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# Operator integrals and sesquilinear forms

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ABSTRACT

We consider various systematic ways of defining unbounded operator valued integrals of complex functions with respect to (mostly) positive operator measures and positive sesquilinear form measures, and investigate their relationships to each other in view of the extension theory of symmetric operators. We demonstrate the associated mathematical subtleties with a physically relevant example involving moment operators of the momentum observable of a particle confined to move on a bounded interval.



## 1. Introduction

Selfadjoint operators represent observables in the traditional (von Neumann) description of quantum mechanics when a quantum system is associated with a Hilbert space $\mathcal{H}$. By the spectral theorem, selfadjoint operators $A$ in $\mathcal{H}$ are in bijective correspondence with spectral measures (normalized projection valued measures) $\mathsf{E}:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ where $\mathcal{B}(\mathbb{R})$ is the Borel $\sigma$-algebra of the real line $\mathbb{R}$ and $\mathcal{L}(\mathcal{H})$ is the space of bounded operators on $\mathcal{H}$. The correspondence in the spectral theorem can be written as an *operator integral*, in the form $A=\int x\,d\mathsf{E}(x)$. More specifically, if $\mathsf{E}:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ is a normalized projection valued measure, and $f:\mathbb{R}\to\mathbb{R}$ a Borel measurable (possibly unbounded) function, there exists a unique operator, denoted $\int f\,d\mathsf{E}$, such that its domain

$$\mathrm{Dom}\left(\int f\,d\mathsf{E}\right)=\left\{\varphi\in\mathcal{H}\;\middle|\;\int\left|f(x)\right|^2 d\mathsf{E}_{\varphi,\varphi}(x)<\infty\right\}\tag{1}$$

is dense, and, for all $\psi\in\mathcal{H}$, $\varphi\in\mathrm{Dom}(\int f\,d\mathsf{E})$,

$$\left\langle\psi\;\middle|\;\left(\int f\,d\mathsf{E}\right)\varphi\right\rangle=\int f(x)\,d\mathsf{E}_{\psi,\varphi}(x)\tag{2}$$

where $\mathsf{E}_{\psi,\varphi}(X):=\langle\psi\mid\mathsf{E}(X)\varphi\rangle$, $X\in\mathcal{B}(\mathbb{R})$. This operator is selfadjoint and its spectral measure is $X\mapsto\mathsf{E}(f^{-1}(X))$. In addition, $\|(\int f\,d\mathsf{E})\varphi\|^2=\int|f(x)|^2\,d\mathsf{E}_{\varphi,\varphi}(x)$, consistent with the feature that the domain consists of exactly those vectors for which the integral of the *square* of $f$ is finite.

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However, from the operational point of view of quantum measurement theory, this definition is often considered too restrictive: in standard modern quantum theory (in particular, quantum information theory), a generalization to (normalized) positive operator (valued) measures (POVMs) is used instead. Before going to the motivation of the present paper, we very briefly give some selected historical remarks on the general role of POVMs in quantum theory.

The generalization goes back to the old probabilistic axiomatization program of G. Ludwig, who observed [18] that the abstract probabilistic description of experiments in terms of preparation and detection naturally leads to the detection events being, in general, represented by positive operators with norm at most one. Events represented by projections then appear as idealizations, allowing the general formulation to describe e.g. imperfections of measurements. We note that such a probabilistic approach to observables has been reintroduced relatively recently in the modern information theoretic context [4]. Allowing imperfections in the measurement makes it possible to e.g. jointly measure position and momentum of a quantum particle (see e.g. [5]). Another point of view comes when one considers the conditional state after the measurement. In particular, with POVMs perfect repeatability of the measurement is lost, and the concept of an instrument is needed to deal with sequential measurements. To our knowledge the first paper to successfully consider this aspect in full generality (involving also observables with continuous outcome sets) was that of Davies and Lewis [7].

An interesting technical difference between spectral measures and general POVMs comes from the fact that there is no functional calculus in the sense of the spectral theorem. Bounded functions can still be integrated with respect to a POVM without difficulty, but the ensuing map $f \mapsto \int f\,d\mathsf{E}$ is multiplicative if and only if $\mathsf{E}$ is projection valued. In the case of *unbounded functions*, even the definition of this operator valued integral is not clear, and this brings us to the topic of the present paper. From the physical point of view, integrating unbounded functions is motivated by the analogue of the moment method for probability measures, and we will return to this application in Section 6.

The difference to the projection valued case already shows in the first moment: In fact, according to Naimark dilation theory (see e.g. [24] or [1]), for any densely defined symmetric operator $A$ in $\mathcal{H}$ there exists a normalized POVM $\mathsf{E}:\mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$, having the properties

$$\langle \psi \mid A\varphi\rangle = \int x\,d\mathsf{E}_{\psi,\varphi}(x), \quad \psi \in \mathcal{H},\ \varphi \in \mathrm{Dom}(A), \tag{3}$$

and

$$\|A\varphi\|^2 = \int x^2\,d\mathsf{E}_{\varphi,\varphi}(x), \quad \varphi \in \mathrm{Dom}(A). \tag{4}$$

However, unlike the case of spectral measures, the domain of $A$ need not coincide with the set of vectors for which the integral in (4) is finite. Moreover, the correspondence does not work the other way: not every POVM $\mathsf{E}:\mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ satisfies (3) and (4) with respect to some symmetric operator $A$. This has been noted in the above references, along with the fact that the integral in the right hand side of (4) may well be infinite for *any* nonzero vector $\varphi$. Moreover, a normalized POVM corresponding to a symmetric operator $A$ as above is unique only if $A$ is maximally symmetric (i.e. has no proper symmetric extension) [1].

For these reasons, going from a POVM to a symmetric operator is not straightforward and choosing a reasonable definition for the domain of the operator integral $\int f\,d\mathsf{E}$ is problematic – except when $f$ is bounded, in which case the domain is all of $\mathcal{H}$.

In fact, the difficulties in choosing the domain have led the authors in [1, p. 132] to consider $\int x\,d\mathsf{E}(x)$ in a symbolic sense only, as a shorthand for Eqs. (3) and (4), provided they hold for the given POVM. As pointed out by Werner [27], however, even the general operator integral $\int f\,d\mathsf{E}$ can be uniquely defined as a symmetric operator on the domain (1), so that (2) holds, in contrast to what appears to be intended in [1, p. 132]. (See the above paper by Werner, and also [15].) The reason why this does not contradict the observation that not every POVM satisfies (3) and (4) for some symmetric operator is simply that (4) does not hold for $A = \int x\,d\mathsf{E}(x)$ in general.

When (4) holds, with (1) for $f(x) = x$ dense, the POVM is called *variance-free* [28]. For a general POVM it may be (and often is) the case that only the inequality

$$\left\| \left( \int f\,d\mathsf{E} \right) \varphi \right\|^2 \leqslant \int \left| f(x) \right|^2 d\mathsf{E}_{\varphi,\varphi} \tag{5}$$

holds. The domain of (1) has a physical meaning as the set of those vector states for which the measurement distribution has finite variance. For this reason, this set is a natural domain for the *variance form*

$$(\psi,\varphi) \mapsto \int x^2\,d\mathsf{E}_{\psi,\varphi} - \langle \tilde{\mathsf{E}}[1]\psi \mid \tilde{\mathsf{E}}[1]\varphi \rangle \in \mathbb{C}$$

where $\tilde{\mathsf{E}}[1] = \int x\,d\mathsf{E}$ is the first moment operator of $\mathsf{E}$ (see Section 6). This definition for the domain of the operator integral appears most frequently in the literature, see e.g. [27,26,1]. For spectral measures, the variance form vanishes identically, due to the multiplicativity of the functional calculus. In fact, the variance form can be understood as a measure of inaccuracy in the measurement described by the POVM [3]; a standard example of this phenomenon is exhibited by the approximate position and momentum observables [5].

However, not all POVMs with zero variance form are spectral measures. Since the inaccuracy aspect of the POVM generalization is manifestly not present in such a case, the difference from being projection valued is quite well captured by the domain questions alone; in fact, if a variance-free POVM has selfadjoint first moment $\tilde{\mathsf{E}}[1]$, then it is necessarily a spectral measure [14]. This observation makes variance-free POVMs particularly interesting from the point of view of the present paper.

In physical applications, a non-projection valued variance-free POVM cannot usually be considered as an "inaccurate" version of some projection valued measure. However, such a POVM can often nevertheless be identified with a quantum version of a classical variable *for which no selfadjoint operator qualifies as a quantization*. Perhaps the most well-known example this is the quantization of *time* [13,27]. Another similar but simpler example is obtained by *spatial confinement* of a quantum particle, which we present in Section 6.

We now return to the domain questions in the general setting. One might think that using Eq. (1) would settle the definition of the operator integral. However, after losing the equality in (5), it is no longer clear whether the finiteness of the integral in the right hand side is actually *needed* to define the operator integral. Loosely speaking, the reason for the square of $f$ appearing in the definition of the domain is connected to the multiplicativity of the projection valued measure, which is no longer true for POVMs. In fact, *the square integrability domain* (1) *is not necessarily the largest possible one where* (2) *defines an operator*. This is easy to see: for example, consider the POVM $X \mapsto \mathsf{E}(X) := \mu(X)I$, where $\mu$ is a probability measure and $I$ the identity operator on any Hilbert space. If $f$ is a $\mu$-integrable function, the integrals $\int f \, d\mathsf{E}_{\psi,\varphi} = \langle \psi \mid (\int f \, d\mu)\varphi \rangle$ determine a well-defined operator with domain all of $\mathcal{H}$, even if $\int |f|^2 \, d\mu = \infty$, collapsing the domain (1) to $\{0\}$. Hence, the natural definition of an operator integral needs closer mathematical examination.

A different definition has been used in [15,16]; we call this the *strong* operator integral. As we will see, even this choice is not the largest reasonable, and we will also define *weak* operator integrals which have still larger domains than the strong one. These are more operationally motivated, as they are constructed from the scalar measures $X \mapsto \langle \psi \mid \mathsf{E}(X)\varphi \rangle$.

To a large extent, our approach depends of the interplay between vector measures and operator theory. We refer the reader to the monograph [20] and its bibliography for various other aspects of this interplay. In the more recent article [11] some connections of vector measure theory to quantum mechanics are expounded from a point of view different from ours.

The structure of the paper is as follows. We begin by considering strong operator integrals in the setting of general Banach spaces. When specializing to Hilbert spaces and positive operator measures, the role of the square integrability domain is explained. Subsequently, we proceed to introduce weak operator integrals, and investigate their connection to operators defined via quadratic forms. A physically motivated example concludes the paper.

## 2. Preliminaries and notation

We begin with a fairly general setting: let $E$ and $F$ be Banach spaces and $L(E, F)$ the space of bounded linear operators $T : E \to F$. (We use complex scalars, as our main applications deal with complex Hilbert spaces.) Consider a measurable space $(\Omega, \mathcal{A})$ (where by definition $\mathcal{A}$ is a $\sigma$-algebra of subsets of $\Omega$). A map $M : \mathcal{A} \to L(E, F)$ is called an *operator measure* if it is strong operator (or briefly, strongly) $\sigma$-additive. This means that for each $x \in E$ the map $X \mapsto M_x(X) := M(X)x$ is a *vector measure*, i.e. $\sigma$-additive with respect to the norm in $F$. By the Orlicz–Pettis theorem it is equivalent to require that for any $x \in E$ and $y' \in F'$ (the topological dual of $F$), the function $X \mapsto M_{y',x}(X) := \langle y', M(X)x \rangle$ on $\mathcal{A}$ is a complex measure. The following definition agrees with the usage in [8]. (We only integrate $\mathcal{A}$-measurable functions, though this restriction could be relaxed somewhat, see e.g. [29].)

**Definition 1.** Let $\mu : \mathcal{A} \to F$ be a vector measure and $f : \Omega \to \mathbb{C}$ an $\mathcal{A}$-measurable function. The function $f$ is $\mu$*-integrable* if there is a sequence $(f_n)$ of simple functions converging to $f$ pointwise and such that $\lim_{n\to\infty} \int_X f_n \, d\mu$ exists for all $X \in \mathcal{A}$. Then $\int_\Omega f \, d\mu := \lim_{n\to\infty} \int_\Omega f_n \, d\mu$ is called the *integral* of $f$ with respect to $\mu$.

**Remark 1.** It turns out to be equivalent to the above definition to require that $f$ is integrable with respect to the complex measure $\mu_{y'} := y' \circ \mu$ for every $y' \in F'$ and for each $X \in \mathcal{A}$ one has a vector $\nu(X) \in F$ (clearly unique) such that $\langle y', \nu(X) \rangle = \int_X f \, d\mu_{y'}$ for all $X \in \mathcal{A}$, $y' \in F'$. (See [17], and [29] for another proof.) If $f$ is integrable with respect to every $\mu_{y'}$, it follows from the dominated convergence theorem and the uniform boundedness principle (as in e.g. [15, p. 328]) that for each $X \in \mathcal{A}$ there is some element $\nu(X) \in F''$ satisfying $\langle y', \nu(X) \rangle = \int_X f \, d\mu_{y'}$ for each $y' \in F'$, and so in case $F$ is reflexive we can conclude that $f$ is $\mu$-integrable. We use this observation especially when $F$ is a Hilbert space.

Let $\mathcal{H}$ be a (complex) Hilbert space, and let $\mathcal{L}(\mathcal{H})$ denote the space of bounded operators on $\mathcal{H}$. We do not have to assume that $\mathcal{H}$ is separable, except in some examples where this is clearly indicated. The identity operator of $\mathcal{H}$ is denoted by $I_{\mathcal{H}}$ or simply by $I$. For $\psi, \varphi \in \mathcal{H}$, we use the symbol $|\psi\rangle\langle\varphi|$ to denote the rank one operator $\eta \mapsto \langle \varphi \mid \eta \rangle \psi$. For a (linear) operator $A$ in $\mathcal{H}$, we let $\mathrm{Dom}(A)$ denote the domain of $A$, i.e. the (linear) subspace of $\mathcal{H}$ on which $A$ is defined. As before, $(\Omega, \mathcal{A})$ is a measurable space. We let $\mathcal{B}(\Omega)$ denote the Borel $\sigma$-algebra of any topological space $\Omega$. We follow the convention $\mathbb{N} = \{0, 1, 2, \ldots\}$, and let $\chi_X$ be the characteristic function of the set $X \in \mathcal{A}$.

**Definition 2.** Let $\mathsf{E}: \mathcal{A} \to \mathcal{L}(\mathcal{H})$ be a function.

(a) $\mathsf{E}$ is a *positive operator* (*valued*) *measure*, or POVM for short, if $\mathsf{E}$ is an operator measure and $\mathsf{E}(X) \geqslant 0$ for all $X \in \mathcal{A}$.
(b) A POVM $\mathsf{E}$ is *normalized* if $\mathsf{E}(\Omega) = I$.
(c) A projection valued POVM (PVM for short) which is normalized is a *spectral measure*.

For a POVM $\mathsf{E}: \mathcal{A} \to \mathcal{L}(\mathcal{H})$ and $\psi, \varphi \in \mathcal{H}$, we let $\mathsf{E}_{\psi,\varphi}$ denote the complex measure $X \mapsto \langle \psi \mid \mathsf{E}(X)\varphi \rangle$ and $\mathsf{E}_\varphi$ denote the $\mathcal{H}$-valued vector measure $X \mapsto \mathsf{E}(X)\varphi$.

*Naimark's dilation theorem* (see e.g. [24]) states that, for any POVM $\mathsf{E}: \mathcal{A} \to \mathcal{L}(\mathcal{H})$, there exists another Hilbert space $\mathcal{K}$, a spectral measure $\mathsf{F}: \mathcal{A} \to \mathcal{L}(\mathcal{K})$, and a bounded linear map $V : \mathcal{H} \to \mathcal{K}$, such that $\mathsf{E}(X) = V^*\mathsf{F}(X)V$ for all $X \in \mathcal{A}$. If the set of the linear combinations of vectors $\mathsf{F}(X)V\varphi$, $X \in \mathcal{A}$, $\varphi \in \mathcal{H}$, is dense in $\mathcal{K}$, then the Naimark dilation $(\mathcal{K}, \mathsf{F}, V)$ is said to be *minimal*. Note that $\mathsf{E}$ is normalized if and only if $V$ is an isometry, i.e. $V^*V = I$. In that case, $\mathcal{H}$ can be identified with the range of $V$, a subspace of $\mathcal{K}$.

We have already discussed integration with respect to a vector measure. Since an operator measure usually fails to be norm $\sigma$-additive, integration with respect to operator measures needs a different approach. For a bounded measurable function $f : \Omega \to \mathbb{C}$, integration with respect to a POVM is, however, quite elementary (see e.g. [2]). One starts by setting $\int f\, d\mathsf{E} := \sum_{n=0}^{k} c_n \mathsf{E}(X_n)$ for $f = \sum_{n=0}^{k} c_n \chi_{X_n}$, $c_n \in \mathbb{C}$, $X_n \cap X_m = \emptyset$, $m \neq n \in \mathbb{N}$. The extension from these simple functions to bounded $\mathcal{A}$-measurable functions $f : \Omega \to \mathbb{C}$ requires the uniform convergence of the integrals of simple functions. Ultimately this depends on the fact that the range of any POVM is norm bounded, and the resulting integral defines a bounded operator. The following lemma is straightforward to prove by using the usual approximation techniques appearing in the construction of the integral.

**Lemma 1.** *Let $(\mathcal{K}, \mathsf{F}, V)$ be a Naimark dilation of $\mathsf{E}$. Then for every bounded $\mathcal{A}$-measurable function $f : \Omega \to \mathbb{C}$, we have $\int f\, d\mathsf{E} = V^*(\int f\, d\mathsf{F})V$.*

For unbounded functions, even defining a domain for the operator valued integral needs attention. We study this question next.

## 3. Strong operator integrals

Let $(\Omega, \mathcal{A})$ be a measurable space. We first consider general Banach spaces $E$ and $F$.

**Definition 3.** Let $M : \mathcal{A} \to L(E, F)$ be an operator measure and $f : \Omega \to \mathbb{C}$ an $\mathcal{A}$-measurable function. We let $D(f, M)$ denote the subset of $E$ consisting of those $x \in E$ for which $f$ is integrable with respect to the vector measure $X \mapsto M_x(X) = M(X)x$. If $x \in D(f, M)$, we denote by $L(f, M)x$ the integral $\int_\Omega f\, dM_x$.

**Proposition 1.** *If $f : \Omega \to \mathbb{C}$ is an $\mathcal{A}$-measurable function, the set $D(f, M)$, the domain of $L(f, M)$, is a vector subspace of $E$, and $L(f, M) : D(f, M) \to F$ is a linear map.*

**Proof.** See e.g. [29, Corollary 3.7]. $\square$

The following proposition is an immediate consequence of Remark 1.

**Proposition 2.** *Assume that the Banach space $F$ is reflexive. For $x \in E$ the following conditions are equivalent*: (i) $x \in D(f, M)$; (ii) $f$ *is* $M_{y',x}$*-integrable for all* $y' \in F'$.

We mainly apply the above results in the case where $F = \mathcal{H}$, a Hilbert space.

**Definition 4.** We say that a measure $\mu : \mathcal{A} \to \mathcal{H}$ is *orthogonally scattered* if

$$\big\langle \mu(X) \,\big|\, \mu(Y) \big\rangle = 0$$

whenever the sets $X, Y \in \mathcal{A}$ are disjoint.

Orthogonally scattered vector measures have a highly developed theory, see e.g. [19]. A basic observation is that if $\mu : \mathcal{A} \to \mathcal{H}$ is an orthogonally scattered vector measure, by denoting $\lambda(X) = \lambda_\mu(X) := \|\mu(X)\|^2$, we get a finite positive measure $\lambda$ on $\mathcal{A}$. The following result is well known and we only give a brief indication of proof.

**Proposition 3.** *Let $\mu : \mathcal{A} \to \mathcal{H}$ be an orthogonally scattered vector measure and $\lambda = \lambda_\mu$ the positive measure defined above. An $\mathcal{A}$-measurable function $f : \Omega \to \mathbb{C}$ is $\mu$-integrable if and only if $|f|^2$ is $\lambda$-integrable, in which case $\|\int_\Omega f\, d\mu\|^2 = \int_\Omega |f|^2\, d\lambda$.*

**Proof.** In one direction, one may use the argument in the proof of Lemma A.2 (b) in [15]. In the other direction a technique from the proof of Proposition 4 below may be adapted. □

**Remark 2.** (a) It follows from the above proposition that if $E$ is a Banach space and $M : \mathcal{A} \to L(E, \mathcal{H})$ is an operator measure such that for each $x \in E$ the vector measure $M_x : \mathcal{A} \to \mathcal{H}$ is orthogonally scattered, then the domain $D(f, M)$ of the strong operator integral $L(f, M)$ consists of precisely those vectors $x \in E$ for which $|f|^2$ is integrable with respect to the measure $X \mapsto \|M_x(X)\|^2$ on $\mathcal{A}$.

(b) If $\mathsf{E} : \mathcal{A} \to \mathcal{L}(\mathcal{H})$ is a PVM, then for each $\varphi \in \mathcal{H}$ the vector measure $\mathsf{E}_\varphi$ is orthogonally scattered and $\|\mathsf{E}_\varphi(X)\|^2 = \langle \varphi \mid \mathsf{E}(X)\varphi \rangle$ whenever $X \in \mathcal{A}$.

(c) Consider the Hilbert space $\ell^2 = \ell^2(\mathbb{N})$. Let $\mathcal{A}$ be the power set of $\mathbb{N}$. Let $g : \mathbb{N} \to \mathbb{C}$ be a bounded function and define $M : \mathcal{A} \to \mathcal{L}(\ell^2)$ by the formula $M(X)\varphi = g\varphi\chi_X$ for all $X \in \mathcal{A}$, $\varphi \in \ell^2$. Then $M$ satisfies the assumption in (a), so that $D(f, M)$ consists of those $\varphi \in \ell^2$ for which $fg\phi \in \ell^2$. Note that $M$ need not be a PVM, nor even a POVM. This example can be easily extended for more general measure spaces.

We have seen (the well-known fact) that for a PVM $\mathsf{E} : \mathcal{A} \to \mathcal{L}(\mathcal{H})$, a vector $\varphi \in \mathcal{H}$ belongs to $D(f, \mathsf{E})$ if and only if $|f|^2$ is integrable with respect to the measure $\mathsf{E}_{\varphi,\varphi}$. More generally, for any POVM $\mathsf{E} : \mathcal{A} \to \mathcal{L}(\mathcal{H})$ we call the set $\tilde{D}(f, \mathsf{E}) := \{\varphi \in \mathcal{H} \mid |f|^2 \text{ is } \mathsf{E}_{\varphi,\varphi}\text{-integrable}\}$ the *square integrability domain* for the integral $\int_\Omega f\, d\mathsf{E}$. This makes sense, as it is known that $\tilde{D}(f, \mathsf{E})$ is a linear subspace of $\mathcal{H}$ contained in $D(f, \mathsf{E})$. In [15] this was given a direct elementary proof. The authors of [15] were unaware that this result essentially had already appeared in [27], where the proof is based on Naimark's dilation theorem. (For completeness, we give a proof below reproducing the idea in [27].) The fact that $\tilde{D}(f, \mathsf{E})$ is a linear subspace is implied by the following easy consequence of the Cauchy–Schwarz inequality. We state it explicitly as it will also have some later use. (The terminology will be recalled at the beginning of Section 4.)

**Lemma 2.** *Let $\mathcal{V}$ be a vector space, and $q : \mathcal{V} \times \mathcal{V} \to \mathbb{C}$ a positive sesquilinear form. Then*

$$q(\varphi + \psi, \varphi + \psi) \leqslant 2q(\varphi, \varphi) + 2q(\psi, \psi), \quad \varphi, \psi \in \mathcal{V}.$$

**Proposition 4.** *The vector valued integral $\int f\, d\mathsf{E}_\varphi$ exists for each $\varphi \in \tilde{D}(f, \mathsf{E})$.*

**Proof.** Let $(\mathcal{K}, \mathsf{F}, V)$ be a Naimark dilation of $\mathsf{E}$ and $(f_n)$ a sequence of simple functions converging pointwise to $f$ with $|f_n| \leqslant |f|$. Then the bounded operator $\int f_n\, d\mathsf{E}$ is defined for each $n$ according to the definition in the preceding section. Fix $\varphi \in \tilde{D}(f, \mathsf{E})$. Using Lemma 1, and the multiplicativity of the spectral measure $\mathsf{F}$, we have for each $X \in \mathcal{A}$, that

$$\begin{aligned} \left\| \int_X (f_n - f_m)\, d\mathsf{E}_\varphi \right\|^2 &= \left\| V^* \int_X (f_n - f_m)\, d\mathsf{F}\, V\varphi \right\|^2 \leqslant \|V^*\|^2 \left\| \int_X (f_n - f_m)\, d\mathsf{F}\, V\varphi \right\|^2 \\ &= \|V^*\|^2 \int_X |f_n - f_m|^2\, d\mathsf{F}_{V\varphi,V\varphi} = \|V^*\|^2 \int_X |f_n - f_m|^2\, d\mathsf{E}_{\varphi,\varphi}. \end{aligned}$$

Since $|f|^2$ is integrable, it thus follows from the dominated convergence theorem that the sequence $(\int_X f_n\, d\mathsf{E}_\varphi)$ of vectors is a Cauchy sequence, and thus converges. This proves the existence of the integral $\int f\, d\mathsf{E}_\varphi$ of $f$ with respect to the vector valued measure $\mathsf{E}_\varphi$. □

According to this result, we can define a linear operator

$$\tilde{L}(f, \mathsf{E}) : \tilde{D}(f, \mathsf{E}) \to \mathcal{H}, \qquad \tilde{L}(f, \mathsf{E})\varphi := \int f\, d\mathsf{E}_\varphi.$$

Since $f$ is integrable with respect to each scalar measure $\mathsf{E}_{\psi,\varphi}$, $\psi \in \mathcal{H}$ if it is integrable with respect to $\mathsf{E}_\varphi$ (see e.g. [8]), it follows that $\langle \psi \mid \tilde{L}(f, \mathsf{E})\varphi \rangle = \int f\, d\mathsf{E}_{\psi,\varphi}$ for all $\varphi \in \tilde{D}(f, \mathsf{E})$, $\psi \in \mathcal{H}$. Since $\tilde{D}(f, \mathsf{E}) = \{\varphi \in \mathcal{H} \mid V\varphi \in \tilde{D}(f, \mathsf{F})\}$, where $\tilde{D}(f, \mathsf{F})$ is the domain of the selfadjoint operator $\tilde{L}(f, \mathsf{F})$, it now follows that

$$\tilde{L}(f, \mathsf{E}) = V^* \tilde{L}(f, \mathsf{F}) V. \tag{6}$$

(See also [16].)

Summarizing, for a POVM $\mathsf{E}$ and a measurable function $f$, we have $\tilde{D}(f, \mathsf{E}) \subset D(f, \mathsf{E})$ and $\tilde{L}(f, \mathsf{E}) \subset L(f, \mathsf{E})$ where

$$D(f, \mathsf{E}) = \left\{ \varphi \in \mathcal{H} \;\middle|\; \int |f|\, d|\mathsf{E}_{\psi,\varphi}| < \infty \text{ for all } \psi \in \mathcal{H} \right\}, \tag{7}$$

$$\big\langle \psi \;\big|\; L(f, \mathsf{E})\varphi \big\rangle = \int f\, d\mathsf{E}_{\psi,\varphi}, \tag{8}$$

for the total variation $|\mathsf{E}_{\psi,\varphi}|$ of $\mathsf{E}_{\psi,\varphi}$.

In Definition 3 we used the notation $L(f, M)$ but did not give it a name. From now on, we call it *the* strong operator integral of $f$ or the *maximal* strong operator integral of $f$ with respect to the operator measure $M$. If $D$ is a linear subspace of $D(f, M)$, we may call the restriction of $L(f, M)$ to $D$ *a* strong operator integral. Thus for a POVM $\mathsf{E}$, the operator $\tilde{L}(f, \mathsf{E})$ is a strong operator integral. In this Hilbert space setting the key to our terminology is the possibility to use the whole of $\mathcal{H}$ as a "test space": for any $\varphi$ in the appropriate domain, the integral of $f$ with respect to $\mathsf{E}_{\psi,\phi}$ for *every* $\psi \in \mathcal{H}$ exists.

**Example 1.** Let $A$ be an unbounded selfadjoint operator in $\mathcal{H}$ and $\mathsf{E}: \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ its spectral measure. Then $A = L(f, \mathsf{E})$ and $D(f, \mathsf{E}) = \{\varphi \in \mathcal{H} \mid f \text{ is } \mathsf{E}_{\psi,\varphi}\text{-integrable for all } \psi \in \mathcal{H}\}$ where $f: \mathbb{R} \to \mathbb{R}$ is the identity map. Since $\mathsf{E}_{\psi,\varphi}(X) = \overline{\mathsf{E}_{\varphi,\psi}(X)}$, we may also observe that if $\psi \in \mathcal{H}$, then $f$ is $\mathsf{E}_{\varphi,\psi}$-integrable for all $\varphi$ in the dense subspace $D(f, \mathsf{E})$ of $\mathcal{H}$. But this does not imply that $D(f, \mathsf{E}) = \mathcal{H}$. In particular, we see that in Proposition 2 it is not enough to assume the $M_{y',x}$-integrability of $f$ for all $y'$ in a dense subspace of $F'$.

The above example may serve as a motivation for considering integration with respect to operator measures where the requirement for the test space described before the example is relaxed. This leads us to a host of possibilities for so-called weak operator integrals whose analysis will be our main concern in the sequel.

## 4. Weak operator integrals

Often in physical applications one is led to consider the scalar measures $X \mapsto \mathsf{E}_{\psi,\varphi}(X) = \langle \psi \mid \mathsf{E}(X)\varphi \rangle$ related to a Hilbert operator measure $\mathsf{E}$ instead of the vector measures $\mathsf{E}_\varphi$. In this section we set up a very general framework for this. For any vector spaces $\mathcal{V}_1$, $\mathcal{V}_2$, a map $S: \mathcal{V}_1 \times \mathcal{V}_2 \to \mathbb{C}$ is said to be a *sesquilinear form*, or just sesquilinear, if it is linear in the second and antilinear (i.e. conjugate linear) in the first argument. Such an $S$ is *positive* if $\mathcal{V}_1 = \mathcal{V}_2$ and $S(\varphi, \varphi) \geqslant 0$ for all $\varphi \in \mathcal{V}_1$. Then $S$ satisfies $S(\psi, \varphi) = \overline{S(\varphi, \psi)}$ for all $\psi, \varphi \in \mathcal{V}_1$.

Any vector space $\mathcal{V}$ may be regarded as a dense linear subspace of a Hilbert space $\mathcal{H}$: take $\mathcal{H} = \ell^2_K$ where $K$ is a Hamel basis of $\mathcal{V}$. In the context of sesquilinear forms there is, however, often a postulated way in which the vector space is embedded as a dense subspace of a Hilbert space. When this is the case, it is clear from the context so that, for example, there is a given norm and hence a topology on $\mathcal{V}$.

Let $\mathcal{V} \subseteq \mathcal{H}$ be a dense (linear) subspace of $\mathcal{H}$ and $\mathcal{S}(\mathcal{V})$ the vector space of sesquilinear forms $S: \mathcal{V} \times \mathcal{V} \to \mathbb{C}$. Assume that $\mathsf{E}: \mathcal{A} \to \mathcal{S}(\mathcal{V})$ is a *positive sesquilinear form valued measure*, i.e.

(a) $\mathsf{E}_{\psi,\varphi}: \mathcal{A} \to \mathbb{C}$, $X \mapsto \mathsf{E}_{\psi,\varphi}(X) := [\mathsf{E}(X)](\psi, \varphi)$, is a complex measure for all $\psi, \varphi \in \mathcal{V}$,
(b) $\mathsf{E}_{\varphi,\varphi}(X) \geqslant 0$ for all $\varphi \in \mathcal{V}$ and $X \in \mathcal{A}$.

We refer the reader to [9,10] for a detailed study of such measures. Note that any POVM $\mathsf{E}': \mathcal{A} \to \mathcal{L}(\mathcal{H})$ defines a unique positive sesquilinear form valued measure $\mathsf{E}: \mathcal{A} \to \mathcal{S}(\mathcal{H})$ by setting $[\mathsf{E}(X)](\psi, \varphi) := \langle \psi \mid \mathsf{E}'(X)\varphi \rangle$ (thus, in the case of POVMs, we may put $\mathcal{V} = \mathcal{H}$ below). We always identify $\mathsf{E}'$ with $\mathsf{E}$ and by an abuse of notation simply write $\mathsf{E}' = \mathsf{E}$. Throughout this section, $f: \mathcal{A} \to \mathbb{C}$ is an $\mathcal{A}$-measurable function.

### 4.1. Definition

We begin with the maximal set of pairs $(\psi, \varphi)$ for which $\int f \, d\mathsf{E}_{\psi,\varphi}$ makes sense:

$$\mathcal{W}(f, \mathsf{E}) := \{(\psi, \varphi) \in \mathcal{V} \times \mathcal{V} \mid f \text{ is } \mathsf{E}_{\psi,\varphi}\text{-integrable}\}.$$

Note that $\overline{\mathsf{E}_{\psi,\varphi}(X)} \equiv \mathsf{E}_{\varphi,\psi}(X)$ by positivity so that $|\mathsf{E}_{\psi,\varphi}| = |\mathsf{E}_{\varphi,\psi}|$ and, hence, $\mathcal{W}(f, \mathsf{E}) \subseteq \mathcal{V} \times \mathcal{V}$ is symmetric, i.e. $(\psi, \varphi) \in \mathcal{W}(f, \mathsf{E})$ implies $(\varphi, \psi) \in \mathcal{W}(f, \mathsf{E})$. We then put

$$\mathcal{W}_\varphi(f, \mathsf{E}) := \{\psi \in \mathcal{V} \mid (\psi, \varphi) \in \mathcal{W}(f, \mathsf{E})\} \tag{9}$$

for each $\varphi \in \mathcal{V}$. Since $\mathsf{E}_{\alpha\psi_1+\beta\psi_2,\varphi} = \overline{\alpha}\mathsf{E}_{\psi_1,\varphi} + \overline{\beta}\mathsf{E}_{\psi_2,\varphi}$, $\alpha, \beta \in \mathbb{C}$, $\psi_1, \psi_2 \in \mathcal{V}$, it follows that each $\mathcal{W}_\varphi(f, \mathsf{E}) \subseteq \mathcal{V} \subseteq \mathcal{H}$ is a linear subspace, and the functional $\psi \mapsto \overline{\int f \, d\mathsf{E}_{\psi,\varphi}}$ is linear on that subspace. A similar argument shows that

$$\mathcal{W}_{\varphi_1}(f, \mathsf{E}) \cap \mathcal{W}_{\varphi_2}(f, \mathsf{E}) \subseteq \mathcal{W}_{\alpha\varphi_1+\beta\varphi_2}(f, \mathsf{E}) \tag{10}$$

for any $\varphi_1, \varphi_2 \in \mathcal{V}$ and $\alpha, \beta \in \mathbb{C}$.

We are now interested in (linear) *operators* $T: \mathrm{Dom}(T) \to \mathcal{H}$ determined by these integrals through $\langle \psi \mid T\varphi \rangle = \int f \, d\mathsf{E}_{\psi,\varphi}$. Accordingly, such an operator should have the property that for each $\varphi \in \mathrm{Dom}(T)$: $\langle \psi \mid T\varphi \rangle = \int f \, d\mathsf{E}_{\psi,\varphi}$, where $\psi$ runs through some subset $\mathcal{S}_\varphi$ of $\mathcal{W}_\varphi(f, \mathsf{E})$ which separates the points of $\mathcal{H}$ in the usual sense of self-duality of $\mathcal{H}$. We make this separation requirement to always guarantee that the vector $T\varphi$ is uniquely determined by the integrals $\int f \, d\mathsf{E}_{\psi,\varphi}$ via the inner products just mentioned. Note that here we really want to determine $T\varphi$, and the vector $\psi$ is just in an auxiliary role.[1] Since each $\mathcal{W}_\varphi(f,\mathsf{E})$ is a linear subspace, the necessarily dense[2] linear span $\mathcal{D}_\varphi$ of such a separating subset $\mathcal{S}_\varphi$ is also included in $\mathcal{W}_\varphi(f,\mathsf{E})$, and by linearity, $\langle\psi \mid T\varphi\rangle = \int f\,d\mathsf{E}_{\psi,\varphi}$ for all $\psi\in\mathcal{D}_\varphi$. Hence, we can take the separating subsets to be dense subspaces without restricting generality.

The above requirements imply, in particular, that $\mathrm{Dom}(T)$ must be a subset of

$$\Gamma(f,\mathsf{E}) := \left\{\varphi\in\mathcal{V} \;\middle|\; \mathcal{W}_\varphi(f,\mathsf{E}) \text{ is dense in } \mathcal{H}\right\}.$$

The requirement of choosing the separating subspaces can now be formulated as follows: Let $\mathcal{C}(f,\mathsf{E})$ denote the family of maps

$$\Phi : \Gamma(f,\mathsf{E}) \to \{\mathcal{D}\subseteq\mathcal{H} \mid \mathcal{D} \text{ is a dense subspace}\},$$
$$\Phi(\varphi)\subseteq\mathcal{W}_\varphi(f,\mathsf{E}) \quad \text{for all } \varphi\in\Gamma(f,\mathsf{E}).$$

Note that $\mathcal{C}(f,\mathsf{E})\neq\emptyset$, because an obvious choice is $\Phi(\varphi)=\mathcal{W}_\varphi(f,\mathsf{E})$ for all $\varphi\in\Gamma(f,\mathsf{E})$. We can now state the definition of a weak operator integral.

**Definition 5.** We say that a linear operator $T:\mathrm{Dom}(T)\to\mathcal{H}$ is a *weak operator integral* of $f$ with respect to $\mathsf{E}$, if $\mathrm{Dom}(T)\subseteq\Gamma(f,\mathsf{E})$, and there exists a map $\Phi\in\mathcal{C}(f,\mathsf{E})$, such that

$$\langle\psi \mid T\varphi\rangle = \int f\,d\mathsf{E}_{\psi,\varphi}, \quad \text{for all } \varphi\in\mathrm{Dom}(T),\ \psi\in\Phi(\varphi). \tag{11}$$

We then also say that the weak operator integral $T$ is *associated with the map* $\Phi$. For each $\Phi\in\mathcal{C}(f,\mathsf{E})$, we let $\mathcal{L}_W(f,\mathsf{E},\Phi)$ denote the set of weak operator integrals associated with $\Phi$.

Note that $\Gamma(f,\mathsf{E})$ always contains the trivial subspace $\mathcal{D}_0=\{0\}$, so for every choice of $\Phi$ there corresponds at least a trivial weak operator integral.

The choice of the function $\Phi$ is crucial; different choices may correspond to different operators $T$, because on the one hand, dense subspaces can have a trivial intersection, see Section 6 for an example, and on the other hand, different choices can lead to the same operator. In particular, we have the following result.

**Proposition 5.** *Let $\mathsf{E}:\mathcal{A}\to\mathcal{L}(\mathcal{H})$ be a POVM. Each strong operator integral is also a weak operator integral associated with every $\Phi\in\mathcal{C}(f,\mathsf{E})$.*

**Proof.** According to (7), the domain of the maximal strong operator integral is given by

$$D(f,\mathsf{E}) = \left\{\varphi\in\mathcal{H} \;\middle|\; \mathcal{W}_\varphi(f,\mathsf{E})=\mathcal{H}\right\},$$

so $D(f,\mathsf{E})\subseteq\Gamma(f,\mathsf{E})$. Given any $\Phi\in\mathcal{C}(f,\mathsf{E})$, Eq. (11) holds because of (7). □

Now, given a map $\Phi\in\mathcal{C}(f,\mathsf{E})$, we set

$$\Gamma_c(f,\mathsf{E},\Phi) := \left\{\varphi\in\Gamma(f,\mathsf{E}) \;\middle|\; \Phi(\varphi)\ni\psi\mapsto\int f\,d\mathsf{E}_{\psi,\varphi} \text{ is continuous}\right\},$$

and use the Frechet–Riesz theorem to define a unique map

$$G(f,\mathsf{E},\Phi):\Gamma_c(f,\mathsf{E},\Phi)\to\mathcal{H}, \quad \left\langle\psi \;\middle|\; G(f,\mathsf{E},\Phi)\varphi\right\rangle = \int f\,d\mathsf{E}_{\psi,\varphi} \quad \text{for all } \psi\in\Phi(\varphi).$$

Clearly, the domain of any weak operator integral associated with the map $\Phi$ is included in $\Gamma_c(f,\mathsf{E},\Phi)$. This observation immediately gives the following characterization.

**Proposition 6.** *Fix a $\Phi\in\mathcal{C}(f,\mathsf{E})$. Given any subspace $\mathcal{D}_0$ of $\mathcal{H}$ which is included in $\Gamma_c(f,\mathsf{E},\Phi)$, the restriction $G(f,\mathsf{E},\Phi)|_{\mathcal{D}_0}$ is a weak operator integral (with domain $\mathcal{D}_0$) associated to $\Phi$. Conversely, every element of $\mathcal{L}_W(f,\mathsf{E},\Phi)$ is obtained this way.*

Since the intersection of two dense subspaces does not have to be dense (it can even be $\{0\}$), it is clear that $\Gamma(f,\mathsf{E})$, and therefore also $\Gamma_c(f,\mathsf{E},\Phi)$, are not themselves linear subspaces in general. Hence, there is no canonical choice for a maximal weak operator integral associated with a given map $\Phi$. However, it follows immediately from the above proposition that

[1] If we were interested in *sesquilinear forms* rather than operators, then we should consider $\psi$ and $\varphi$ in an equal footing. However, here we want to consider *operator* integrals, so the given requirement is clearly the most natural one.

[2] Note that the orthogonal complement of a separating subset $\mathcal{S}$ is $\mathcal{H}$, so $\mathcal{S}$ generates a dense subspace.

given two operators $T, T'$, such that $T' \subseteq T$ (that is, $\mathrm{Dom}(T') \subseteq \mathrm{Dom}(T)$ and $T'\varphi = T\varphi$, $\varphi \in \mathrm{Dom}(T')$), and $T \in \mathcal{L}_W(f, \mathsf{E}, \Phi)$, it follows that $T' \in \mathcal{L}_W(f, \mathsf{E}, \Phi)$. In particular, the (nonempty) set $\mathcal{L}_W(f, \mathsf{E}, \Phi)$ is partially ordered via the usual operator ordering, or, equivalently, the inclusion of domains. Moreover, every (nonempty) totally ordered subset of $\mathcal{L}_W(f, \mathsf{E}, \Phi)$ has an upper bound in $\mathcal{L}_W(f, \mathsf{E}, \Phi)$ (the upper bound is obtained by taking the union of the domains of the operators in the chain). Hence, by Zorn's lemma, there exists at least one maximal element in $\mathcal{L}_W(f, \mathsf{E}, \Phi)$. We call such an element a *maximal weak operator integral* associated to $\Phi$.

**Example 2.** For a POVM $\mathsf{E}$ and a bounded function $f$, we have $\Gamma_c(f, \mathsf{E}, \Phi) = \mathcal{H}$ regardless of the choice of $\Phi$, so every weak operator integral is a restriction of the bounded operator $\int f\, d\mathsf{E}$ to some subspace.

**Example 3.** Let $\mathsf{E}(X) := \mu(X)I$, where $\mu$ is a probability measure, and let $f$ be a $\mu$-integrable function. Then $\mathcal{W}(f, \mathsf{E}) = \mathcal{H} \times \mathcal{H}$, and $\Gamma_c(f, \mathsf{E}, \Phi) = \mathcal{H}$, regardless of the choice of $\Phi$, so that weak operator integrals are simply restrictions of $\varphi \mapsto (\int f\, d\mu)\varphi$ to some subspaces of $\mathcal{H}$. If $f$ is not $\mu$-integrable, then $\mathcal{W}(f, \mathsf{E}) = \{(\psi, \varphi) \in \mathcal{H} \times \mathcal{H} \mid \langle \psi \mid \varphi \rangle = 0\}$, and $\mathcal{W}_\varphi(f, \mathsf{E})$ is the orthogonal complement of $\{\varphi\}$. This is dense only for $\varphi = 0$, so $\Gamma(f, \mathsf{E}) = \{0\}$. Hence, there exists only one weak operator integral, which is the zero operator defined on $\{0\}$.

### 4.2. Weak operator integrals determined by a fixed separating subspace

We now look at the class $\mathcal{L}_W(f, \mathsf{E}, \Phi)$ with particular choices of $\Phi$. The canonical choice would be to take, for each $\varphi \in \Gamma(f, \mathsf{E})$, the separating subspace to be the maximal one, i.e. $\Phi(\varphi) = \mathcal{W}_\varphi(f, \mathsf{E})$ for each $\varphi$. However, in practice, it often happens that a dense subspace (of e.g. smooth functions) is fixed. For example, this can be a linear space spanned by some physically relevant orthonormal basis of $\mathcal{H}$ (e.g. the photon number basis of a single mode optical field).

Accordingly, we now investigate the case where a fixed *dense* subspace $\mathcal{D}_s$ is given ($s$ stands for separating). For $\varphi \in \Gamma(f, \mathsf{E})$ we define $\Phi_{\mathcal{D}_s}(\varphi) = \mathcal{D}_s$ if $\mathcal{D}_s \subseteq \mathcal{W}_\varphi(f, \mathsf{E})$ and $\Phi_{\mathcal{D}_s}(\varphi) = \mathcal{W}_\varphi(f, \mathsf{E})$ otherwise. Then we have the following result.

**Proposition 7.** *The set*

$$\hat{D}_{\mathcal{D}_s}(f, \mathsf{E}) := \left\{ \varphi \in \mathcal{V} \,\middle|\, \mathcal{D}_s \subseteq \mathcal{W}_\varphi(f, \mathsf{E}),\ \mathcal{D}_s \ni \psi \mapsto \int f\, d\mathsf{E}_{\psi,\varphi} \in \mathbb{C} \text{ is continuous} \right\}$$

*is the domain of a (clearly unique) element $\hat{L}_{\mathcal{D}_s}(f, \mathsf{E}) \in \mathcal{L}_W(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$. In the case where $\mathsf{E}$ is a POVM, this operator is an extension of the maximal strong operator integral $L(f, \mathsf{E})$.*

**Proof.** Clearly, $\hat{D}_{\mathcal{D}_s}(f, \mathsf{E}) = \{\varphi \in \Gamma_c(f, \mathsf{E}, \Phi_{\mathcal{D}_s}) \mid \mathcal{D}_s \subseteq \mathcal{W}_\varphi(f, \mathsf{E})\}$; in particular, $\hat{D}_{\mathcal{D}_s}(f, \mathsf{E})$ is a subset of $\Gamma_c(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$. We have to show that it is a linear space. Let $\varphi_1, \varphi_2 \in \hat{D}_{\mathcal{D}_s}(f, \mathsf{E})$, and $\alpha, \beta \in \mathbb{C}$. Now $\mathcal{D}_s \subseteq \mathcal{W}_{\varphi_1}(f, \mathsf{E}) \cap \mathcal{W}_{\varphi_2}(f, \mathsf{E}) \subseteq \mathcal{W}_{\alpha\varphi_1+\beta\varphi_2}(f, \mathsf{E})$ (see (10)); in particular, the latter is dense, so $\alpha\varphi_1 + \beta\varphi_2 \in \Gamma(f, \mathsf{E})$, and $\Phi(\alpha\varphi_1 + \beta\varphi_2) = \mathcal{D}_s$. Since $\psi \mapsto \int f\, d\mathsf{E}_{\psi,\varphi_i}$ is continuous on $\mathcal{D}_s$ for $i = 1, 2$, then $\psi \mapsto \int f\, d\mathsf{E}_{\psi,\alpha\varphi_1+\beta\varphi_2}$ is continuous on $\mathcal{D}_s$. Hence, $\alpha\varphi_1 + \beta\varphi_2 \in \Gamma_c(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$. We have shown that $\hat{D}_{\mathcal{D}_s}(f, \mathsf{E})$ is a linear space. By Proposition 6, the restriction of $G(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$ to $\hat{D}_{\mathcal{D}_s}(f, \mathsf{E})$ is an element of $\mathcal{L}_W(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$. It remains to prove that in the case where $\mathsf{E}$ is a POVM, the domain of the maximal strong operator integral is included in $\hat{D}_{\mathcal{D}_s}(f, \mathsf{E})$. But this is so because for $\varphi \in D(f, \mathsf{E})$, we have $\mathcal{D}_s \subseteq \mathcal{H} = \mathcal{W}_\varphi(f, \mathsf{E})$, regardless of $\mathcal{D}_s$. $\square$

Since $L(f, \mathsf{E}) \subseteq \hat{L}_{\mathcal{D}_s}(f, \mathsf{E})$ for any POVM $\mathsf{E}$, one can ask when these two operators are the same. Since $\|\eta\| = \sup\{|\langle \psi \mid \eta \rangle| \mid \psi \in \mathcal{D}_s,\ \|\psi\| \leqslant 1\}$ (as $\mathcal{D}_s$ is dense), the following result is a direct consequence of [29, Theorem 3.5] (see also [17]).

**Proposition 8.** *Suppose $\mathsf{E}$ is a POVM, and let $\mathcal{D}_s \subseteq \mathcal{H}$ be a dense subspace. Then $L(f, \mathsf{E}) = \hat{L}_{\mathcal{D}_s}(f, \mathsf{E})$ if and only if for each $\varphi \in \hat{D}_{\mathcal{D}_s}(f, \mathsf{E})$, we have*

$$\lim_{n\to\infty} \sup_{\psi \in \mathcal{D}_s,\ \|\psi\| \leqslant 1} \int_{X_n} |f|\, d|\mathsf{E}_{\psi,\varphi}| = 0$$

*whenever the sets $X_n \in \mathcal{A}$ satisfy $X_{n+1} \subseteq X_n$, $n \in \mathbb{N}$, and $\bigcap_n X_n = \emptyset$.*

### 4.3. Symmetric weak operator integrals

Since the integrals $\int f\, d\mathsf{E}_{\psi,\varphi}$ are symmetric in the sense that $(\psi, \varphi) \in \mathcal{W}(f, \mathsf{E})$ implies $(\varphi, \psi) \in \mathcal{W}(f, \mathsf{E})$, and $\overline{\int f\, d\mathsf{E}_{\psi,\varphi}} = \int \overline{f}\, d\mathsf{E}_{\varphi,\psi}$, it is natural to ask when a weak operator integral is a symmetric operator. We will not look at the most general case, but concentrate on the elements of $\mathcal{L}_W(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$, with the fixed separating subspace $\mathcal{D}_s \subseteq \mathcal{V}$. Since continuity properties of the integral $\int f\, d\mathsf{E}_{\psi,\varphi}$ with respect to the vectors $\varphi$, $\psi$ are rather weak (even in the case where $\mathsf{E}$ is POVM), we cannot expect that knowing

$$\langle \psi \mid \hat{L}_{\mathcal{D}_s}(f,\mathsf{E})\varphi\rangle = \int f\, d\mathsf{E}_{\psi,\varphi} = \overline{\int \bar{f}\, d\mathsf{E}_{\varphi,\psi}}$$

for all $\psi \in \mathcal{D}_s$, $\varphi \in \hat{D}_{\mathcal{D}_s}(f,\mathsf{E})$, would be sufficient to connect this to the case where $\varphi \in \mathcal{D}_s$ and $\psi \in \hat{D}_{\mathcal{D}_s}(f,\mathsf{E})$. Therefore, we now assume that the dense subspace $\mathcal{D}_s$ satisfies the equivalent conditions of the following trivial lemma.

**Lemma 3.** *Let $\mathcal{D}_s \subseteq \mathcal{V}$ be a subspace. Then $\mathcal{D}_s \subseteq \{\varphi \in \mathcal{H} \mid \mathcal{D}_s \subseteq \mathcal{W}_\varphi(f,\mathsf{E})\}$ if and only if $\mathcal{D}_s \times \mathcal{D}_s \subseteq \mathcal{W}(f,\mathsf{E})$.*

**Proposition 9.** *Suppose that $\mathcal{D}_s \subseteq \mathcal{V}$ is a dense subspace satisfying $\mathcal{D}_s \times \mathcal{D}_s \subseteq \mathcal{W}(f,\mathsf{E})$. We define a (clearly unique) operator $L'_{\mathcal{D}_s}(f,\mathsf{E})$ whose domain and action are given by*

$$D'_{\mathcal{D}_s}(f,\mathsf{E}) := \left\{\varphi \in \mathcal{D}_s \;\middle|\; \mathcal{D}_s \ni \psi \mapsto \int f\, d\mathsf{E}_{\psi,\varphi} \in \mathbb{C} \text{ is continuous}\right\},$$

$$\langle \psi \mid L'_{\mathcal{D}_s}(f,\mathsf{E})\varphi\rangle = \int f\, d\mathsf{E}_{\psi,\varphi}, \quad \psi \in \mathcal{D}_s,\ \varphi \in D'_{\mathcal{D}_s}(f,\mathsf{E}).$$

*Then $L'_{\mathcal{D}_s}(f,\mathsf{E}) \subseteq \hat{L}_{\mathcal{D}_s}(f,\mathsf{E})$. In particular, $L'_{\mathcal{D}_s}(f,\mathsf{E})$ is a weak operator integral, with $L'_{\mathcal{D}_s}(f,\mathsf{E}) \in \mathcal{L}_W(f,\mathsf{E},\Phi_{\mathcal{D}_s})$. Moreover, if $f$ is real valued, then $L'_{\mathcal{D}_s}(f,\mathsf{E})$ is a symmetric operator.*

**Proof.** It is clear that $L'_{\mathcal{D}_s}(f,\mathsf{E})$ is a well-defined operator on the given domain $D'_{\mathcal{D}_s}(f,\mathsf{E})$. (Note that the condition $\mathcal{D}_s \times \mathcal{D}_s \subseteq \mathcal{W}(f,\mathsf{E})$ ensures that the integral is defined.) We now show that $D'_{\mathcal{D}_s}(f,\mathsf{E}) \subseteq \hat{D}_{\mathcal{D}_s}(f,\mathsf{E})$, which by Proposition 6 implies that $L'_{\mathcal{D}_s}(f,\mathsf{E}) \in \mathcal{L}_W(f,\mathsf{E},\Phi_{\mathcal{D}_s})$ and $L'_{\mathcal{D}_s}(f,\mathsf{E}) \subseteq \hat{L}_{\mathcal{D}_s}(f,\mathsf{E})$. Accordingly, let $\varphi \in D'_{\mathcal{D}_s}(f,\mathsf{E})$. In particular, $\varphi \in \mathcal{D}_s$. Since $\mathcal{D}_s \times \mathcal{D}_s \subseteq \mathcal{W}(f,\mathsf{E})$, we have $\mathcal{D}_s \subseteq \mathcal{W}_\varphi(f,\mathsf{E})$. But $\psi \mapsto \int f\, d\mathsf{E}_{\psi,\varphi}$ is continuous on $\mathcal{D}_s$, so $\varphi \in \hat{D}_{\mathcal{D}_s}(f,\mathsf{E})$. It remains to show that $L'_{\mathcal{D}_s}(f,\mathsf{E})$ is symmetric if $f$ is real valued. For that, let $\psi,\varphi \in D'_{\mathcal{D}_s}(f,\mathsf{E})$. Then both of them are also in $\mathcal{D}_s$. Hence,

$$\langle \psi \mid L'_{\mathcal{D}_s}(f,\mathsf{E})\varphi\rangle = \int f\, d\mathsf{E}_{\psi,\varphi} = \overline{\int f\, d\mathsf{E}_{\varphi,\psi}} = \overline{\langle \varphi \mid L'_{\mathcal{D}_s}(f,\mathsf{E})\psi\rangle} = \langle L'_{\mathcal{D}_s}(f,\mathsf{E})\psi \mid \varphi\rangle. \qquad \square$$

We call an operator $L'_{\mathcal{D}_s}(f,\mathsf{E})$ *symmetric weak operator integral* determined by $\mathcal{D}_s$. (Even in the case where $f$ is not real valued.)

**Example 4.** Suppose that $\mathcal{H}$ is separable, let $\{\varphi_n\}_{n\in\mathbb{N}}$ be an orthonormal basis of $\mathcal{H}$, and put $\mathcal{V} := \operatorname{lin}\{\varphi_n \mid n \in \mathbb{N}\}$, and $\mathsf{E} : \mathcal{A} \to \mathcal{S}(\mathcal{V})$ a positive sesquilinear form measure. Let $f : \mathcal{A} \to \mathbb{C}$ be such that

$$\sum_{n\in\mathbb{N}} \left|\int f\, d\mathsf{E}_{\varphi_n,\varphi_m}\right|^2 < \infty \quad \text{for all } m \in \mathbb{N}. \tag{12}$$

In particular, $\int f\, d\mathsf{E}_{\varphi_n,\varphi_m}$ exists for all $n,m \in \mathbb{N}$, that is, $(\varphi_n,\varphi_m) \in \mathcal{W}(f,\mathsf{E})$ for each $n$. By sesquilinearity, it follows that $(\psi,\varphi) \in \mathcal{W}(f,\mathsf{E})$ for all $\psi,\varphi \in \mathcal{V}$, i.e. $\mathcal{W}(f,\mathsf{E}) = \mathcal{V} \times \mathcal{V}$. Hence, $\mathcal{V}$ itself satisfies the conditions of Proposition 9, and we have the symmetric weak operator integral $L'_{\mathcal{V}}(f,\mathsf{E})$. It now follows from (12) that for each $m \in \mathbb{N}$,

$$\mathcal{V} \ni \psi \mapsto \int f\, d\mathsf{E}_{\psi,\varphi_m} = \sum_{n\in N} \langle \psi \mid \varphi_n\rangle \int f\, d\mathsf{E}_{\varphi_n,\varphi_m} \in \mathbb{C}$$

is continuous. Since each $\varphi \in \mathcal{V}$ is a (finite) linear combination of the vectors $\varphi_m$, the continuity holds for each $\varphi \in \mathcal{V}$. Hence, the domain of the symmetric weak operator integral $L'_{\mathcal{V}}(f,\mathsf{E})$ is the whole of $\mathcal{V}$, and its action is determined by

$$L'_{\mathcal{V}}(f,\mathsf{E})\varphi_m = \sum_{n\in N} \left(\int f\, d\mathsf{E}_{\varphi_n,\varphi_m}\right)\varphi_n, \quad \text{for all } m \in \mathbb{N}.$$

Of course, an operator defined via this same formula may have a larger domain; for example, if

$$\mathsf{E}_{\varphi_n,\varphi_m}(X) = \delta_{nm}\mu_n(X), \quad n,m \in N,\ X \in \mathcal{A},$$

where $\delta_{nm}$ is the Kronecker delta and $\{\mu_n\}$ is a sequence[3] of bounded positive measures on $\mathcal{A} \subseteq 2^\Omega$ then $\int f\, d\mathsf{E}_{\varphi_n,\varphi_m} = \delta_{nm} f_m$, where $f_m := \int f\, d\mu_m$, and the largest possible domain of an extension of the weak operator integral $L'_{\mathcal{V}}(f,\mathsf{E})$

[3] Evidently $\mathsf{E}$ defines a POVM if and only if $\sup_{n\in\mathbb{N}} \mu_n(\Omega) < \infty$.

is $\{\varphi \in \mathcal{H} \mid \sum_m |f_m\langle\varphi_m \mid \varphi\rangle|^2 < \infty\}$. Note that this extension is bounded if and only if $\sup_{m\in\mathbb{N}} |f_m| < \infty$. However, the extension is *not* a weak operator integral, because its domain is larger than the form domain $\mathcal{V}$ of the sesquilinear form valued measure $\mathsf{E}$.

We immediately make the following observation.

**Proposition 10.** *Suppose* $\mathsf{E}$ *is a POVM, and the strong operator integral* $L(f,\mathsf{E})$ *is densely defined. Set* $\mathcal{D}_s = D(f,\mathsf{E})$*. Then* $L(f,\mathsf{E}) = L'_{\mathcal{D}_s}(f,\mathsf{E})$*, i.e. the strong operator integral is the symmetric weak operator integral determined by its domain.*

**Proof.** If $\varphi \in \mathcal{D}_s$ then $\int f\, d\mathsf{E}_{\psi,\varphi}$ exists for all $\psi \in \mathcal{H}$, so $\mathcal{D}_s \times \mathcal{D}_s \subseteq \mathcal{H} \times \mathcal{D}_s \subseteq \mathcal{W}(f,\mathsf{E})$. Hence, $L'_{\mathcal{D}_s}(f,\mathsf{E})$ is defined. Moreover, if $\varphi \in \mathcal{D}_s$ then $\psi \mapsto \int f\, d\mathsf{E}_{\psi,\varphi}$ is continuous on the whole $\mathcal{H}$, and hence also on the subspace $\mathcal{D}_s$. Thus $\mathcal{D}_s \subseteq D'_{\mathcal{D}_s}(f,\mathsf{E}) \subseteq \mathcal{D}_s$, and the proof is complete. □

Hence, the domain of the strong operator integral, when dense, is one choice for a separating subspace $\mathcal{D}_s$ of a weak operator integral when $\mathsf{E}$ is a POVM. It is easy to see that even in the general case there is a *maximal choice* for this subspace, which can be explicitly written down:

**Proposition 11.** *The set*

$$\mathcal{D}_F(f,\mathsf{E}) := \left\{\varphi \in \mathcal{H} \;\middle|\; \int |f|\, d\mathsf{E}_{\varphi,\varphi} < \infty\right\} = \left\{\varphi \in \mathcal{H} \;\middle|\; \varphi \in \mathcal{W}_\varphi(f,\mathsf{E})\right\}$$

*is the largest subspace* $\mathcal{D} \subseteq \mathcal{H}$ *such that* $\mathcal{D} \times \mathcal{D} \subseteq \mathcal{W}(f,\mathsf{E})$ *(in the sense that any subspace* $\mathcal{D}$ *with this property, is included in* $\mathcal{D}_F(f,\mathsf{E})$*).*

**Proof.** The fact that the set $\mathcal{D}_F(f,\mathsf{E})$ is a linear subspace of $\mathcal{H}$ follows immediately from Lemma 2. Next we note that given $\varphi, \psi \in \mathcal{H}$, the measure $\mathsf{E}_{\psi,\varphi}$ is a linear combination of four measures of the form $\mathsf{E}_{\psi+i^k\varphi,\psi+i^k\varphi}$, $k = 0, 1, 2, 3$. If $(\psi,\psi) \in \mathcal{W}(f,\mathsf{E})$ and $(\varphi,\varphi) \in \mathcal{W}(f,\mathsf{E})$ then $f$ is integrable with respect to each of the four measures, since $\mathcal{D}_F(f,\mathsf{E})$ is a linear subspace. Hence, $f$ is also integrable with respect to $\mathsf{E}_{\psi,\varphi}$, that is, $(\psi,\varphi) \in \mathcal{W}(f,\mathsf{E})$. Thus, $\mathcal{D}_F(f,\mathsf{E}) \times \mathcal{D}_F(f,\mathsf{E}) \subseteq \mathcal{W}(f,\mathsf{E})$. On the other hand, if $\mathcal{D} \subseteq \mathcal{H}$ is any subspace with $\mathcal{D} \times \mathcal{D} \subseteq \mathcal{W}(f,\mathsf{E})$, then $(\varphi,\varphi) \in \mathcal{W}(f,\mathsf{E})$ for all $\varphi \in \mathcal{D}$, so that $\mathcal{D} \subseteq \mathcal{D}_F(f,\mathsf{E})$. Thus, $\mathcal{D}_F(f,\mathsf{E})$ is the largest of such subspaces $\mathcal{D}$. □

We can now state the following definition.

**Definition 6.** Assume that $\mathcal{D}_F(f,\mathsf{E})$ is dense. The operator

$$L'(f,\mathsf{E}) := L'_{\mathcal{D}_F(f,\mathsf{E})}(f,\mathsf{E}),$$

is called *the largest symmetric weak operator integral* determined by $f$ and $\mathsf{E}$.

All other symmetric operator integrals are restrictions of the largest one. In particular, if $\mathsf{E}$ is a POVM, Proposition 10 gives

$$L(f,\mathsf{E}) \subseteq L'(f,\mathsf{E}).$$

Note that this inclusion holds even in the case where $L(f,\mathsf{E})$ is not dense (which can easily happen even if $\mathcal{D}_F(f,\mathsf{E})$ is dense), because if $\int f\, d\mathsf{E}_{\psi,\varphi}$ exists for all $\psi$ then $\int |f|\, d\mathsf{E}_{\varphi,\varphi} < \infty$.

The following result deals with the case of spectral measures.

**Proposition 12.** *Suppose that* $\mathsf{E}$ *is projection valued. Then*

$$\tilde{L}(f,\mathsf{E}) = L(f,\mathsf{E}) = L'(f,\mathsf{E}).$$

**Proof.** Since $\tilde{L}(f,\mathsf{E}) = L(f,\mathsf{E})$ is densely defined (the usual spectral integral), the weak operator integral $L'(f,\mathsf{E})$ exists, and is an extension of $L(f,\mathsf{E})$. Hence, we only need to show that $\mathrm{Dom}(L'(f,\mathsf{E})) \subseteq \tilde{D}(f,\mathsf{E})$. Define $g : \Omega \to \mathbb{C}$ by $g = \sqrt{|f|}$, and $h : \Omega \to \mathbb{C}$ by setting $h(x) = f(x)/(|f(x)|)$ if $f(x) \neq 0$, and $h(x) = 0$ otherwise. Then $h$ and $g$ are measurable, $h$ is bounded, $g \geqslant 0$, and $f = g^2 h$. Now

$$L(g,\mathsf{E})^* L(gh,\mathsf{E}) \subseteq L\big(g^2 h,\mathsf{E}\big) = L(f,\mathsf{E}), \tag{13}$$

by the usual rules of spectral calculus of unbounded functions. Now

$$\mathcal{D}_F(f,\mathsf{E}) = \left\{\varphi \in \mathcal{H} \;\middle|\; \int |f|\, d\mathsf{E}_{\varphi,\varphi} < \infty\right\} = \mathrm{Dom}\big(L(g,\mathsf{E})\big) = \mathrm{Dom}\big(L(gh,\mathsf{E})\big).$$

According to what has been concluded earlier by using polarization, $f$ is $\mathsf{E}_{\psi,\varphi}$-integrable whenever *both* $\psi$ and $\varphi$ belong to $\mathcal{D}_F(f,\mathsf{E})$. Since $\mathsf{E}$ is a spectral measure, we have

$$\int f\,d\mathsf{E}_{\psi,\varphi} = \int g(gh)\,d\mathsf{E}_{\psi,\varphi} = \big\langle L(g,\mathsf{E})\psi \bigm| L(gh,\mathsf{E})\varphi\big\rangle, \quad \varphi,\psi \in \mathcal{D}_F(f,\mathsf{E}).$$

Indeed, if $g$ is bounded, then this follows from the multiplicativity of the spectral measure, and in the general case, we approximate $g$ with the sequence $(g_n)$, where $g_n(x) = g(x)$ if $g(x) \leqslant n$, and $g_n(x) = 0$ otherwise, and conclude that on the one hand, $L(g_n h,\mathsf{E})\varphi \to L(gh,\mathsf{E})$, $L(g_n,\mathsf{E})\varphi \to L(g,\mathsf{E})$ strongly, and on the other hand, $\int g_n^2 h\,d\mathsf{E}_{\psi,\varphi} \to \int g^2 h\,d\mathsf{E}_{\psi,\varphi}$ by dominated convergence (since $|f| = g^2$ is $\mathsf{E}_{\psi,\varphi}$-integrable).

Now if $\varphi \in \mathrm{Dom}(L'(f,\mathsf{E}))$ then by definition, $\psi \mapsto \int f\,d\mathsf{E}_{\psi,\varphi}$ is continuous in $\mathcal{D}_F(f,\mathsf{E}) = \mathrm{Dom}(L(g,\mathsf{E}))$. By the formula obtained, this implies that $L(gh,\mathsf{E})\varphi$ belongs to $\mathrm{Dom}(L(g,\mathsf{E})^*)$, i.e. $\varphi \in \mathrm{Dom}(L(g,\mathsf{E})^* L(gh,\mathsf{E}))$, so $\varphi \in \mathrm{Dom}(L(f,\mathsf{E}))$. The proof is complete. □

## 5. Sesquilinear form valued integral

### 5.1. The sesquilinear form valued integral of a sesquilinear form valued measure and a measurable function

Since $\mathsf{E}$ is a sesquilinear form valued measure, it is natural to consider the *sesquilinear form valued integral* of a measurable function with respect to $\mathsf{E}$. In this section, we first define this integral, and then consider its connection to weak operator integrals.

We start by defining a function

$$F_{f,\mathsf{E}} : \mathcal{W}(f,\mathsf{E}) \to \mathbb{C}, \quad (\psi,\varphi) \mapsto F_{f,\mathsf{E}}(\psi,\varphi) = \int f\,d\mathsf{E}_{\psi,\varphi}.$$

This function satisfies e.g. $(\alpha\psi_1 + \beta\psi_2, \varphi) \in \mathcal{W}(f,\mathsf{E})$ and $F_{f,\mathsf{E}}(\alpha\psi_1 + \beta\psi_2,\varphi) = \overline{\alpha} F_{f,\mathsf{E}}(\psi_1,\varphi) + \overline{\beta} F_{f,\mathsf{E}}(\psi_2,\varphi)$, for any $(\psi_1,\varphi), (\psi_2,\varphi) \in \mathcal{W}(f,\mathsf{E})$. In addition, $(\psi,\varphi) \in \mathcal{W}(f,\mathsf{E})$ if and only if $(\varphi,\psi) \in \mathcal{W}(f,\mathsf{E})$, and

$$\overline{F_{f,\mathsf{E}}(\psi,\varphi)} = F_{\overline{f},\mathsf{E}}(\varphi,\psi), \quad (\psi,\varphi) \in \mathcal{W}(f,\mathsf{E}). \tag{14}$$

In order to consider $F_{f,\mathsf{E}}$ as a sesquilinear form, we have to restrict its domain of definition to a set of the form $\mathcal{D} \times \mathcal{D} \subseteq \mathcal{W}(f,\mathsf{E})$, where $\mathcal{D} \subseteq \mathcal{V}$ is a subspace. (Clearly, any such restriction is sesquilinear.) According to Proposition 11, there is a canonical choice for $\mathcal{D}$, namely the largest one $\mathcal{D}_F(f,\mathsf{E})$. We denote the restriction of $F_{f,\mathsf{E}}$ to $\mathcal{D}_F(f,\mathsf{E})$ by the same symbol. We say that

$$F_{f,\mathsf{E}} : \mathcal{D}_F(f,\mathsf{E}) \times \mathcal{D}_F(f,\mathsf{E}) \to \mathbb{C}$$

is *the form integral of $f$ with respect to* $\mathsf{E}$. The subspace $\mathcal{D}_F(f,\mathsf{E})$ is the *form domain*.

It follows from (14) that $F_{f,\mathsf{E}}$ is symmetric if $f$ is real valued. It is clearly positive if $f$ is a positive function.

**Remark 3.** The form domain should not be confused with the square integrability domain, which is the form domain of the form integral of $|f|^2$ with respect to $\mathsf{E}$.

In order to consider the connection between the (unique) form integral of $f$ with respect to $\mathsf{E}$, and the various weak operator integrals, we need some preliminaries on the standard extension theory of quadratic forms.

### 5.2. Preliminaries on quadratic forms

We start with some basic preliminaries on the theory of quadratic forms (see e.g. [22,12]). *A quadratic form* is a sesquilinear form $q : \mathcal{D} \times \mathcal{D} \to \mathbb{C}$, where $\mathcal{D} \subseteq \mathcal{H}$ is a *dense* subspace, called the *form domain*. If $q(\psi,\varphi) = \overline{q(\varphi,\psi)}$, for all $\psi,\varphi \in \mathcal{D}$, then $q$ is called *symmetric*, and if $q(\varphi,\varphi) \geqslant 0$ for all $\varphi \in \mathcal{D}$, it is called *positive*.

The *adjoint form* $q^*$ of $q$ is defined on the same domain $\mathcal{D}$, via

$$q^*(\varphi,\psi) = \overline{q(\psi,\varphi)}, \quad \varphi,\psi \in \mathcal{D}.$$

Inclusion $q' \subseteq q$ between two quadratic forms is defined via the corresponding inclusion of the form domains. A linear combination of two quadratic forms is defined in the obvious way, with the domain being the intersection of the form domains. In particular, the *real* and *imaginary parts* of a quadratic form $q$ are defined by

$$\Re q := \frac{1}{2}\big(q + q^*\big), \qquad \Im q := \frac{1}{2i}\big(q - q^*\big).$$

A positive quadratic form $q : \mathcal{D} \times \mathcal{D} \to \mathbb{C}$ is said to be *closed* if $\varphi_n \in \mathcal{D}$, $\varphi_n \to \varphi \in \mathcal{H}$, and

$$\lim_{n,m\to\infty} q(\varphi_n - \varphi_m, \varphi_n - \varphi_m) = 0$$

imply $\varphi \in \mathcal{D}$ and

$$\lim_{n\to\infty} q(\varphi_n - \varphi, \varphi_n - \varphi) = 0.$$

It follows that $q$ is closed if and only if $\Re q$ is closed (see [12, p. 313]).

There is a canonical way of associating a positive selfadjoint operator to a positive closed quadratic form. It is given by the following theorem (see [12,6]).

**Theorem 1.** *Let $q$ be a closed symmetric positive quadratic form with dense form domain $\mathcal{D}$. Then there exists a positive selfadjoint operator $T$ such that* $\mathrm{Dom}(\sqrt{T}) = \mathcal{D}$, *and*

$$q(\psi, \varphi) = \langle \sqrt{T}\psi \mid \sqrt{T}\varphi \rangle, \quad \text{for all } \psi, \varphi \in \mathcal{D}.$$

We say that $T$ given by the above theorem is the *operator associated to the quadratic form* $q$. We will make use of the following simple corollary; it also shows that $T$ is uniquely determined, hence the definite article.

**Proposition 13.** *Let $q$ be a closed symmetric positive quadratic form with dense form domain $\mathcal{D} \subseteq \mathcal{H}$ and $T$ the positive selfadjoint operator associated to it as in Theorem 1. Then*

$$\begin{aligned}
&\mathrm{Dom}(T) = \{\varphi \in \mathcal{D} \mid \mathcal{D} \ni \psi \mapsto q(\psi, \varphi) \in \mathbb{C} \text{ is continuous}\},\\
&q(\psi, \varphi) = \langle \psi \mid T\varphi \rangle, \quad \text{for all } \psi \in \mathcal{D},\ \varphi \in \mathrm{Dom}(T).
\end{aligned} \tag{15}$$

*If there is a Hilbert space $\mathcal{K}$, and an operator $A : \mathcal{D} \to \mathcal{K}$, such that*

$$q(\psi, \varphi) = \langle A\psi \mid A\varphi \rangle, \quad \text{for all } \psi, \varphi \in \mathcal{D},$$

*then $A^*A = T$.*

**Proof.** If $A$ is as in the lemma, we have, by the definition of the adjoint, that

$$\begin{aligned}
\mathrm{Dom}(A^*A) &= \{\varphi \in \mathcal{D} \mid A\varphi \in \mathrm{Dom}(A^*)\}\\
&= \{\varphi \in \mathcal{D} \mid \mathcal{D} \ni \psi \mapsto \langle A\psi \mid A\varphi \rangle \in \mathbb{C} \text{ is continuous}\}\\
&= \{\varphi \in \mathcal{D} \mid \mathcal{D} \ni \psi \mapsto q(\psi, \varphi) \in \mathbb{C} \text{ is continuous}\}.
\end{aligned}$$

In particular, this holds for $\mathcal{K} = \mathcal{H}$ and $A = \sqrt{T}$, which gives (15), because $T = (\sqrt{T})^*\sqrt{T}$. It follows that $\mathrm{Dom}(A^*A) = \mathrm{Dom}(T)$, and if $\varphi \in \mathrm{Dom}(T)$, $\psi \in \mathcal{D}$, we have

$$\langle \psi \mid A^*A\varphi \rangle = \langle A\psi \mid A\varphi \rangle = q(\psi, \varphi) = \langle \psi \mid T\varphi \rangle.$$

As $\mathcal{D}$ is dense, this implies that $A^*A = T$. □

**Remark 4.** Note that it is nontrivial that the domain of $A^*A$ in the above proposition is actually dense. This fact follows from the above theorem. Note also that the operator $A$ is automatically closed, because the form $q$ was assumed to be closed. A special case of this result is the well-known theorem of von Neumann (see e.g. [23, p. 180]), which says that $A^*A$ is selfadjoint if $A$ is a closed densely defined operator.

### 5.3. Connection between form and weak operator integrals

In the case where $\mathcal{D}_F(f, \mathsf{E})$ is dense, the sesquilinear form $F_{f,\mathsf{E}}$ is a quadratic form. In general, the adjoint form is given by

$$F^*_{f,\mathsf{E}}(\psi, \varphi) = \int \overline{f}\, d\mathsf{E}_{\psi,\varphi}, \quad \psi, \varphi \in \mathcal{D}_F(f, \mathsf{E}).$$

Moreover,

$$\Re(F_{f,\mathsf{E}}) \subseteq F_{\Re(f),\mathsf{E}}, \qquad \Im(F_{f,\mathsf{E}}) \subseteq F_{\Im(f),\mathsf{E}},$$

where $\Re(f)$ and $\Im(f)$ are the real and imaginary parts of the function $f$, respectively. We can further decompose these into positive and negative parts, so that

$$f = f_1 - f_2 + i(f_3 - f_4),$$
$$f_i \geqslant 0, \qquad \left|\Re(f)\right| = f_1 + f_2, \qquad \left|\Im(f)\right| = f_3 + f_4.$$

Then clearly $\mathcal{D}_F(f, \mathsf{E}) = \bigcap_{i=1}^4 \mathcal{D}_F(f_i, \mathsf{E})$, so the form integral decomposes naturally as the linear combination of the corresponding positive forms:

$$F_{f,\mathsf{E}} = F_{f_1,\mathsf{E}} - F_{f_2,\mathsf{E}} + iF_{f_3,\mathsf{E}} - iF_{f_4,\mathsf{E}}.$$

Unfortunately, the situation is not so simple in case of the weak operator integrals. However, the following result holds:

**Proposition 14.** *Suppose that $\mathcal{D}_F(f, \mathsf{E})$ is dense. Then*

$$L'(f, \mathsf{E}) \supseteq L'(f_1, \mathsf{E}) - L'(f_2, \mathsf{E}) + iL'(f_3, \mathsf{E}) - iL'(f_4, \mathsf{E}) \in \mathcal{L}_W(f, \mathsf{E}, \Phi_{\mathcal{D}_s}),$$

*where $\mathcal{D}_s = \mathcal{D}_F(f, \mathsf{E})$, and the inclusion can be interpreted as the ordering relation in the class $\mathcal{L}_W(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$ of weak operator integrals.*

**Proof.** First note that since $\mathcal{D}_F(f, \mathsf{E})$ is dense, so is each $\mathcal{D}_F(f_i, \mathsf{E})$; hence, the weak operator integrals $L'(f_i, \mathsf{E})$ are defined. Denote $A := L'(f_1, \mathsf{E}) - L'(f_2, \mathsf{E}) + iL'(f_3, \mathsf{E}) - iL'(f_4, \mathsf{E})$. By definition,

$$\mathrm{Dom}(A) = \bigcap_{i=1}^{4} \mathrm{Dom}\bigl(L'(f_i, \mathsf{E})\bigr),$$

so that $\mathrm{Dom}(A) \subseteq \mathcal{D}_F(f, \mathsf{E})$. If $\varphi \in \mathrm{Dom}(A)$, each functional $\psi \mapsto \int f_i \, d\mathsf{E}_{\psi,\varphi}$ is continuous on $\mathcal{D}_F(f, \mathsf{E}) = \bigcap_{i=1}^4 \mathcal{D}_F(f_i, \mathsf{E})$, and coincides with $\psi \mapsto \langle \psi \mid L'(f_i, \mathsf{E})\varphi \rangle$ there. This implies that $\varphi \in \mathrm{Dom}(L'(f, \mathsf{E}))$. Hence, $A \subseteq L'(f, \mathsf{E})$. Since $L'(f, \mathsf{E}) \in \mathcal{L}_W(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$, it follows from Proposition 6 that also $A \in \mathcal{L}_W(f, \mathsf{E}, \Phi_{\mathcal{D}_s})$. This completes the proof. $\square$

We now consider the relationship between $F_{f,\mathsf{E}}$ and $L'(f, \mathsf{E})$ in the case of a positive function $f$, and a POVM $\mathsf{E}$.

**Proposition 15.** *Let $\mathsf{E}$ be a POVM and $f : \Omega \to \mathbb{C}$ a positive measurable function, such that $\mathcal{D}_F(f, \mathsf{E})$ is dense. Then the quadratic form $F_{f,\mathsf{E}}$ is symmetric, positive and closed. The associated positive selfadjoint operator $T$ (see Theorem 1), is given by*

$$T = \bigl(L(\sqrt{f}, \mathsf{F})V\bigr)^* L(\sqrt{f}, \mathsf{F})V,$$

*where $(\mathcal{K}, \mathsf{F}, V)$ is any Naimark dilation of $\mathsf{E}$. Moreover,*

$$T = L'(f, \mathsf{E}),$$

*i.e., $T$ is the largest symmetric weak operator integral determined by $f$ and $\mathsf{E}$. In particular, $L'(f, \mathsf{E})$ is selfadjoint.*

**Proof.** Clearly, $F_{f,\mathsf{E}}(\varphi, \varphi) \geqslant 0$ for all $\varphi \in F_{f,\mathsf{E}}$. Let $(\mathcal{K}, \mathsf{F}, V)$ be a Naimark dilation of $\mathsf{E}$, so that $\mathsf{E}(X) = V^*\mathsf{F}(X)V$ and $\mathsf{F}$ is projection valued. Then

$$\mathcal{D}_F(f, \mathsf{E}) = \bigl\{\varphi \in \mathcal{H} \bigm| V\varphi \in D(\sqrt{f}, \mathsf{F})\bigr\},$$
$$F_{f,\mathsf{E}}(\varphi, \varphi) = \bigl\|L(\sqrt{f}, \mathsf{F})V\varphi\bigr\|^2, \quad \text{for all } \varphi \in \mathcal{D}_F(f, \mathsf{E}). \tag{16}$$

Now if $\varphi_n \in \mathcal{D}_F(f, \mathsf{E})$, such that $\varphi_n \to \varphi \in \mathcal{H}$, and $\lim_{n,m\to\infty} F_{f,\mathsf{E}}(\varphi_n - \varphi_m, \varphi_n - \varphi_m) = 0$, it follows that $V\varphi_n \to V\varphi$, and $(L(\sqrt{f}, \mathsf{F})V\varphi_n)_n$ converges in $\mathcal{K}$. Since $\mathsf{F}$ is projection valued, $L(\sqrt{f}, \mathsf{F})$ is a closed operator on its domain, so $V\varphi \in D(\sqrt{f}, \mathsf{F})$, and $\lim_{n\to\infty} L(\sqrt{f}, \mathsf{F})V\varphi_n = L(\sqrt{f}, \mathsf{F})V\varphi$. But this implies that $\varphi \in \mathcal{D}_F(f, \mathsf{E})$, and $\lim_{n\to\infty} F_{f,\mathsf{E}}(\varphi_n - \varphi, \varphi_n - \varphi) = 0$. Hence the form $F_{f,\mathsf{E}}$ is closed. From (16) it now follows by polarization and Proposition 13 that $(L(\sqrt{f}, \mathsf{F})V)^* L(\sqrt{f}, \mathsf{F})V$ is the selfadjoint operator associated to the form $F_{f,\mathsf{E}}$. From Proposition 13, we immediately see that $T = L'(f, \mathsf{E})$. This completes the proof. $\square$

**Remark 5.** Notice that in the above proposition, $V^*L(f, \mathsf{F})V \subseteq T = L'(f, \mathsf{E})$, because

$$V^*L(\sqrt{f}, \mathsf{F}) \subseteq \bigl(L(\sqrt{f}, \mathsf{F})V\bigr)^*. \tag{17}$$

From (6), we know that $V^*L(f, \mathsf{F})V = \tilde{L}(f, \mathsf{E})$. Hence, in this case, the difference between the strong operator integral on the square integrability domain and the maximal symmetric weak operator integral is in the operator inclusion (17), which can be proper because continuity of the functional $\psi \mapsto \langle L(\sqrt{f}, \mathsf{F})\psi \mid \varphi \rangle$ on $V(\mathcal{H}) \cap \mathrm{Dom}(L(\sqrt{f}, \mathsf{F}))$ does not necessarily imply its continuity on the full domain $\mathrm{Dom}(L(\sqrt{f}, \mathsf{F}))$.

## 6. Application: moment operators of variance-free POVMs

In the introduction we motivated the above theory with quantum mechanics, where observables are represented by positive operator valued measures. Here we conclude the paper by applying this theory to the determination of moment operators of variance-free POVMs. Recall that the physical interpretation of such a POVM is an observable that cannot be "sharpened" to a projection valued (i.e. von Neumann type) observable with the same first moment, unless it is already projection valued; see Proposition 16 below. We first derive some general results, and then present an application involving the momentum observable of a spatially confined quantum system.

### 6.1. Moment operators and forms of a POVM

Let $\mathsf{E}:\mathcal{B}(\mathbb{R})\to\mathcal{L}(\mathcal{H})$ be a normalized POVM. The most straightforward way of looking at the moments of the physically relevant measurement outcome distributions $\mathsf{E}_{\varphi,\varphi}$ is via the *moment forms*

$$F_{x^k,\mathsf{E}}(\psi,\varphi)=\int x^k\,d\mathsf{E}_{\psi,\varphi},\quad \psi,\varphi\in\mathcal{D}_F\left(x^k,\mathsf{E}\right).$$

However, it is often desirable to look at *operator valued moments* (or *moment operators*) instead. They are defined as operator integrals $\int x^k\,d\mathsf{E}$ of the real functions $x\mapsto x^k$ where $k\in\mathbb{N}$.[4] We have three natural ways to define these operators: $\tilde{\mathsf{E}}[k]:=\tilde{L}(x^k,\mathsf{E})$, $\mathsf{E}[k]:=L(x^k,\mathsf{E})$, and $\mathsf{E}'[k]:=L'(x^k,\mathsf{E})$. Recall that $\tilde{\mathsf{E}}[k]\subseteq\mathsf{E}[k]\subseteq\mathsf{E}'[k]$ and their domains are

$$\operatorname{Dom}\left(\tilde{\mathsf{E}}[k]\right)=\left\{\varphi\in\mathcal{H}\;\middle|\;\int x^{2k}\,d\mathsf{E}_{\varphi,\varphi}(x)<\infty\right\},$$

$$\operatorname{Dom}\left(\mathsf{E}[k]\right)=\left\{\varphi\in\mathcal{H}\;\middle|\;\int |x|^k\,d|\mathsf{E}_{\psi,\varphi}|<\infty\text{ for all }\psi\in\mathcal{H}\right\},$$

$$\operatorname{Dom}\left(\mathsf{E}'[k]\right)=\left\{\varphi\in\mathcal{D}_F\left(x^k,\mathsf{E}\right)\;\middle|\;\mathcal{D}_F\left(x^k,\mathsf{E}\right)\ni\psi\mapsto\int x^k\,d\mathsf{E}_{\psi,\varphi}\in\mathbb{C}\text{ is continuous}\right\}$$
$$\text{if }\mathcal{D}_F\left(x^k,\mathsf{E}\right)=\left\{\varphi\in\mathcal{H}\;\middle|\;\int |x|^k\,d\mathsf{E}_{\varphi,\varphi}<\infty\right\}\text{ is dense in }\mathcal{H}.$$

As mentioned in the Introduction, the *variance form* is defined on $\operatorname{Dom}(\tilde{\mathsf{E}}[1])=\mathcal{D}_F(x^2,\mathsf{E})$ via

$$(\psi,\varphi)\mapsto F_{x^2,\mathsf{E}}(\psi,\varphi)-\left\langle\tilde{\mathsf{E}}[1]\psi\;\middle|\;\tilde{\mathsf{E}}[1]\varphi\right\rangle.$$

If $\operatorname{Dom}(\tilde{\mathsf{E}}[1])$ is dense and this variance form is identically zero, the POVM $\mathsf{E}$ is called *variance-free*. We then have the following result.

**Proposition 16.** *(See [14].) If $\mathsf{E}$ is variance-free, and $\tilde{\mathsf{E}}[1]$ is selfadjoint, then $\mathsf{E}$ is projection valued (with $\tilde{E}[1]$ the associated selfadjoint operator).*

The variance form, and also higher moments, can be conveniently investigated in terms of a Naimark dilation $(\mathcal{K},\mathsf{F},V)$ of $\mathsf{E}$; recall that

$$\mathsf{E}(X)=V^*\mathsf{F}(X)V,\quad\text{for all }X\in\mathcal{B}(\mathbb{R}).$$

From Proposition 12 one sees that $\tilde{\mathsf{F}}[k]=\mathsf{F}[k]=\mathsf{F}'[k]$ for all $k\in\mathbb{N}$. Moreover, $\operatorname{Dom}(\mathsf{F}[k]V)=\operatorname{Dom}(\tilde{\mathsf{E}}[k])$ and

$$\tilde{\mathsf{E}}[k]=V^*\mathsf{F}[k]V.\tag{18}$$

(This was also proved in [16].) The variance-free case is characterized by the following proposition, essentially proved in [28]. We include the proof for completeness.

**Proposition 17.** *Suppose that $\operatorname{Dom}(\tilde{\mathsf{E}}[1])$ is dense. The following conditions are equivalent:*

(i) $\mathsf{E}$ *is variance-free;*
(ii) $\mathsf{F}[1](\operatorname{Dom}(\mathsf{F}[1])\cap V(\mathcal{H}))\subseteq V(\mathcal{H})$;
(iii) $\mathsf{F}[j](\operatorname{Dom}(\mathsf{F}[j])\cap V(\mathcal{H}))\subseteq V(\mathcal{H})$ *for all* $j\in\mathbb{N}$.

*If the conditions hold, then $\tilde{\mathsf{E}}[j]=\tilde{\mathsf{E}}[1]^j$ for all $j\in\mathbb{N}$.*

[4] For simplicity, we will use the symbol $x^k$ to denote the function $x\mapsto x^k$.

**Proof.** If $\mathsf{E}$ is variance-free, then

$$\|VV^*\mathsf{F}[1]V\varphi\|^2 = \|V\tilde{\mathsf{E}}[1]\varphi\|^2 = \|\tilde{\mathsf{E}}[1]\varphi\|^2 = \int x^2\,d\mathsf{E}_{\varphi,\varphi}(x) = \int x^2\,d\mathsf{F}_{V\varphi,V\varphi}(x) = \|\mathsf{F}[1]V\varphi\|^2,$$

for all $\varphi \in \mathrm{Dom}(\tilde{\mathsf{E}}[1])$, where we have used the fact that $\mathsf{F}$ is always variance-free because it is projection valued. This shows that $\mathsf{F}[1]V\varphi \in V(\mathcal{H})$ for all $\varphi \in \mathrm{Dom}(\tilde{\mathsf{E}}[1]) = \mathrm{Dom}(\mathsf{F}[1]V)$, which is equivalent to (ii). That (ii) implies (iii) follows by induction and the fact that $\mathsf{F}[j+1] = \mathsf{F}[j]\mathsf{F}[1]$. Condition (iii) trivially implies (ii), and assuming (ii) implies $VV^*\mathsf{F}[1]V = \mathsf{F}[1]V$, which implies (i) by the same computation as above. This condition also gives the last statement by induction. □

The proposition shows that for variance-free POVMs, we have $\tilde{\mathsf{E}}[j] = \tilde{\mathsf{E}}[1]^j$, i.e. moment operators defined via the strong operator integral on the square integrability domain behave exactly in the same way as in the case of spectral measures. We now proceed to look at the weak operator integrals $\mathsf{E}'[k]$.

In general, if $k$ is even, i.e. $k = 2j$, $j \in \mathbb{N}$, and $\mathcal{D}_F(x^{2j}, \mathsf{E}) = \mathrm{Dom}(\tilde{\mathsf{E}}[j])$ is dense, it follows from Proposition 15 that

$$\mathsf{E}'[2j] = \big(\mathsf{F}[j]V\big)^*\big(\mathsf{F}[j]V\big) \tag{19}$$

is positive and selfadjoint. In particular, $\mathrm{Dom}(\mathsf{E}'[2j])$ consists of exactly those vectors $\varphi \in \mathrm{Dom}(\tilde{\mathsf{E}}[j])$ for which $\mathsf{F}[j]V\varphi \in \mathrm{Dom}((\mathsf{F}[j]V)^*)$. Note that

$$V^*\mathsf{F}[j] \subseteq \big(\mathsf{F}[j]V\big)^* \tag{20}$$

always holds; this is consistent with the general fact $\tilde{\mathsf{E}}[2j] \subseteq \mathsf{E}'[2j]$.

**Proposition 18.** *Suppose that* $\mathsf{E}$ *is variance-free, and* $j \in \mathbb{N}$ *is such that* $\mathrm{Dom}(\tilde{\mathsf{E}}[j])$ *is dense. Then* $\mathsf{E}'[2j] = \tilde{\mathsf{E}}[j]^*\tilde{\mathsf{E}}[j]$.

**Proof.** We use (ii) in Proposition 17, which implies $\mathsf{F}[j]V = VV^*\mathsf{F}[j]V = V\tilde{\mathsf{E}}[j]$. Now a vector $\varphi \in \mathcal{H}$ satisfies $V\varphi \in \mathrm{Dom}((V\tilde{\mathsf{E}}[j])^*)$ if and only if $\psi \mapsto \langle V\tilde{\mathsf{E}}[j]\psi \mid V\varphi\rangle = \langle \tilde{\mathsf{E}}[j]\psi \mid \varphi\rangle$ is continuous on $\mathrm{Dom}(\tilde{\mathsf{E}}[j])$, which happens exactly when $\varphi \in \mathrm{Dom}(\tilde{\mathsf{E}}[j]^*)$. Hence, $(\mathsf{F}[j]V)^*V = (V\tilde{\mathsf{E}}[j])^*V = \tilde{\mathsf{E}}[j]^*$ and $\mathsf{E}'[2j] = (\mathsf{F}[j]V)^*(\mathsf{F}[j]V) = (V\tilde{\mathsf{E}}[j])^*(V\tilde{\mathsf{E}}[j]) = \{(V\tilde{\mathsf{E}}[j])^*V\}\tilde{\mathsf{E}}[j] = \tilde{\mathsf{E}}[j]^*\tilde{\mathsf{E}}[j]$. □

This proposition suggests that even though the strong operator integral $\tilde{\mathsf{E}}[2]$ factorizes as $\tilde{\mathsf{E}}[2] = \tilde{\mathsf{E}}[1]^2$ for every variance-free POVM, this is not necessarily true for the corresponding weak operator integral. And in fact, in the next subsection we exhibit a simple explicit example of a non-projection valued variance-free POVM with $\tilde{\mathsf{E}}[1] = \mathsf{E}[1] = \mathsf{E}'[1]$, and $\tilde{\mathsf{E}}[2] = \mathsf{E}[2] = \mathsf{E}[1]^2$, but $\mathsf{E}'[2] = \mathsf{E}[1]^*\mathsf{E}[1] \neq \mathsf{E}'[1]^2$.

We conclude that the first two moment operators can (at least in some cases) distinguish spectral measures from variance-free POVMs, *provided that the weak operator integral is used in defining the moments.*

### *6.2. Momentum observable for a confined quantum system*

The application we shall discuss here comes under the general heading of *quantum confinement*. At the start of quantum theory proper, it was realized that Schrödinger's equation for the energy spectrum of a system could be written so as to model particles confined to a spatial region, in particular, to a compact interval along the line, say $\mathcal{I} = [0, \ell]$. This was a toy model at the time, but had the merit that the spectrum and eigenfunctions could be written down simply, in terms of circular functions. Along with this model were associated models in which the particles were only weakly confined and could get out if their energy was great enough, the so-called finite well – or barrier – systems. Indeed, tunneling through a potential barrier was one of the early triumphs of wave mechanics.

With the passage of time, experimental methods of confinement have improved very considerably. Nowadays it is feasible to confine small number of atoms, molecules, or other small systems fairly strictly, and for impressive intervals of time (by atomic standards of time). This is done by a combination of electromagnetic fields, including laser beams, and low temperature methods. Atoms can even be attached to the interior of *buckyballs* and studied there, which seems iconic [25].

At the general level, confinement can be understood as a restriction of the set of states of a quantum system with a Hilbert space $\mathcal{K}$. An obvious way to do this is to restrict to a closed subspace $\mathcal{H} \subset \mathcal{K}$, which will then be the Hilbert space for the confined system. We let $U : \mathcal{H} \to \mathcal{K}$ be the canonical isometry. Now if $\mathsf{F} : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{K})$ is a spectral measure, describing some projection valued observable in the large system, we can define a corresponding POVM $\mathsf{E} : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ for the confined system via

$$\mathsf{E}(X) := U^*\mathsf{F}(X)U. \tag{21}$$

This brings us the setup described above, where $(\mathcal{K}, \mathsf{F}, U)$ is a Naimark dilation of $\mathsf{E}$. However, the possible physical meaning of $\mathsf{E}$ is not necessarily directly obtainable from that of $\mathsf{F}$, unless the physical meaning of the confinement is made more clear. We return to this below.

Since the purpose of the present discussion is to give a physically relevant example rather than a full analysis of confinement, we will now restrict consideration to *spatial confinement*, and consider the simplest case of a massive nonrelativistic particle (in the sequel of mass $m$) moving in one dimension, in units where $\hbar = 1$. Similar analysis could be done in a more realistic three-dimensional case, with more additional technicalities obscuring the essential features already present in the one-dimensional case.

The Hilbert space of the system is $\mathcal{K} = L^2(\mathbb{R})$, and the (sharp) position observable is $\mathsf{Q}_{\mathbb{R}} : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(L^2(\mathbb{R}))$,

$$\big(\mathsf{Q}_{\mathbb{R}}(X)\psi\big)(x) := \chi_X(x)\psi(x), \quad X \in \mathcal{B}(\mathbb{R}),\ \psi \in L^2(\mathbb{R}),\ x \in \mathbb{R}.$$

The (sharp) momentum observable is $\mathsf{P}_{\mathbb{R}} : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(L^2(\mathbb{R}))$

$$\mathsf{P}_{\mathbb{R}}(Y) := \mathcal{F}^*\mathsf{Q}_{\mathbb{R}}(Y)\mathcal{F}, \quad Y \in \mathcal{B}(\mathbb{R}),$$

where $\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is the Fourier–Plancherel operator determined by

$$(\mathcal{F}\psi)(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ixt}\psi(t)\,dt, \quad \psi \in L^1(\mathbb{R}) \cap L^2(\mathbb{R}),\ x \in \mathbb{R}.$$

Since $\mathsf{Q}_{\mathbb{R}}$ and $\mathsf{P}_{\mathbb{R}}$ are spectral measures, there is no ambiguity in defining their moment operators, see Proposition 12. In particular, $\mathsf{Q}_{\mathbb{R}}[1]$ and $\mathsf{P}_{\mathbb{R}}[1]$ are the usual selfadjoint position and momentum operators[5]

$$\big(\mathsf{Q}_{\mathbb{R}}[1]\psi\big)(x) = x\psi(x), \qquad \big(\mathsf{P}_{\mathbb{R}}[1]\psi\big)(x) = -i\psi'(x)$$

where $\psi'(x) := d\psi(x)/dx$ (and similarly $\psi''(x) := d^2\psi(x)/dx^2$). Recall that, e.g., $\mathrm{Dom}(\mathsf{P}_{\mathbb{R}}[1])$ consists of those absolutely continuous functions $\psi \in L^2(\mathbb{R})$ for which $\psi' \in L^2(\mathbb{R})$. The Hamiltonian, or energy operator, is $(2m)^{-1}\mathsf{P}_{\mathbb{R}}[1]^2 = (2m)^{-1}\mathsf{P}_{\mathbb{R}}[2]$ whose spectrum is absolutely continuous and equal to $[0, \infty)$. We observe that there is no potential acting and $(2m)^{-1}\mathsf{P}_{\mathbb{R}}[2]$ is therefore the kinetic energy operator.

Now suppose that the particle is confined to move on a (fixed) bounded interval taken to be $\mathcal{I} = [0, \ell]$, where $\ell > 0$ is the length of the interval. The confined system has the Hilbert space $L^2([0, \ell])$, with the isometry $U : L^2([0, \ell]) \to L^2(\mathbb{R})$ given by $(U\psi)(x) = \psi(x)$ if $x \in [0, \ell]$ and $(U\psi)(x) = 0$ otherwise.

If the confinement is considered as being effected by a deep potential well, the perfect confinement being an idealization, one can argue that the POVMs obtained from the observables for the free particle via the compression (21), retain their physical meaning also for the confined system. It is worth noting that POVMs on $L^2([0, \ell])$ can alternatively be understood as observables of an entirely different physical system, namely the free particle *on the circle* (i.e. the one obtained by identifying the endpoints of the interval). This system has translational symmetry modulo $\ell$, the translations being generated by the selfadjoint extensions of $-id/dx$ corresponding to boundary conditions periodic up to a phase,[6] each of which qualifies as a momentum observable for that system. As expected, the corresponding kinetic energy operators are obtained by squaring these, in a way analogous to the free particle on a line. However, these operators do not have a physical meaning when $L^2([0, \ell])$ is considered as a *confined* system, which does not have translation symmetry.

Applying (21) to the position observable, we end up with an obvious position observable for the confined system: the (restricted) spectral measure $\mathsf{Q} : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(L^2(\mathcal{I}))$,

$$\big(\mathsf{Q}(X)\varphi\big)(x) := \chi_X(x)\varphi(x), \quad X \in \mathcal{B}(\mathbb{R}),\ \varphi \in L^2(\mathcal{I}),\ x \in \mathcal{I}.$$

Again, there is no ambiguity in calculating the moments of $\mathsf{Q}$. However, the situation is totally different for the case of momentum: we define $\mathsf{P} : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(L^2(\mathcal{I}))$ via

$$\mathsf{P}(Y) := U^*\mathsf{P}_{\mathbb{R}}(Y)U, \quad Y \in \mathcal{B}(\mathbb{R}).$$

This is now a normalized POVM which is *not* projection valued, because the projection $UU^*$ is a function of the position operator, and thus does not commute with $\mathsf{P}_{\mathbb{R}}(Y)$, in general. It is therefore interesting to look at the first moment operators, $\tilde{\mathsf{P}}[1]$, $\mathsf{P}[1]$, and $\mathsf{P}'[1]$, which *would be* all equal and selfadjoint if $\mathsf{P}$ were a spectral measure.

We first note that if an absolutely continuous function $\psi$ vanishes identically outside the interval $[0, \ell]$, then so does its derivative $\psi'$. According to Proposition 17, this shows that $\mathsf{P}$ is variance-free, and we have $\tilde{\mathsf{P}}[n] = \tilde{\mathsf{P}}[1]^n$ for all $n \in \mathbb{N}$. In order to determine $\tilde{\mathsf{P}}[1]$, we use the fact that $\mathrm{Dom}(\tilde{\mathsf{P}}[1]) = \mathrm{Dom}(\mathsf{P}_{\mathbb{R}}[1]U)$. Now this domain consists of exactly those functions $\varphi \in L^2(\mathcal{I})$ for which $U\varphi$ is absolutely continuous, with $(U\varphi)' \in L^2(\mathbb{R})$. But $U\varphi$ is absolutely continuous precisely when $\varphi$ is absolutely continuous in the interval $\mathcal{I} = [0, \ell]$, *and vanishes at the endpoints*. (If it did not vanish, then there would be a discontinuity.)

The set of absolutely continuous functions $\varphi \in L^2(\mathcal{I})$ with $\varphi' \in L^2(\mathcal{I})$ and $\varphi(0) = \varphi(\ell) = 0$ is denoted by $\mathrm{Dom}(P_0)$, and the corresponding version of the differential operator $-id/dx$ by $P_0$, acting in $L^2(\mathcal{I})$. Hence, $\mathsf{P}_{\mathbb{R}}[1]U = UP_0$. This implies

[5] This is the well-known Schrödinger representation of the canonical commutation relations, see e.g. [21].

[6] This is the standard example used in functional analysis textbooks (see e.g. [22]) to demonstrate the fact that a symmetric operator can have a multitude of selfadjoint extensions.

$\tilde{\mathsf{P}}[1] = U^*\mathsf{P}_{\mathbb{R}}[1]U = U^*UP_0 = P_0$. The operator is well known to be densely defined and closed, but *not* selfadjoint (see e.g. [22]). This is consistent with the fact that $\mathsf{P}$ is variance-free (see Proposition 16).

Note that $P_0$ does have selfadjoint extensions, but these are given by the boundary conditions of the form $\psi(0) = e^{i\theta}\psi(\ell)$, and are related to the circle system mentioned above.

We have shown that $\tilde{\mathsf{P}}[n] = P_0^n$. In Appendix A we will show that the same is true for the full strong operator integrals. In particular, for the first two moments we have

$$\tilde{\mathsf{P}}[1] = \mathsf{P}[1] = P_0, \qquad \tilde{\mathsf{P}}[2] = \mathsf{P}[2] = P_0^2 = \mathsf{P}[1]^2, \tag{22}$$

i.e. the moment operators factorize exactly as if $\mathsf{P}$ were projection valued. The domain of $\mathsf{P}[2]$ is characterized by the boundary conditions $\psi(0) = \psi(\ell) = \psi'(0) = \psi'(\ell) = 0$ (and the usual requirements that $\psi$ be continuously differentiable with $\psi'$ absolutely continuous and $\psi'' \in L^2(\mathcal{I})$).

We now look at the weak operator integrals $\mathsf{P}'[j]$. Since $\mathsf{P}$ is variance-free, it follows from Proposition 18 that $\mathsf{P}'[2j] = \tilde{\mathsf{P}}[j]^*\tilde{\mathsf{P}}[j] = (P_0^j)^*P_0^j$. Most importantly, the weak operator integral version of the second moment operator is $\mathsf{P}'[2] = P_0^*P_0$. We will show in Appendix A that $\mathsf{P}'[1] = P_0$, so we can conclude with

$$\mathsf{P}'[1] = P_0, \qquad \mathsf{P}'[2] = P_0^*P_0 \neq P_0^2 = \mathsf{P}'[1]^2. \tag{23}$$

In contrast to the corresponding strong integral $\mathsf{P}[2]$, the domain of $\mathsf{P}'[2]$ is characterized by the less restrictive Dirichlet boundary condition $\psi(0) = \psi(\ell) = 0$, which makes the second derivative selfadjoint. The operator $(2m)^{-1}\mathsf{P}'[2]$ is precisely the Hamiltonian operator for the particle of mass $m$ confined to move in the interval $\mathcal{I}$ (the infinite square well). Its spectrum consists of isolated eigenvalues $\lambda_n = n^2\pi^2/(2m\ell^2)$, all of unit multiplicity, with corresponding eigenvectors

$$\psi_n(x) = \sqrt{\frac{2}{\ell}}\sin(n\pi x/\ell), \quad n \in \mathbb{Z},\ 0 \leqslant x \leqslant \ell,$$

comprising an orthonormal basis of $L^2([0,\ell])$.

We are now ready to conclude and summarize the above discussion. For a free particle on a line, as well as a free particle in the circle, the kinetic energy operator is the square of the (selfadjoint) momentum operator. This can be regarded as a basic *quantization rule*. For the confined system of a particle on the interval $[0,\ell]$, the momentum observable is no longer projection valued but instead described by the variance-free POVM $\mathsf{P}$, and the "square" is replaced by the second moment operator. In order to retain the quantization rule, the domain of the second moment operator must be appropriately chosen; for the three available choices $\tilde{\mathsf{P}}[2]$, $\mathsf{P}[2]$, and $\mathsf{P}'[2]$, the first two coincide, but are too small. However, the weak operator integral $\mathsf{P}'[2]$ coincides exactly with the appropriate kinetic energy operator.

This example demonstrates that the domain of the strong operator integral (Definition 3) can be too small for a proper physical interpretation, the appropriate enlargement being captured by the general definition (Definition 6) of the largest symmetric weak operator integral.

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**Appendix A**

In this appendix, we show that $\mathsf{P}[n] = P_0^n$ for all $n$, and $\mathsf{P}[1] = P_0$. The notations refer to the example in Section 6.

First we define, for all $n = 1, 2, \ldots$, the Sobolev–Hilbert spaces

$$H^n(\mathcal{I}) = \left\{\varphi \in C^{n-1}(\mathcal{I}) \,\middle|\, \varphi^{(n-1)} \text{ is absolutely continuous and } \varphi^{(n)} \in L^2(\mathcal{I})\right\}$$

where $C^k(\mathcal{I})$ is the space of $k$-times continuously differentiable complex functions on $\mathcal{I}$ (and $C^0(\mathcal{I})$ stands for continuous functions). For $n = 1$ we write $H^1(\mathcal{I}) = H(\mathcal{I})$.

We begin with the observation that both the strong operator integral $\mathsf{P}[n]$ and the weak one $\mathsf{P}'[n]$ are symmetric extensions of $\tilde{\mathsf{P}}[n] = P_0^n$. Hence, it follows that $\mathrm{Dom}(\mathsf{P}[n]) \subseteq \mathrm{Dom}(\mathsf{P}'[n]) \subseteq H^n(\mathcal{I})$, and these operators just act as $(-i)^n d^n/dx^n$ on their respective domains.

We will first show that $\mathsf{P}[n] = P_0^n$, for all $n = 1, 2, \ldots$ (see Proposition 19 below). The following two lemmas are needed. Let $\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the Fourier–Plancherel operator.[7] Hence,

$$(\mathcal{F}\varphi)(x) = \frac{1}{\sqrt{2\pi}}\int_0^\ell e^{-ixt}\varphi(t)\,dt, \quad x \in \mathbb{R},\ \varphi \in L^2(\mathcal{I}).$$

[7] Here we want to apply $\mathcal{F}$ to functions in $L^2(\mathcal{I})$. In our notation this would be written as $\mathcal{F}U$; in order to simplify the notations, we will write $\mathcal{F}$ instead.

(Note that every element of $L^2(\mathcal{I})$ is integrable by the Cauchy–Schwarz inequality.) The function $\mathcal{F}\varphi : \mathbb{R} \to \mathbb{C}$ is continuous, bounded, and belongs to $L^2(\mathbb{R})$.

**Lemma 4.**

(a) *For any* $\varphi \in H(\mathcal{I})$, *we have*

$$[\mathcal{F}\varphi'](x) = ix[\mathcal{F}\varphi](x) + \frac{1}{\sqrt{2\pi}}\big[\varphi(\ell)e^{-ix\ell} - \varphi(0)\big], \quad x \in \mathbb{R}.$$

(b) *For any* $\varphi \in H^n(I) \cap \mathrm{Dom}(P_0^{n-1})$, *we have*

$$x^n[\mathcal{F}\varphi](x) = (-i)^n\big[\mathcal{F}\varphi^{(n)}\big](x) + \frac{i^n}{\sqrt{2\pi}}\big[\varphi^{(n-1)}(\ell)e^{-i\ell x} - \varphi^{(n-1)}(0)\big], \quad x \in \mathbb{R}.$$

**Proof.** Straightforward application of absolute continuity and integration-by-parts. $\square$

**Lemma 5.** *Let* $a, b \in \mathbb{C}$. *Then* $x \mapsto F_\psi(x) := \overline{[\mathcal{F}\psi](x)}[ae^{-i\ell x} - b]$ *is Lebesgue-integrable over* $\mathbb{R}$ *for all* $\psi \in L^2(\mathcal{I})$, *if and only if* $a = b = 0$.

**Proof.** We only need to consider functions $\psi_\theta \in L^2(\mathcal{I})$, where $\psi_\theta(t) := e^{-i\theta t}$, with $\theta \in \mathbb{R}$. Then

$$F_{\psi_\theta}(x) = \frac{[e^{i(x+\theta)\ell} - 1][e^{-ix\ell}a - b]}{i(x+\theta)\sqrt{2\pi}}.$$

If $|a| \neq |b|$, then $|F_{\psi_0}(x)| \geqslant 2|\sin(x\ell/2)|\alpha/(i|x|\sqrt{2\pi}\,)$, with $\alpha = ||a| - |b||$, so $F_{\psi_0}$ is not integrable. If $|a| = |b|$, take $\theta$ so that $a = -e^{-i\theta\ell}b$. Then $F_{\varphi_\theta}(x) = -2b\sin((x+\theta)\ell)/(\sqrt{2\pi}(x+\theta))$, which is again not integrable. The only remaining possibility is $a = b = 0$, and then $F_\psi = 0$ is trivially integrable. $\square$

**Proposition 19.** $\mathsf{P}[n] = P_0^n$ *for all* $n = 1, 2, \dots$.

**Proof.** We have already noted that $\mathsf{P}[n]$ is a restriction of $(-i)^n d^n/dx^n : H^n(\mathcal{I}) \to L^2(\mathcal{I})$. In particular, $\mathrm{Dom}(\mathsf{P}[n]) \subseteq H^n(\mathcal{I})$. Thus, we only need to show that the vectors in $\mathrm{Dom}(\mathsf{P}[n])$ are exactly those elements of $H^n(\mathcal{I})$ which satisfy the boundary conditions defining $\mathrm{Dom}(P_0^n)$. Proceeding by induction, we first consider the case $n = 1$. Using Lemma 4, we get

$$x\overline{[\mathcal{F}\psi](x)}[\mathcal{F}\varphi](x) = -i\overline{[\mathcal{F}\psi](x)}\big[\mathcal{F}\varphi'\big](x) + \frac{i}{\sqrt{2\pi}}\overline{[\mathcal{F}\psi](x)}\big[\varphi(\ell)e^{-i\ell x} - \varphi(0)\big], \tag{24}$$

for $\psi \in L^2(\mathcal{I})$ and $\varphi \in H(\mathcal{I})$. By definition, $\varphi \in \mathrm{Dom}(\mathsf{P}[1])$ if and only if $x \mapsto \overline{[\mathcal{F}\psi](x)}[\mathcal{F}\varphi](x)$ is integrable over $\mathbb{R}$ for all $\psi \in L^2(\mathcal{I})$. Since $\varphi' \in L^2(\mathcal{I})$, so that both $\mathcal{F}\psi$ and $\mathcal{F}\varphi'$ are in $L^2(\mathbb{R})$, the first term in the right hand side of (24) is integrable in any case. Hence $\varphi \in \mathrm{Dom}(\mathsf{P}[1])$ if and only if the second term is integrable for all $\psi \in L^2(\mathcal{I})$. But by Lemma 5, this happens exactly when $\varphi(0) = \varphi(\ell) = 0$, i.e. $\varphi \in \mathrm{Dom}(P_0)$. Thus, $\mathsf{P}[1] = P_0$. Now we assume inductively that $\mathsf{P}[n-1] = P_0^{n-1}$. Since $|x^{n-1}| \leqslant 1 + |x^n|$ for all $x \in \mathbb{R}$, and the relevant complex measures are finite, it follows that $\mathsf{P}[n] \subseteq \mathsf{P}[n-1] = P_0^{n-1}$, where the last equality follows from the induction assumption. Hence, $\mathrm{Dom}(\mathsf{P}[n]) \subseteq H^n(\mathcal{I}) \cap \mathrm{Dom}(P_0^{n-1})$. Letting $\varphi \in H^n(\mathcal{I}) \cap \mathrm{Dom}(P_0^{n-1})$ we get from Lemma 4 (b) that

$$x^n\overline{[\mathcal{F}\psi](x)}[\mathcal{F}\varphi](x) = (-i)^n\overline{[\mathcal{F}\psi](x)}\big[\mathcal{F}\varphi^{(n)}\big](x) + \frac{i^n}{\sqrt{2\pi}}\overline{[\mathcal{F}\psi](x)}\big[\varphi^{(n-1)}(\ell)e^{-i\ell x} - \varphi^{(n-1)}(0)\big]$$

for all $\psi \in L^2(\mathcal{I})$. Since now $\varphi^{(n)} \in L^2(\mathcal{I})$ (because $\varphi \in H^n(\mathcal{I})$), we can again use the same argument as before to conclude by Lemma 5 that $\varphi \in \mathrm{Dom}(\mathsf{P}[n])$ if and only if $\varphi^{(n-1)}(\ell) = \varphi^{(n-1)}(0) = 0$, i.e. $\varphi \in \mathrm{Dom}(P_0^n)$. The proof is complete. $\square$

The remaining result concerns the weak operator integral.

**Proposition 20.** $\mathsf{P}'[1] = P_0$.

**Proof.** Recall first that $\mathsf{P}'[1]$ is a symmetric extension of $\tilde{\mathsf{P}}[1]$, and hence coincides with one of the selfadjoint extensions[8] $P^{(\theta)}$ of $P_0$, or $P_0$ itself. We show that $\mathrm{Dom}(\mathsf{P}'[1])$ is a proper subspace of $\mathrm{Dom}(P^{(\theta)})$, so that $\mathsf{P}'[1] = P_0$ must hold. For any $a, b \in \mathbb{C}$, define $\varphi_{a,b} : \mathbb{R} \to \mathbb{C}$ by $\varphi_{a,b}(t) := (b-a)t/\ell + a$. This is obviously infinitely differentiable, and satisfies the boundary conditions $\varphi_{a,b}(0) = a$ and $\varphi_{a,b}(\ell) = b$, so for a suitable choice of the two constants, the vector $\varphi_{a,b}$ will belong

[8] Selfadjoint extensions of $P_0$ are $-id/dx$ on the domains given by the boundary conditions $\psi(\ell) = e^{i\theta}\psi(0)$.

to the domain of a given $P^{(\theta)}$. We will show that it does not belong to the form domain $\mathcal{D}_F(x, \mathsf{P})$ (which is even larger than the domain of $\mathsf{P}'[1]$), unless $a = b = 0$. In order to prove this, it suffices to show that $xG(x)$ is not integrable over $[1, \infty)$, where $G : \mathbb{R} \to \mathbb{C}$ is the density of the measure $\mathsf{P}_{\varphi_{a,b},\varphi_{a,b}}$, i.e. $G(x) := |(\mathcal{F}\varphi_{a,b})(x)|^2 = (2\pi)^{-1}|\int_0^\ell e^{-ixt}\varphi_{a,b}(t)\,dt|^2$. Now in case $a = b \neq 0$, we have simply $xG(x) = 2|a|^2[1 - \cos(x\ell)]/(2\pi x)$, which is not integrable. In case $a \neq b$, we put $a' := (b - a)\ell^{-1} \neq 0$, $b' := a/a'$; then we get $2\pi\,|a|^{-2}xG(x) = h(x) + x^{-2}(f(x) + x^{-1}g(x))$, where $h(x) := x^{-1}|\ell + b' - b'e^{ix\ell}|^2$, and $f$ and $g$ are bounded real functions. Now $\int xG(x)\,dx = \infty$ is equivalent to $\int_1^\infty h(x)\,dx = \infty$, which is true because $h(x) \geqslant x^{-1}(|\ell + b| - |b|)^2$ in case $|\ell + b| \neq |b|$, while $h(x) = 2|b|^2x^{-1}[1 - \cos(x\ell + \beta)]$ for some $\beta \in [0, 2\pi)$ in case $|\ell + b| = |b|$. The proof is complete. □

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