the standard selfadjoint *momentum operator* in $L^2(\mathbb{R}, dx)$. ■

6 Conclusions and open problems

Before going to the summary we state our overall conclusions:

(a) When dealing with $*$-algebras the notion of algebraic observable – $a = a^* \in \mathfrak{A}$ – and quantum observable – $\pi_\omega(a)$ (essentially) self-adjoint for a given ω – do not necessarily agree as we proved by discussing some simple counterexamples. This raises a problem with the physical interpretation of those algebraic observables which do not produce quantum observables in some GNS representation. This issue does not arise in the C^*-algebraic setting where an algebraic observable always defines quantum observables in every GNS representation. However, the use of $*$-algebras that are not C^*-algebras is in particular mandatory in some important cases as perturbative QFT and the afore-mentioned problem cannot avoided.

(b) The notion of POVM turned out to be of pivotal interest in our investigation. On the one hand it provides a universally recognized notion of generalized observable (as is well known from other areas of quantum physics like quantum information) that can be used in the interpretation of $\pi_\omega(a)$ when it is not essentially selfadjoint for an algebraic observable a. On the other hand, we also proved that POVMs have a nice interplay with the moment problem of the pair (a, ω) and those of the deformations (a, ω_b), $b \in \mathfrak{A}$. The moment problem should be tackled for accepting the popular intepretation of $\omega(a)$ as the expectation value of the algebraic observable a. The moment problem admits a unique (spectral) solution if $\mathfrak{A}$ is a C^*-algebra, but as before, it involves some subtle issues when dealing with $*$-algebras. However, we proved that, for an algebraic observable a in a $*$-algebra $\mathfrak{A}$, if the moment problems of the class of (a, ω_b), $b \in \mathfrak{A}$, admit unique solutions, then $\pi_\omega(a)$ is essentially selfadjoint (quantum observable) and the POVM of $\pi_\omega(a)$ is a PVM. In the general case, the class of POVMs decomposing a given GNS representation $\pi_\omega(a)$ of an algebraic observable a are one-to-one with a class of special, physically meaningful, families of solutions of the moment problems for the pairs (a, ω_b). There is only one such family if and only if $\pi_\omega(a)$ admits a unique POVM, i.e., it is maximally symmetric. From this viewpoint, a maximally symmetric $\pi_\omega(a)$ seems to define a good generalization of a quantum observable.

6.1 Summary

Issue A concerned the fact that an Hermitian element $a^* = a \in \mathfrak{A}$ may be represented in a GNS representation of some non-normalized state ω by means of an operator $\pi_\omega(a)$ which is not essentially selfadjoint and which can or cannot have selfadjoint extensions (see (1) and (2) in Example 3). Stated differently, an algebraic observable does not always define a quantum observables. If $\mathfrak{A}$ is a C^*-algebra, $\pi_\omega(a)$ is always selfadjoint, but there are some cases in physics as QFT where the use of C^*-algebras is not technically convenient. Therefore Issue A must be therefore seriously considered. We have proved, however, that it is always possible to interpret the symmetric operator $\pi_\omega(a)$ as a *generalized observable* just by fixing a normalized POVM associated to it which decomposes the operator $\pi_\omega(a)$ according to Definition 25 into a generalized version of the spectral theorem of selfadjoint operators. The POVM decomposing $\pi_\omega(a)$ is unique if and only if $\overline{\pi_\omega(a)}$ is *maximally symmetric* (Definition 19) and this unique normalized POVM is a PVM when $\pi_\omega(a)$ is essentially selfadjoint. This provides a sufficient condition for an algebraic observable to uniquely define a generalized observable in a given GNS representation. However, in the general case there are many POVMs associated to a given symmetric operator $\pi_\omega(a)$. The reduction of the number of those POVMs is entangled with the next issue.

Issue B regarded the popular expectation-value interpretation of $\omega(a)$. Form an operational point of view in common with the formulation of classical physics, $\mu_\omega^{(a)}$ can be fixed looking for a measure giving rise to the known momenta $\omega(a^n)$, that is solving the moment problem (9). If $\overline{\pi_\omega(a)}$ is selfadjoint, a physically meaningful way (10) to define $\mu_\omega^{(a)}$ uses the PVM of $\overline{\pi_\omega(a)}$. In general, many measures $\mu_\omega^{(a)}$ associated with the class of moments $\omega(a^n)$ as in (9) exist even if $\overline{\pi_\omega(a)}$ does not admit selfadjoint extensions. The physical meaning of these measures is dubious. The number of the measures $\mu_\omega^{(a)}$ is reduced by considering the information provided by other elements $b \in \mathfrak{A}$ in terms of deformed non-normalized states ω_b (Definition 7) and considering $\mu_\omega^{(a)}$ as an element of the class of measures $\mu_{\omega_b}^{(a)}$ solving separately the moment problem for a and each ω_b. These measures are expected to enjoy a list of physically meaningful mutual relations (49)-(50) able to considerably reduce their number. A class of such measures, for a and ω fixed is called *consistent class of measures* (Definition 29). (If $\mathfrak{A}$ is a C^*-algebra, there is exactly one measure $\mu_\omega^{(a)}$ spectrally obtained implementing the expectation value interpretation of $\omega(a)$ and Issue B is harmless.) Theorem 31 established that every normalized POVM decomposing the symmetric operator $\pi_\omega(a)$ defines a unique class of consistent measures $\{\nu_b^{(a)}\}_{b\in\mathfrak{A}}$ in the natural way (53). These measures solve the moment problem for ω_b, thus corroborating the expectation-value interpretation of $\omega_b(a)$ and $\omega(a)$ in particular. When the POVM is a PVM, the standard relation (10) between PVMs and Borel spectral measures is recovered. The result is reversed in Theorem 33, which is the main achievement of this paper: for a Hermitian element $a \in \mathfrak{A}$ and a non-normalized state ω, an associated consistent class of measures $\mu_{\omega_b}^{(a)}$ solving the moment problem for every corresponding deformation ω_b always determines a unique POVM which decomposes the symmetric operator $\pi_\omega(a)$. Also the measures $\mu_{\omega_b}^{(a)}$ arise from POVMs $Q^{(a,\omega_b)}$ (59) which, as expected, decompose the respective generalized observables $\pi_{\omega_b}(a)$. The POVMs $Q^{(a,\omega_b)}$ are all induced by the initial POVM $Q^{(a,\omega)}$ (58). As a complement, Corollary 35 establishes that $\overline{\pi_\omega(a)}$ is maximally symmetric (selfadjoint in particular) if and only if there is only a unique class of consistent measures $\mu_{\omega_b}^{(a)}$ solving the moment problem for every corresponding deformation ω_b. Part of Corollary 35 admits a stronger version established in Theorem 9 which refers to the whole class of measures $\mu_{\omega_b}^{(a)}$ solving the moment problem for every corresponding deformation ω_b without imposing constrains (49)-(50). If $a = a^*$ and ω are fixed and there is exactly one measure solving the moment problem for each deformation ω_b, then $\overline{\pi_\omega(a)}$ is selfadjoint and therefore has the interpretation of a standard observable in the usual Hilbert space formulation of quantum theories. The converse assertion of this very strong result is untenable, as explicitly proved with two counterexamples from elementary QM and elementary QFT (Example 11).

6.2 Open issues

There are at least two important open issues after the results established in this work. One concerns the fact that, when $\pi_\omega(a)$ is only symmetric, its interpretation as generalized observable depends on the choice of the normalized POVM associated to it. This POVM is unique if and only if $\overline{\pi_\omega(a)}$ is maximally symmetric (selfadjoint in particular). It is not clear if the information contained in the triple $\mathfrak{A}$, a, ω permits one to fix this choice or somehow reduce the number of possibilities. The second open issue regards the option of simultaneous measurements of compatible (i.e., pairwise commuting) abstract observables $a_1, \ldots, a_n$ with associated joint measures on $\mathbb{R}^n$ accounting for the expectation-value interpretation. The many-variables moment problem is not a straightforward generalization of the one-variable moment problem [21] and also the notion of joint POVM presents some non-trivial technical difficulties [2]. Already at the level of selfadjoint observables, commutativity of symmetric operators (say $\pi_\omega(a_1)$ and $\pi_\omega(a_2)$) on a dense invariant domain of essential selfadjointness ($\mathcal{D}_\omega$) does not imply the much more physically meaningful commutativity of their respective PVMs (as proved by Nelson [24]) and the existence of a joint PVM. These aspects have been investigated in [3], where a stronger positivity condition for the state ω has been imposed to ensure the existence of self-adjoint extensions for the operators $\pi_\omega(a_1), \ldots, \pi_\omega(a_n)$ whose spectral measures mutually commute. We plan to investigate this issue in the light of our results in a forthcoming publication.

Acknowledgments

The authors thank C. Capoferri, C. Dappiaggi, S. Mazzucchi and N. Pinamonti for useful discussions. We are grateful to C. Fewster for helpful comments and for pointing out to us reference [3] and to the anonymous referees for their the helpful suggestions.

A Appendix

A.1 Reducing subspaces

Definition 37: If $D(T) \subset \mathsf{H}$ is a subspace of the Hilbert space H, let $T : D(T) \to \mathsf{H}$ be an operator and $\mathsf{H}_0 \subset \mathsf{H}$ a closed subspace with $\{0\} \neq \mathsf{H}_0 \neq \mathsf{H}$, P_0 denoting the orthogonal projector onto H_0. In this case, H_0 is said to **reduce** T if both conditions are true

(i) $T(D(T) \cap \mathsf{H}_0) \subset \mathsf{H}_0$ and $T(D(T) \cap \mathsf{H}_0^\perp) \subset \mathsf{H}_0^\perp$,

(ii) $P_0(D(T)) \subset D(T)$,

so that the direct orthogonal decomposition holds

$$D(T) = (D(T) \cap \mathsf{H}_0) \oplus (D(T) \cap \mathsf{H}_0^\perp) \quad \text{and} \quad T = T\restriction_{D(T)\cap\mathsf{H}_0} \oplus T\restriction_{D(T)\cap\mathsf{H}_0^\perp} . \tag{66}$$

The operator $T_0 = T\restriction_{D(T)\cap\mathsf{H}_0}$ is called the **part of T on H_0**. ■

Remark 38:
(1) It is worth stressing that (i) does *not* imply (ii). (A counterexample is given by $\mathsf{H} := L^2([0,+\infty), dx)$, $T := -i\frac{d}{dx}$ with $D(T) := C_c^\infty((0,+\infty))$ and $\mathsf{H}_0 := \text{span}\{\varphi\}$, where $\varphi(x) = e^{-x}$. Here $D(T) \cap \mathsf{H}_0 = \{0\}$ so that the former inclusion in (i) is trivially valid, whereas the latter is valid by integrating by parts. However, it is easy to pick out $\psi \in D(T)$ such that $\langle\psi|\varphi\rangle \neq 0$, so that $(P_0\psi)(x)$ has the support of φ itself given by the whole $[0,+\infty)$ and $P_0\psi \notin D(T)$.) *Moreover, without (ii) the direct orthogonal decomposition (66) cannot take place.*
(2) *Evidently H_0 reduces T iff $\mathsf{H}_0^\perp$ reduces T, since $I - P_0$ projects onto $\mathsf{H}_0^\perp$.*
(3) *A condition equivalent to (i)-(ii) is $P_0T \subset TP_0$ as the reader immediately proves.* ■

Proposition 39: *If the closed subspace H_0 reduces the symmetric (selfadjoint) operator T on H, then also $T\restriction_{D(T)\cap\mathsf{H}_0}$ and $T\restriction_{D(T)\cap\mathsf{H}_0^\perp}$ are symmetric (resp. selfadjoint) in H_0 and $\mathsf{H}_0^\perp$ respectively.*

Proof. Direct inspection. □

A useful technical fact is presented in the following proposition [20].

Proposition 40: *Let T be a closed symmetric operator on a Hilbert space H. Let D_0 be a dense subspace of a closed subspace H_0 of H such that $D_0 \subset D(T)$ and $T(D_0) \subset \mathsf{H}_0$. Suppose that $T_0 := T\restriction_{D_0}$ is essentially self-adjoint on H_0. Then H_0 reduces T and $\overline{T_0}$ is the part of T on H_0.*

Proof. See [20, Prop.1.17]. □

A.2 More on generalized symmetric and selfadjoint extensions

According to definition 21 we have

$$D(A) \subset D(B) \cap \mathsf{H} \subset D(B)\,, \tag{67}$$

where $D(B)$ is dense in K and $D(A)$ is dense in H. Generalized extensions B with $B \supsetneq A$ are classified accordingly to the previous inclusions following [1], in particular:

(i) B is said to be of **kind I** if $D(A) \neq D(B) \cap \mathsf{H} = D(B)$ – that is, if B is a standard extension of A;

(ii) B is said to be of **kind II** if $D(A) = D(B) \cap \mathsf{H} \neq D(B)$;

(iii) B is said to be of **kind III** if $D(A) \neq D(B) \cap \mathsf{H} \neq D(B)$;

Proposition 41: *If $A : D(A) \to \mathsf{H}$ with $D(A) \subset \mathsf{H}$ is maximally symmetric and $B \supsetneq A$ is a generalized symmetric extension, then B is of kind II.*

Proof. The kind I is not possible *a priori* since A does not admit proper symmetric extensions in H. Let us assume that B is either of kind II or III and consider the operator $P_\mathsf{H}BP_\mathsf{H}$, with its natural domain $D(P_\mathsf{H}BP_\mathsf{H}) = D(BP_\mathsf{H})$, where $P_\mathsf{H} \in \mathscr{L}(\mathsf{K})$ is the orthogonal projector onto H. Since this is a symmetric extension of A in H which is maximally symmetric, we have $A = P_\mathsf{H}BP_\mathsf{H}$, in particular $D(BP_\mathsf{H}) = D(A)$. As a consequence, if $x \in D(B) \cap \mathsf{H}$, then $x \in D(BP_\mathsf{H}) = D(A)$ so that $D(A) \supset D(B) \cap \mathsf{H}$ and thus $D(A) = D(B) \cap \mathsf{H}$ because the other inclusion is true from (67). We have proved that B is of kind II. □

We have an important technical result

Theorem 42: *A non-selfadjoint symmetric operator A always admits a generalized selfadjoint extension B. Such an extension can be chosen of kind II when A is closed.*

Proof. See [1, Thm. 1. p.127 Vol II] for the former statement. The latter statement relies on the comment under the proof of [1, Thm. 1. p.127 Vol II] and it is completely proved in [17, Thm.13][11]. The fact that the selfadjoint extensions can be chosen in order to satisfy (iii) of Definition 21 is proved in [18, Thm.7]. □

A.3 Proof of some propositions

Lemma 43: *Referring to (1) in example 11, $\psi_\omega \in \mathcal{D}_{\omega_B}$.*

Proof. To prove that $\psi_\omega \in \mathcal{D}_{\omega_B}$ observe that, since A and A^* are generators of $\mathfrak{A}_{\mathrm{CCR},1}$ satisfying $[A, A^*] = I$, we can always rearrange every element $B \in \mathfrak{A}_{\mathrm{CCR},1}$ into the form

$$B = \sum_{n,m} c^{(B)}_{n,m} A^{*n} A^m ,$$

where $A^0 := A^{*0} := I$ and where only a finite number of coefficients $c^{(B)}_{n,m} \in \mathbb{C}$ depending on B are different from 0. Here, (13) implies

$$\psi_{\omega_B} = \sum_{n,m} c^{(B)}_{n,m} A^{*n} A^m \psi_\omega = \sum_{k\in\mathbb{N}} d^{(B)}_k \psi_k , \tag{68}$$

where again only a finite number of coefficients $d^{(B)}_k \in \mathbb{C}$ depending on B are different from 0 and to pass from the first sum to the second one we took advantage of the standard harmonic oscillator algebra of the Hermite basis where $A\psi_k = \sqrt{k}\psi_{k-1}$, $A^*\psi_k = \sqrt{k+1}\psi_{k+1}$ with $\psi_0 := \psi_\omega$. To conclude, notice that, if $C \in \mathfrak{A}_{\mathrm{CCR},1}$, (13) also implies that $\pi_{\omega_B}(C)\psi_{\omega_B} = \pi_\omega(C)\psi_{\omega_B}$. Therefore, if $k_B \in \mathbb{N}$ is the largest natural such that $d^{(B)}_k \neq 0$ in (68), choosing $C := \frac{1}{d^{(B)}_{k_B}\sqrt{k_B!}} A^{k_B} \in \mathfrak{A}_{\mathrm{CCR},1}$, we have

$$\pi_{\omega_B}(C)\psi_{\omega_B} = \sum_{k\in\mathbb{N}} d^{(B)}_k \frac{1}{d^{(B)}_{k_B}\sqrt{k_B!}} A^{k_B}\psi_k = 0 + \frac{d^{(B)}_{k_B}\sqrt{k_B!}}{d^{(B)}_{k_B}\sqrt{k_B!}}\psi_0 = \psi_0 = \psi_\omega .$$

In other words, $\psi_\omega \in \mathcal{D}_{\omega_B}$ as argued. □

Lemma 44: *Referring to (2) in example 11, $\psi_\omega \in \mathcal{D}_{\omega_b}$ if (29) is valid.*

Proof. First define the elements of the algebra $\mathfrak{A}[M, g]$

$$A_\varphi := \frac{1}{2}\left(\Phi[\varphi] + i\Phi[\varphi']\right) \quad \text{and} \quad A^*_\varphi := \frac{1}{2}\left(\Phi[\varphi] - i\Phi[\varphi']\right) .$$

[11]Unfortunately the necessary closedness requirement disappeared passing from [17, Thm.13] to the comment under [1, Thm. 1. p.127 Vol II].

We stress that the elements A^*_φ and A_φ form a set of generators of $\mathfrak{A}[M,g]$, because the $\Phi[\varphi]$ are generators and the previous relations can be inverted to

$$\Phi[\varphi] = A_\varphi + A^*_\varphi$$

By using (26), linearity of $x \mapsto a^+_x$, anti-linearity of $x \mapsto a_x$, and (29), we immediately find

$$\pi_\omega\left(A_\varphi\right) = a_{K\varphi}|_{\mathcal{D}_\omega} \quad \text{and} \quad \pi_\omega\left(A^*_\varphi\right) = a^+_{K\varphi}|_{\mathcal{D}_\omega} \tag{69}$$

The algebraic relations reflecting (25) are also valid from (b) and (c) in item (2) of example 11,

$$[A_\varphi, A^*_{\tilde{\varphi}}] = \langle K\varphi, K\tilde{\varphi}\rangle I\,, \quad [A_\varphi, A_{\tilde{\varphi}}] = [A^*_\varphi, A^*_{\tilde{\varphi}}] = 0\,.$$

Exploiting the found results, we can prove that $\psi_\omega \in \mathcal{D}_{\omega_b}$ as wanted. The generic element $b \in \mathfrak{A}[M,g]$, taking advantage of the generators A_φ and A^*_φ and their commutation relations, is always of the form (where we adopt the convention that $\prod_{j=1}^0 A^{(*)}_{\varphi_j} := \mathbb{I}$)

$$b = \sum_{k,h=0}^{N} c_{kh}^{j_1\ldots j_k i_1 \ldots i_h} A^*_{\varphi^{(k)}_{j_1}} \cdots A^*_{\varphi^{(k)}_{j_k}} A_{\tilde{\varphi}^{(h)}_{i_1}} \cdots A_{\tilde{\varphi}^{(h)}_{i_h}} \tag{70}$$

for sets of solutions $\{\varphi^{(k)}_j\}_{j\in\{1,\ldots,D_k\}}$ and $\{\tilde{\varphi}^{(h)}_i\}_{i\in\{1,\ldots,E_h\}}$ in $Sol[M,g]$ and where we adopted Einstein's summation convention. Obviously, N, D_h, E_h, and the complex coefficients $c_{k,h}^{j_1\ldots j_k i_1\ldots i_h}$ depend on b and these coefficients are completely symmetric separately in the indices j_r and in the indices i_r due to the fact that the elements $A^*_{\varphi_{j_1}}, \cdots, A^*_{\varphi_{j_k}}$ and $A_{\varphi_{i_1}}, \cdots, A_{\varphi_{i_h}}$ separately pairwise commute. Hence, (69) entails

$$\psi_{\omega_b} = \pi_\omega(b)\psi_\omega = \sum_{k=0}^{N} c_{k0}^{j_1\ldots j_k} a^+_{\psi^{(k)}_{j_1}} \cdots a^+_{\psi^{(k)}_{j_k}} \psi_\omega \tag{71}$$

where $\psi^{(k)}_j := K\varphi^{(k)}_j$ and we henceforth assume that not all coefficients $c_{N0}^{j_1\ldots j_N}$ vanish and all vectors $\psi^{(N)}_j = K\varphi^{(N)}_j$ for $j = 1, \ldots, D_N$ do not vanish (otherwise the N-th addend in (71) would give no contribution). Defining

$$d := \overline{c_{N0}^{i_1\cdots i_N}} A_{K\varphi^{(N)}_{i_1}} \cdots A_{K\varphi^{(N)}_{i_N}} \in \mathfrak{A}[M,g]$$

(25) yields, if $c^{j_1\cdots j_N} := c_{N0}^{j_1\cdots j_N}$ and $\psi_j := \psi^{(N)}_j$

$$\mathcal{D}_{\omega_b} \ni \pi_\omega(d)\pi_\omega(b)\psi_\omega = \overline{c^{i_1\cdots i_N}} c^{j_1\cdots j_N} a_{\psi_{i_1}} \cdots a_{\psi_{i_N}} a^+_{\psi_{j_1}} \cdots a^+_{\psi_{j_N}} \psi_\omega\,. \tag{72}$$

At this juncture we can fix an orthonormal basis $\{e_l\}_{i=1,\ldots,D}$ in the span of the vectors $\{\psi_j\}_{j=1,\ldots,D_N}$ and we can rearrange the identity above as

$$\pi_\omega(d)\pi_\omega(b)\psi_\omega = \overline{c'^{i_1\cdots i_N}} c'^{j_1\cdots j_N} a_{e_{i_1}} \cdots a_{e_{i_N}} a^+_{e_{j_1}} \cdots a^+_{e_{j_N}} \psi_\omega$$

where not all the symmetric coefficients $c'^{j_1\cdots j_N}$ vanish (since they are the components in a new basis of the non-vanishing tensor defined by the components $c^{j_1\cdots j_N}$). Expanding the contractions we find, where P_N denotes the group of permutations of N objects

$$\pi_\omega(d)\pi_\omega(b)\psi_\omega = \sum_{\sigma\in P_N} \overline{c'^{i_1\cdots i_N}} c'^{j_1\cdots j_N} \delta_{i_1 j_{\sigma(1)}} \cdots \delta_{i_N j_{\sigma(N)}} \psi_\omega$$

$$= \sum_{\sigma\in P_N} \overline{c'^{i_1\cdots i_N}} c'^{j_{\sigma^{-1}(1)}\cdots j_{\sigma^{-1}(N)}} \delta_{i_1 j_1} \cdots \delta_{i_N j_N} \psi_\omega = \sum_{\sigma\in P_N} \overline{c'^{i_1\cdots i_N}} c'^{j_1\cdots j_N} \delta_{i_1 j_1} \cdots \delta_{i_N j_N} \psi_\omega \,.$$

(In the second line, $c'^{j_{\sigma^{-1}(1)}\cdots j_{\sigma^{-1}(N)}} = c'^{j_1\cdots j_N}$ arises from the symmetry of the coefficients.) That is

$$\pi_\omega(d)\pi_\omega(b)\psi_\omega = \left(N! \sum_{j_1,\ldots,j_N=1}^{D} |c'^{j_1\cdots c_N}|^2 \right) \psi_\omega \in \mathcal{D}_{\omega_b} \,. \tag{73}$$

Since the coefficient in front of ψ_ω in (73) does not vanish, then $\psi_\omega \in \mathcal{D}_{\omega_b}$ as wanted. □

Proof of Proposition 22. Let B be a generalized symmetric extension in the Hilbert space K of the selfadjoint operator A in the Hilbert space H with $\mathsf{H} \subset \mathsf{K}$. The closed symmetric operator $B' = \overline{B}$ in K extends A. In view of Proposition 39-40, since $B'\restriction_{D(A)} = A$ is selfadjoint on H, then H reduces B' and $\overline{B} = \overline{B'\restriction_{D(A)}} \oplus B''$, where the two addends are symmetric operators respectively on H and $\mathsf{H}^\perp$. Requirement (iii) in Definition 21 imposes that $\mathsf{H}^\perp = \{0\}$, so that $\mathsf{K} = \mathsf{H}$ and B is a standard symmetric extension of the selfadjoint operator A which entails $B = A$. □

Proof of Theorem 23. (a) and (b). If A is symmetric, for each generalized selfadjoint extension B as in Definition 21 (they exist in view of Theorem 42 and, if A is selfadjoint, $B := A$), one can define a corresponding normalized POVM $Q^{(A)} \colon \mathscr{B}(\mathbb{R}) \to \mathfrak{B}(\mathsf{H})$ as follows. Let $P \colon \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathsf{K})$ be the unique PVM associated with B

$$B := \int_{\mathbb{R}} \lambda dP(\lambda) \,, \tag{74}$$

(see, e.g. [15, Thm. 9.13]) and let $P_\mathsf{H} \in \mathscr{L}(\mathsf{K})$ denote the orthogonal projection onto H viewed as a closed subspace of K. A normalized POVM $Q^{(A)} \colon \mathscr{B}(\mathbb{R}) \to \mathfrak{B}(\mathsf{H})$ is then defined by setting

$$Q^{(A)}(E) := P_\mathsf{H} P(E)\restriction_\mathsf{H} \qquad \forall E \in \mathscr{B}(\mathbb{R}) \,. \tag{75}$$

The POVM $Q^{(A)}$ is linked to A by the following identities as the reader easily proves from standard spectral theory:

$$\langle\psi|A\varphi\rangle = \int_{\mathbb{R}} \lambda dQ^{(A)}_{\psi,\varphi}(\lambda) \,, \qquad \|A\varphi\|^2 = \int_{\mathbb{R}} \lambda^2 dQ^{(A)}_{\varphi,\varphi}(\lambda) \,, \qquad \forall \psi \in \mathsf{H}, \varphi \in D(A) \,, \tag{76}$$

The above relation implies the following facts, where λ^k henceforth denotes the map $\mathbb{R} \ni \lambda \to \lambda^k \in \mathbb{R}$ for $k \in \mathbb{N} := \{0, 1, 2, \ldots\}$,

$$\begin{aligned} A = B\restriction_{D(A)} \,, \quad D(A) \subset \{\psi \in \mathsf{H} |\, \lambda \in L^2(\mathbb{R}, Q^{(A)}_{\psi,\psi})\} &= \{\psi \in \mathsf{H} |\, \lambda \in L^2(\mathbb{R}, P_{\psi,\psi})\} \\ &= D(B) \cap \mathsf{H} \subset D(B) \,, \end{aligned} \tag{77}$$

the second equality arising from the identity

$$\int_{\mathbb{R}} \lambda^2 dP_{\psi,\psi}(\lambda) = \int_{\mathbb{R}} \lambda^2 dQ^{(A)}_{\psi,\psi}(\lambda) \qquad \forall \psi \in \mathsf{H}\,,$$

which descends from equation (75). [1, Thm. 2, p. 129 Vol II] proves that every POVM (it is equivalent to a *spectral function* used therein, see Remark 14) satisfying (76) arises from a PVM of a generalized selfadjoint extension B of A as above, so that (77) are satisfied. The proof of (a) and (b) is over.
(c) If the selfadjoint operator B extending A as in (b) is a standard extension of A, then $\mathsf{H} = \mathsf{K}$ so that $P_{\mathsf{K}} = I$ and $Q^{(A)} = P$ so that $Q^{(A)}$ is a PVM. If $Q^{(A)}$ is a PVM, $B := \int_{\mathbb{R}} \lambda dQ^{(A)}(\lambda)$ with domain $D(B) = \{\psi \in \mathsf{H} \mid \int_{\mathbb{R}} \lambda^2 dQ^{(A)}_{\psi,\psi}(\lambda) < +\infty\}$ is a standard selfadjoint extension of A and the associated trivial dilation triple $\mathsf{K} := \mathsf{H}$, $P_{\mathsf{H}} := I$, $P := Q^{(A)}$ trivially generates $Q^{(A)}$ as in (b).
(d) Referring to the proof of (a) and (b) above, for generalized selfadjoint extensions B of kind II, and this choice for B is always feasible when A is closed in view of Theorem 42, we have $D(A) = D(B) \cap \mathsf{H}$ and therefore

$$A = B{\restriction}_{D(B)\cap\mathsf{H}}\,, \quad D(A) = \{\psi \in \mathsf{H} |\, \lambda \in L^2(\mathbb{R}, Q^{(A)}_{\psi,\psi})\} = \{\psi \in \mathsf{H} |\, \lambda \in L^2(\mathbb{R}, P_{\psi,\psi})\} = D(B) \cap \mathsf{H}\,. \tag{78}$$

Since (77) is valid for every POVM satisfying (76), we have that the identity $D(A) = \{\psi \in \mathsf{H} |\, \lambda \in L^2(\mathbb{R}, P_{\psi,\psi})\}$ holds if and only if $A = B{\restriction}_{D(B)\cap\mathsf{H}}$, namely B is an extension of type II of A.
(e) and (f). They are established in [1, Thm. 2, p. 135 Vol II], taking Theorem 42 into account and (d) above. □

Proof of Theorem 26. Consider Naimark's dilation triple of Q, $(\mathsf{K}, P_{\mathsf{H}}, P)$ and define the selfadjoint operator $B := \int_{\mathbb{R}} \lambda dP(\lambda)$. By hypothesis $D(A^{(Q)}) = D(B) \cap \mathsf{H}$. Since $D(B)$ is a subspace of K, it also holds that $D(A^{(Q)})$ is a subspace of H proving (a). A well-known counterexample due to Naimark [1] proves that, in some cases, $D(A^{(Q)}) = \{0\}$ though Q is not trivial. It is clear that, if an operator $A^{(Q)} : D(A^{(Q)}) \to \mathsf{H}$ satisfies (39) then it is unique due to the arbitrariness of $\varphi \in \mathsf{H}$. So we prove (b) and (d) simultaneously just checking that $P_{\mathsf{H}} \int_{\mathbb{R}} \lambda dP(\lambda){\restriction}_{D(A^{(Q)})}$ satisfies (39). The proof is trivial since, from standard properties of the integral of a PVM, if $\psi \in D(A^{(Q)}) \subset D(B)$ and $\varphi \in \mathsf{H}$, then

$$\left\langle \varphi \middle| P_{\mathsf{H}} \int_{\mathbb{R}} \lambda dP(\lambda)\psi \right\rangle = \left\langle P_{\mathsf{H}}\varphi \middle| \int_{\mathbb{R}} \lambda dP(\lambda)\psi \right\rangle = \int_{\mathbb{R}} \lambda dP_{P_{\mathsf{H}}\varphi,\psi}(\lambda) = \int_{\mathbb{R}} \lambda dQ_{\varphi,\psi}(\lambda)\,.$$

(c) immediately arises with the same argument taking advantage of the fact that $B = B^*$ and $P_{\mathsf{H}}\psi = \psi$ if $\psi \in \mathsf{H}$. Regarding (e), it is sufficient observing that (see, e.g. [15]), if $\psi \in D(B)$, then $||B\psi||^2 = \int_{\mathbb{R}} \lambda^2 dP_{\psi,\psi}(\lambda)$ and next taking advantage of $D(A^{(Q)}) = D(B) \cap \mathsf{H}$ and (d) observing in particular that $P^*_{\mathsf{H}} P_{\mathsf{H}}\varphi = P_{\mathsf{H}} P_{\mathsf{H}}\varphi = P_{\mathsf{H}}\varphi = \varphi$ if $\varphi \in \mathsf{H}$. The fact that $A^{(Q)}$ is closed immediately follows from the fact that B is closed (because selfadjoint) and $A = B|_{D(B)\cap\mathsf{H}}$ where H is closed. □

Proof of Proposition 32. What we have to prove is just that the right-hand side of (54) is a positive semi definite Hermitian scalar product over X. Indeed, with that definition of the scalar product $(\,|\,)_p$, the identity $p(x) = \sqrt{(x|x)_p}$ is valid (see below) and this fact automatically implies that p is a seminorm. Uniqueness of the scalar product generating a seminorm p is a trivial consequence of the polarization identity. Let us prove that $(\,|\,)_p$ defined in (54) is a positive semidefinite Hermitian scalar product over X. From the definition of $(\,|\,)_p$ and property (i) of $p\colon X \to [0,+\infty)$, it is trivial business to prove the following facts per direct inspection:

1. $(x|x)_p = p(x)^2 \geq 0$,
2. $(x|0)_p = 0$,
3. $(x|y)_p = \overline{(y|x)_p}$,
4. $(x|iy)_p = i(x|y)_p$.

With these identities, we can also prove

5. $(x|y+z)_p = (x|y)_p + (x|z)_p$,
6. $(x|-y)_p = -(x|y)_p$,

by exploiting property (ii) of p. Actually, (6) immediately arises form (2) and (5). We will prove (5) as the last step of this proof. Iterating property (5), we easily obtain $(x|ny)_p = n(x|y)_p$ for every $n \in \mathbb{N}$, so that $(1/n)(x|z)_p = (x|(1/n)z)_p$ when replacing ny for z. As a consequence, $\lambda(x|y)_p = (x|\lambda y)_p$ if $\lambda \in \mathbb{Q}$. This results extends to $\lambda \in \mathbb{R}$ if the map $\mathbb{R} \ni \lambda \mapsto (x|\lambda y)_p$ is right-continuous because, for every $x \in [0,+\infty)$ there is a decreasing sequence of rationals tending to it. The definition (54) of $(x|y)_p$ proves that map is in fact right-continuous since property (iii) of p implies that, if $\lambda_0 \in [0,+\infty)$,

$$p(x + \lambda i^k y) = p((x + \lambda_0 i^k y) + (\lambda - \lambda_0) i^k y) \to p(x + \lambda_0 i^k y) \quad \text{for } \mathbb{R} \ni \lambda \to \lambda_0^+ \,.$$

We can therefore add the further property

7. $\lambda(x|y)_p = (x|\lambda y)_p$ if $\lambda \in [0,+\infty)$.

Collecting properties (1), (3), (5), (7), (6), (4) together, we obtain that $X \times X \ni (x,y) \mapsto (x|y)_p$ defined as in (54) is a positive semi definite Hermitian scalar product over X whose associated seminorm is p as wanted.
To conclude the proof, we establish property (5) from requirement (ii) on p.

$$4(x|y+z)_p = \sum_{k=0}^{3} (-i)^k p(x + i^k(y+z))^2 = \sum_{k=0}^{3} (-i)^k p((x/2 + i^k y) + (x/2 + i^k z))^2 \,.$$

Since, from (i) of the requirements on p,

$$\sum_{k=0}^{3} (-i)^k p((x/2 + i^k y) - (x/2 + i^k z))^2 = \sum_{k=0}^{3} (-i)^k p(i^k(y-z))^2 = \sum_{k=0}^{3} (-i)^k p((y-z))^2 = 0,$$

we can re-arrange the found decomposition of $4(x|y+z)_p$ as

$$4(x|y+z)_p = \sum_{k=0}^{3}(-i)^k \left[p((x/2+i^k y)+(x/2+i^k z))^2 - p((x/2+i^k y)-(x/2+i^k z))^2\right] .$$

From (ii) of the requirements on p,

$$4(x|y+z)_p = \sum_{k=0}^{3}(-i)^k \left[2p(x/2+i^k y)^2 + 2p(x/2+i^k z)^2\right] = 8(x/2|y)_p + 8(x/2|z)_p .$$

The special case $z=0$ and (2) yield $2(x/2|y)_p = (x|y)_p$ which, exploited again above, yields the wanted result (5) $4(x|y+z)_p = 4(x|y)_p + 4(x|z)_p$. □

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