Abstract. This chapter uses categorical techniques to describe relations between various sets of operators on a Hilbert space, such as self-adjoint, positive, density, effect and projection operators. These relations, including various Hilbert-Schmidt isomorphisms of the form $\text{tr}(A - B)$, are expressed in terms of dual adjunctions, and maps between them. Of particular interest is the connection with quantum structures, via a dual adjunction between convex sets and effect modules. The approach systematically uses categories of modules, via their description as Eilenberg-Moore algebras of a monad.

§1. Introduction. There is a recent exciting line of work connecting research in the semantics of programming languages and logic, and research in the foundations of quantum physics, including quantum computation and logic, see [9] for an overview. This paper fits in that line of work. It concentrates on operators (on Hilbert spaces) and organises and relates these operators according to their algebraic structure. This is to a large extent not more than a systematic presentation of known results and connections in the (modern) language of category theory. However, the approach leads to clarifying results, like Theorem 14 that relates density operators and effects via a dual adjunction between convex sets and effect modules (extending earlier work [25]). It is in line with many other dual adjunctions and dualities that are relevant in programming logics [31, 1, 30]. Indeed, via this dual adjunction we can put the work [11] on quantum weakest preconditions in perspective (see especially Remark 15).

The article begins by describing the familiar sets of operators (bounded, self-adjoint, positive) on a (finite-dimensional) Hilbert space in terms of functors to categories of modules. The dual adjunctions involved are made explicit, basically via dual operation $V \mapsto V^*$, see Section 2. Since the algebraic structure of these sets of operators is described in terms of modules over various semirings, namely over complex numbers $\mathbb{C}$ (for bounded operators), over real numbers $\mathbb{R}$ (for self-adjoint operators), and over non-negative real numbers $\mathbb{R}_{\geq 0}$ (for positive operators), it is useful to have a uniform description of such modules. It is provided in Section 3, via the notion of algebra of
a monad (namely the multiset monad). This abstract description provides (co)limits and the monoidal closed structure of such algebras (from [33]) for free. We then use that convex sets can also be described as such algebras of a monad (namely the distribution monad), and elaborate the connection with effect modules (also known as convex effect algebras, see [36]). In this setting we discuss various ‘Gleason-style’ correspondences, between projections, effects, and density matrices. We borrow the probabilistic Gelfand duality between (Banach) effect modules and (compact) convex sets from [29] for the final steps in our analysis. This duality formalises the difference between the approaches of Heisenberg (focusing on observables/effects) and Schrödinger (focusing on states), see e.g. [22]. It allows us to reconstruct all sets of operators on a Hilbert space from its projections, see Table 1 for an overview. The main contribution of the paper thus lies in a systematic description.

We should emphasise that the investigations in this paper concentrate on finite-dimensional Hilbert and vector spaces.

1.1. Operator overview. For a (finite-dimensional) Hilbert space $H$ we shall study the following sets of operators $H \to H$.

$$
\begin{align*}
&\mathcal{B}(H) \quad \xleftarrow{\text{SA}(H)} \quad \mathcal{P}o\!s\!(H) \quad \xleftarrow{\mathcal{E}f(H)} \quad \mathcal{D}M(H) \\
&\mathcal{B}(H) \quad \mathcal{SA}(H) \quad \mathcal{P}o\!s!(H) \quad \mathcal{E}f(H) \quad \mathcal{D}M(H)
\end{align*}
$$

(1)

where:

| Notation | Description | Structure |
|----------|-------------|-----------|
| $\mathcal{B}(H)$ | bounded/continuous linear | vector space over $\mathbb{C}$ |
| $\mathcal{SA}(H)$ | self-adjoint $A^\dagger = A$ | vector space over $\mathbb{R}$ |
| $\mathcal{P}o\!s\!(H)$ | positive: $A \geq 0$ | module over $\mathbb{R}_{\geq 0}$ |
| $\mathcal{E}f(H)$ | effect: $0 \leq A \leq I$ | effect module over $[0, 1]$ |
| $\mathcal{P}r(H)$ | projection: $A^2 = A = A^\dagger$ | orthomodular lattice |
| $\mathcal{D}M(H)$ | density: $A \geq 0$ and $\text{tr}(A) = 1$ | convex set |

The emphasis lies on the ‘structure’ column. It describes the algebraic structure of the sets of operators that will be relevant here. It is not meant to capture all the structure that is present. For instance, the set $\mathcal{B}(H)$ of endomaps is not only a vector space over the complex numbers, but actually a $C^*$-algebra.

As is well-known, operators on Hilbert spaces behave in a certain sense as numbers. For instance, by taking $H$ to be the trivial space $\mathbb{C}$ of complex
numbers, the diagram (1) becomes:

$$
\begin{array}{cccc}
\mathbb{C} & \leftrightarrow & \mathbb{R} & \leftrightarrow \\
\downarrow & & \downarrow & \\
\mathbb{R}_{\geq 0} & \leftrightarrow & [0, 1] \leftarrow \{0, 1\}
\end{array}
$$

§2. Operators and duality. This section concentrates on the first three sets of operators in (1), namely on $\mathcal{B}(H) \leftrightarrow \mathcal{S} \mathcal{A}(H) \leftrightarrow \mathcal{P} \mathcal{O}s(H)$. It will focus on isomorphisms $V \cong V^*$, for $V = \mathcal{B}(H), \mathcal{S} \mathcal{A}(H), \mathcal{P} \mathcal{O}s(H)$. These isomorphisms turn out to be natural in $H$, in categories of modules (or vector spaces). This serves as motivation for further investigation of the structures involved, in subsequent sections. Only later will we study the density and effect operators $\mathcal{D} \mathcal{M}(H)$ and $\mathcal{E} \mathcal{F}(H)$, capturing ‘states and statements’ in quantum logic. The material in this section thus serves as preparation. It is not new, except possibly for the presentation in terms of maps of adjunctions.

We start by recalling that the category $\mathbf{Vect}_\mathbb{C}$ of vector spaces over the complex numbers $\mathbb{C}$ carries an involution given by conjugation: for a vector space $V$ we write $\overline{V}$ for the conjugate space, with the same vectors as $V$, but with scalar multiplication given by $z \cdot \overline{v} = \overline{\overline{z}} \cdot v$, where the complex number $z \in \mathbb{C}$ has conjugate $\overline{z} \in \mathbb{C}$. This yields an ‘involution’ endofunctor $(-)^\ast : \mathbf{Vect}_\mathbb{C} \to \mathbf{Vect}_\mathbb{C}$ which is the identity on morphisms. A linear map $f : V \to W$ is sometimes called conjugate linear, because it satisfies $f(z \cdot v) = \overline{z} \cdot f(v)$. Complex conjugation $z \mapsto \overline{z}$ is an example of a conjugate linear (isomorphism) $\overline{\mathbb{C}} \cong \mathbb{C}$ in $\mathbf{Vect}_\mathbb{C}$.

We shall write $V \to W$ for the ‘exponent’ vector space of linear maps $V \to W$ between vector spaces $V$ and $W$. There is the standard correspondence between linear functions $U \to (V \to W)$ and $U \otimes V \to W$.

One uses this exponent $\to$ to form the dual space $V^\ast = \overline{V} \to \mathbb{C}$. If $V$ is finite-dimensional, say with a basis $e_1, \ldots, e_n$, written in ‘ket’ notation as $|j\rangle = e_j$, there is the familiar isomorphism of $V$ with its dual space $V^\ast = \overline{V} \to \mathbb{C}$ given as:

$$
\begin{array}{cccc}
V & \cong & V^\ast & \cong & \overline{V} \to \mathbb{C} \\
(\sum_j z_j |j\rangle) & \mapsto & (\sum_j z_j \langle j|)
\end{array}
$$

where the ‘bra’ $\langle j| : \overline{V} \to \mathbb{C}$ sends a vector $w = (\sum_k w_k |k\rangle$ to its $j$-th coordinate $\langle j| w\rangle = \sum_k \overline{w}_k \langle j| k\rangle = \overline{w}_j$. Clearly, this yields an isomorphism $V \cong V^\ast$, because these functions $\langle j|$ form a ‘dual’ basis for $V^\ast$. This isomorphism (2) is a famous example of a non-natural mapping, depending on a choice of basis. It will play a crucial role below, where $\overline{V}$ is a vector space of operators on a Hilbert space.
The mapping \( V \mapsto V^* = (V \to \mathbb{C}) \) yields a functor \( \text{Vect}_\mathbb{C} \to (\text{Vect}_\mathbb{C})^{\text{op}} \); for a map \( C : H \to K \) we have \( C^* : K^* \to H^* \) given by \( f \mapsto f \circ C \). This functor \((-)^*\) is adjoint to itself, in the sense that there is a bijective correspondence (suggested by the double lines) as on the left below, forming an adjunction as on the right.

\[
\begin{align*}
\text{Vect}_\mathbb{C} & \xrightarrow{\neg} (\text{Vect}_\mathbb{C})^{\text{op}} \\
\text{ Vect}_\mathbb{C}(V) & \cong \text{ Vect}_\mathbb{C}(W) \\
\text{ Vect}_\mathbb{C}(W) & \cong \text{ Vect}_\mathbb{C}(V) \\
\text{ Vect}_\mathbb{C}(V) & \cong \text{ Vect}_\mathbb{C}(W)
\end{align*}
\]

In the next step, let \( \text{FdHilb} \) be the category of finite-dimensional Hilbert spaces with bounded linear maps between them. One can drop the boundedness requirement, because a linear map between finite-dimensional spaces is automatically bounded (i.e. continuous). As is usual, we write \( \mathcal{B}(H) \) for the homset of endomaps \( H \to H \) in \( \text{FdHilb} \). This set \( \mathcal{B}(H) \) of “operators on \( H \)” is a vector space over \( \mathbb{C} \), of dimension \( n^2 \) with the outer products \( | j \rangle \langle k | \), for \( j, k \leq n \), as basis—assuming a basis \( | 1 \rangle, \ldots, | n \rangle \) for \( H \). Such outer product projections \( | j \rangle \langle k | \) may be understood as the matrix with only 0s except for a single 1 in the \( j \)-th row of the \( k \)-th column. In general, an operator \( A : H \to H \) can be written as matrix \( A = \sum_{j,k} A_{jk} | j \rangle \langle k | \), where the matrix entries \( A_{jk} \) may be described as \( \langle j | A | k \rangle \).

The mapping \( H \mapsto \mathcal{B}(H) \) is functorial, and will be used here as functor \( \mathcal{B} : \text{FdHilb} \to \text{Vect}_\mathbb{C} \). On a map \( C : H \to K \) it yields a linear function \( \mathcal{B}(H) \to \mathcal{B}(K) \), written as \( \mathcal{B}(C) \), and given by:

\[
\mathcal{B}(C) \left( H \xrightarrow{A} H \right) = \left( K \xrightarrow{C^\dagger} H \xrightarrow{A} H \xrightarrow{C} K \right).
\]

The operator \( C^\dagger = C^T \) is the conjugate transpose of \( C \), satisfying \( \langle Cv | w \rangle = \langle v | C^\dagger w \rangle \). It makes \( \text{FdHilb} \) into a dagger category, see e.g. [2]. This dagger forms an involution on the vector space \( \mathcal{B}(H) \). Also, it is adjoint to itself, as in:

\[
\begin{align*}
\text{FdHilb} & \xrightarrow{\neg} \text{FdHilb}^{\text{op}} \\
\text{ FdHilb}(V) & \cong \text{ FdHilb}(W) \\
\text{ FdHilb}(W) & \cong \text{ FdHilb}(V)
\end{align*}
\]

In the next result we apply the duality isomorphism \( V \cong V^* \) in (2) for \( V = \mathcal{B}(H) \). As we shall see, it involves the trace operation \( \text{tr} : \mathcal{B}(H) \to \mathbb{C} \) of which we first recall some basic facts. For \( A \in \mathcal{B}(H) \) the trace \( \text{tr}(A) \) can be defined as the sum \( \sum_j A_{jj} \) of the diagonal matrix values. This definition is independent of the choice of matrix/basis. This trace \( \text{tr} \) satisfies the following
basic properties.

\[ \text{tr}(A + B) = \text{tr}(A) + \text{tr}(B) \]

\[ \text{tr}(zA) = z \text{tr}(A) \]

where \( z \in \mathbb{C} \)

\[ \text{tr}(AB) = \text{tr}(BA) \]

the so-called cyclic property

\[ \text{tr}(A^T) = \text{tr}(A) \]

where \((-)^T\) is the transpose operation

\[ \text{tr}(A^+) = \overline{\text{tr}(A)} \]

which results from previous points

\[ \text{tr}(A) \geq 0 \]

when \( A \) is positive: \( A \geq 0 \), i.e. \( \langle v | A v \rangle \geq 0 \).

**Proposition 1.** For a finite-dimensional Hilbert space \( H \) the duality isomorphism (2) applied to the vector space \( \mathcal{B}(H) \) of endomaps boils down to a trace calculation, namely:

\[ \mathcal{B}(H) \xrightarrow{\mathfrak{h}_B} \mathcal{B}(H)^* = \overline{\mathcal{B}(H)} \rightarrow \mathbb{C} \]

is \( \mathfrak{h}_B(A) = \lambda B. \text{tr}(AB^+) \),

where the \( \lambda \)-notation is borrowed from the \( \lambda \)-calculus, and used for function abstraction: \( \lambda B. \cdots \) describes the function \( B \mapsto \cdots \).

This map \( \mathcal{B}(H) \xrightarrow{\cong} \mathcal{B}(H)^* \) is independent of the choice of basis. More categorically, it yields a natural isomorphism involving adjoint \((-)^\dagger\) and dual \((-)^* = (-)^{\mathbb{C}}\) in:

\[ \mathcal{B} \circ (-)^\dagger \xrightarrow{\mathfrak{h}_B} (-)^* \circ \mathcal{B} \]

Pictorially, this \( \mathfrak{h}_B \) is a natural transformation \( \mathsf{FdHilb} \xrightarrow{\cong} \mathsf{Vect}^\text{op} \) between the two functors \( \mathsf{FdHilb} \Rightarrow \mathsf{Vect}^\text{op} \) given in:

\[ \begin{array}{ccc}
\mathsf{FdHilb} & \xrightarrow{(-)^\dagger} & \mathsf{FdHilb}^\text{op} \\
\mathcal{B} & \downarrow & \mathcal{B} \\
\mathsf{Vect} & \xrightarrow{(-)^*} & \mathsf{Vect}^\text{op}
\end{array} \]

Moreover, this \( \mathfrak{h}_B \) is part of a map of adjunctions (see [34, IV.7]) in the following situation.

\[ \begin{array}{ccc}
\mathsf{FdHilb} & \xrightarrow{(-)^\dagger} & \mathsf{FdHilb}^\text{op} \\
\mathcal{B} & \downarrow & \mathcal{B} \\
\mathsf{Vect} & \xrightarrow{(-)^*} & \mathsf{Vect}^\text{op}
\end{array} \]

The letters ‘h’ and ‘s’ in the map \( \mathfrak{h}_B \) stand for Hilbert and Schmidt, since the inner product \( (A, B) \mapsto \text{tr}(AB^+) = \mathfrak{h}_B(A)(B) \) is commonly named after them. The subscript \( B \) is added because we shall encounter analogues of this isomorphism for other operators. We drop the subscript when confusion is unlikely.
Proof. If \( |1\rangle, \ldots, |n\rangle \) is a basis for \( H \), then the map \( \mathfrak{h}_s : B(H) \to B(H)^* \) becomes, according to (2),

\[
A = \left( \sum_{j,k} A_{jk} |j\rangle \langle k| \right) \mapsto \lambda B. \sum_{j,k} A_{jk} B_{kj} = \lambda B. \sum_{j,k} A_{jk} (B^\dagger)_{kj} = \lambda B. \sum_j (AB^\dagger)_{jj} = \lambda B. \text{tr}(AB^\dagger).
\]

Since the trace of a matrix is basis-independent, so is this isomorphism \( \mathfrak{h}_s \). Naturality amounts to commutation of the following diagram, for each map \( C : H \to K \) in \( \text{FdHilb} \).

\[
\begin{array}{ccc}
B(H) & \xrightarrow{\mathfrak{h}_s_H} & B(H)^* = B(H) \circ \mathbb{C} \\
\uparrow{\mathfrak{h}_s_C} & & \uparrow{B(C)^*} \\
B(K) & \xrightarrow{\mathfrak{h}_s_K} & B(K)^* = B(K) \circ \mathbb{C}
\end{array}
\]

This diagram commutes because:

\[
(B(C)^* \circ \mathfrak{h}_s_K)(A)(B) = (\mathfrak{h}_s_K(A) \circ B(C))(B) \\
= \mathfrak{h}_s_K(A)(B(C)(B)) \\
= \mathfrak{h}_s_K(A)(CBC^\dagger) \\
= \text{tr}(A(CBC^\dagger)) \\
= \text{tr}(ACB^\dagger) \quad \text{by the cyclic property} \\
= \mathfrak{h}_s_H(C^\dagger AC)(B) \\
= \mathfrak{h}_s_H(B(C^\dagger)(A))(B) \\
= (\mathfrak{h}_s_H \circ B(C^\dagger))(A)(B).
\]

Finally, we use the basic fact that, because these \( \mathfrak{h}_s_H \)'s are natural in \( H \) and componentwise isomorphisms, the inverses \( \mathfrak{h}_s_H^{-1} \) are also natural in \( H \), see e.g. [4, Lemma 7.11]. The details of the map of adjunctions in the above diagram are left to the interested reader.

The remarkable thing about this result is that whereas the maps \( V \xrightarrow{\cong} V^* \) in (2) are not natural, the instantiations \( \mathfrak{h}_s : B(H) \xrightarrow{\cong} B(H)^* \) are, because they involve a trace calculation that is base-independent. We briefly describe the inverse of \( \mathfrak{h}_s = \lambda A. \text{tr}(A\cdot) : \text{B}(H) \xrightarrow{\cong} \text{B}(H)^* = (\text{B}(H) \circ \mathbb{C}) \), via a choice of basis \( |1\rangle, \ldots, |n\rangle \) for \( H \). So suppose we have a linear map \( f : B(H) \to \mathbb{C} \). Define an operator \( \mathfrak{h}_s^{-1}(f) \in B(H) \) with matrix entries:

\[
(\mathfrak{h}_s^{-1}(f))_{jk} = f(|j\rangle \langle k|).
\]
Then we recover $f$ via the trace calculation:

$$\text{hs}\left(\text{hs}^{-1}(f)\right)(B) = \text{tr}\left(\text{hs}^{-1}(f) B^\dagger\right)$$

$$= \text{tr}\left(\sum_{j,k} \text{hs}^{-1}(f)_{jk} |j\rangle\langle k| B^\dagger\right)$$

$$= \sum_{j,k} \text{hs}^{-1}(f)_{jk} \text{tr}\left(|j\rangle\langle k| B^\dagger\right)$$

$$= \sum_{j,k} f(|j\rangle\langle k|) \text{tr}\left((B^\dagger)_{kj}\right)$$

$$= \sum_{j,k} f(|j\rangle\langle k|) \overline{B_{jk}}$$

$$= \sum_{j,k} f(B_{jk}|j\rangle\langle k|), \text{ because } f \text{ is conjugate linear}$$

$$= f\left(\sum_{j,k} B_{jk}|j\rangle\langle k|\right)$$

$$= f(B).$$

Again, this mapping $f \mapsto A_f$ is independent of a choice of basis, because its inverse $A \mapsto \text{tr}(A^-)$ does not depend on such a choice.

**Self-adjoint operators.** We now restrict ourselves to self-adjoint operators $\mathcal{S}A(H) \hookrightarrow \mathcal{B}(H)$. We recall that an operator $A: H \rightarrow H$ is called self-adjoint (or Hermitian) if $A^\dagger = A$. In terms of matrices this means that $A_{jk} = \overline{A_{kj}}$. In particular, all entries $A_{jj}$ on the diagonal are real numbers, and so is the trace (as sum of these $A_{jj}$). The set of self-adjoint operators $\mathcal{S}A(H)$ forms a vector space over $\mathbb{R}$. The mapping $H \mapsto \mathcal{S}A(H)$ can be extended to a functor $\mathcal{S}A: \text{Hilb} \rightarrow \text{Vect}_\mathbb{R}$, by:

$$\mathcal{S}A(C)(H \xrightarrow{A} H) = (K \xrightarrow{C^\dagger} H \xrightarrow{A} H \xrightarrow{C} K).$$

like for $\mathcal{B}$ in (3). This is well-defined since if $A$ is self-adjoint then so is $\mathcal{S}A(C)(A)$, since:

$$\left(\mathcal{S}A(C)(A)\right)^\dagger = \left(CAC^\dagger\right)^\dagger = C^\dagger A^\dagger C^\dagger = CAC^\dagger = \mathcal{S}A(C)(A).$$

There are several ways to turn a linear operator into a self-adjoint one. For instance, for each complex number $z \in \mathbb{C}$ and $B \in \mathcal{B}(H)$ we have self-adjoint operators:

$$zB + \overline{z}B^\dagger \quad \text{and} \quad izB - i\overline{z}B^\dagger. \quad (5)$$
In this way we obtain mappings \( \mathcal{B}(H) \to \mathcal{S}A(H) \) in \( \text{Vect}_\mathbb{R} \). If the real part \( \text{Re}(z) \) is non-zero, the mapping:

\[
B \mapsto \frac{1}{2\text{Re}(z)} (zB + \overline{z}B^\dagger)
\]

is a left-inverse of the inclusion \( \mathcal{S}A(H) \hookrightarrow \mathcal{B}(H) \), making it a split mono.

By moving from \( \mathcal{B} \) to \( \mathcal{S}A \) we get the following analogue of Proposition 1.

**Proposition 2.** For \( H \in \text{FdHilb} \), the subset \( \mathcal{S}A(H) \hookrightarrow \mathcal{B}(H) \) of self-adjoint operators on \( H \) is a vector space over \( \mathbb{R} \), for which one obtains a natural isomorphism in \( \text{Vect}_\mathbb{R} \):

\[
\mathcal{S}A(H) \xrightarrow{\text{hs}_{S\mathcal{A}}} \mathcal{S}A(H)^* = \mathcal{S}A(H) \to \mathbb{R} \quad \text{by} \quad \text{hs}_{S\mathcal{A}}(A)(B) = \text{tr}(AB).
\]

It gives rise to a map of adjunctions:

\[
\begin{array}{ccc}
\text{FdHilb} & \xleftarrow{\top} & \text{FdHilb}^\text{op} \\ \\
\mathcal{S}A & \xrightarrow{(-)^\dagger} & \mathcal{S}A \\
\text{Vect}_\mathbb{R} & \xleftarrow{(-)_{-\to \mathbb{R}}} & \text{Vect}_\mathbb{R}^\text{op} \\
\end{array}
\]

**Proof.** If \( A, B : H \to H \) are self-adjoint operators, then \( \text{tr}(AB^\dagger) = \text{tr}(AB) \) is a real number, since:

\[
\text{tr}(AB) = \text{tr}((AB)^\dagger) = \text{tr}(B^\dagger A^\dagger) = \text{tr}(BA) = \text{tr}(AB).
\]

Conversely, suppose we have a (linear) map \( f : \mathcal{S}A(H) \to \mathbb{R} \) in \( \text{Vect}_\mathbb{R} \). It can be extended to a function \( f' : \overline{\mathcal{B}(H)} \to \mathbb{C} \) via

\[
f'(B) = \frac{1}{2} \left( f(B + B^\dagger) + if(iB - iB^\dagger) \right)
\]

using, as described in (5), that \( B + B^\dagger \) and \( iB - iB^\dagger \) are self-adjoint. It is not hard to see that \( f' \) preserves sums of operators and satisfies \( f'(zB) = \overline{z} f'(B) \). This \( f' \) really extends \( f \) since in the special case when \( B \) is self-adjoint we get \( f'(B) = \frac{1}{2} \left( f(2B) + if(0) \right) = f(B) \) by linearity.

By Proposition 1 there is a unique \( A \in \mathcal{B}(H) \) with:

\[
f' = \text{hs}_\mathcal{B}(A) = \text{tr}(A(-)^\dagger) : \overline{\mathcal{B}(H)} \to \mathbb{C}.
\]

We now put \( \text{hs}_{S\mathcal{A}}^{-1}(f) = \frac{1}{2}(A + A^\dagger) \in \mathcal{S}A(H) \), and check for \( B \in \mathcal{S}A(H) \):

\[
\begin{align*}
\text{hs}_{S\mathcal{A}} \left( \text{hs}_{S\mathcal{A}}^{-1}(f) \right)(B) \\
= \text{tr} \left( \text{hs}_{S\mathcal{A}}^{-1}(f) B \right) \\
= \frac{1}{2} \left( \text{tr}(AB) + \text{tr}(A^\dagger B) \right)
\end{align*}
\]

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\[ \frac{1}{2} (\operatorname{tr}(AB^\dagger) + \operatorname{tr}((BA)^\dagger)) \text{ since } B \text{ is self-adjoint} \]

\[ = \frac{1}{2} (f'(B) + \operatorname{tr}(BA)) \]

\[ = \frac{1}{2} (f(B) + \overline{\operatorname{tr}(AB)}) \text{ since } f(B) = f'(B) \text{ when } B \in \mathcal{S} \mathcal{A}(H) \]

\[ = \frac{1}{2} (f(B) + f(B)) \text{ because } f(B) \text{ is real valued} \]

\[ = f(B) \text{ since } f \text{ is linear.} \]

In the other direction, one obtains \( \mathcal{H}_{\mathcal{S} \mathcal{A}}^{-1}(\mathcal{H}_{\mathcal{S} \mathcal{A}}(A)) = A \) by uniqueness.

We prove uniqueness in the self-adjoint case too. Assume a self-adjoint operator \( C \in \mathcal{S} \mathcal{A}(H) \) also satisfies \( f = \mathcal{H}_{\mathcal{S} \mathcal{A}}(C) : \mathcal{S} \mathcal{A}(H) \to \mathbb{R} \). We need to prove \( C = A = \frac{1}{2}(A^* + A^\dagger) \). We plan to show \( A_{jk} = C_{jk} \) wrt. an arbitrary basis, and thus \( A = C \). We prove the equality \( A_{jk} = C_{jk} \) in two steps, by proving that both their real and imaginary parts are the same.

\[ \operatorname{Re}(C_{jk}) = \frac{1}{2} (C_{jk} + \overline{C_{jk}}) \]

\[ = \frac{1}{2} (C_{jk} + (C^\dagger)_{kj}) \]

\[ = \frac{1}{2} (C_{jk} + C_{kj}) \]

\[ = \frac{1}{2} (\langle j | C | k \rangle + \langle k | C | j \rangle) \]

\[ = \frac{1}{2} (\operatorname{tr}(\langle j | C | k \rangle) + \operatorname{tr}(\langle k | C | j \rangle)) \]

\[ = \frac{1}{2} (\operatorname{tr}(C(|k\rangle \langle j |) + |j\rangle \langle k |)) \]

\[ = \frac{1}{2} (\operatorname{tr}(A(|k\rangle \langle j | + |j\rangle \langle k |)) \]

by assumption, using that \( |k\rangle \langle j | + |j\rangle \langle k | \) is self-adjoint

\[ = \ldots \text{ (as before)} \]

\[ = \operatorname{Re}(A_{jk}). \]

Similarly, \( \operatorname{Im}(C_{jk}) = \operatorname{Im}(A_{jk}) \), by writing \( \operatorname{Im}(C_{jk}) = \frac{1}{2} (-iC_{jk} + i\overline{C_{jk}}) \) and using the self-adjoint operator \(-i|j\rangle \langle k | + i|k\rangle \langle j |\).

Implicitly, the proof gives a formula for the inverse \( \mathcal{H}_{\mathcal{S} \mathcal{A}}^{-1} \) of the Hilbert-Schmidt map for self-adjoint operators.

**Positive operators.** An operator \( A : H \to H \) is called positive if the inner product \( \langle Ax | x \rangle \) is a non-negative real number, for each \( x \in H \). In that case
one writes $A \geq 0$. This is equivalent to: $A = BB^\dagger$, for some operator $B$, and also to: all eigenvalues are non-negative reals. In a spectral decomposition $A = \sum_j \lambda_j |j\rangle\langle j|$ a positive operator $A$ has eigenvalues $\lambda_j \in \mathbb{R}_{\geq 0}$ for all $j$. Hence the trace $\text{tr}(A)$ is a non-negative real number. The set of positive operators on $H$ is written here as $\mathcal{P}os(H)$. It forms a module over the semiring $\mathbb{R}_{\geq 0}$ of non-negative reals since positive operators are closed under addition and under scalar multiplication with $r \in \mathbb{R}_{\geq 0}$. A positive operator is clearly self-adjoint, since $A^\dagger = (BB^\dagger)^\dagger = B^\dagger B^\dagger = BB^\dagger = A$. Thus there are inclusion maps $\mathcal{P}os(H) \hookrightarrow \mathcal{S}A(H) \hookrightarrow \mathcal{B}(H)$. We can describe taking positive operators as a functor $\mathcal{P}os : \mathcal{H}ilb \rightarrow \mathcal{M}od_{\mathbb{R}_{\geq 0}}$ from Hilbert spaces to modules over the non-negative real numbers. The action of $\mathcal{P}os$ on maps is like for $\mathcal{S}A$ and $\mathcal{B}$ in (3), and is well-defined, since if $C : H \rightarrow K$ in $\mathcal{H}ilb$ and $A \geq 0$, then $\mathcal{P}os(C)(A) = CAC^\dagger \geq 0$ since for each $x \in K$,

$$\langle CAC^\dagger x | x \rangle = \langle AC^\dagger x | C^\dagger x \rangle \geq 0.$$ 

As an aside we recall that via positivity one obtains the Löwner order on arbitrary operators $A, B$, defined as: $A \leq B$ iff $B - A \geq 0$. Thus: $A \leq B$ iff $\exists P \in \mathcal{P}os(H). A + P = B$. Hence the spaces $\mathcal{P}os(H) \hookrightarrow \mathcal{S}A(H) \hookrightarrow \mathcal{B}(H)$ are actually ordered (see also [37, 15]).

**Proposition 3.** For $H \in \mathcal{F}d\mathcal{H}ilb$, the subset $\mathcal{P}os(H) \hookrightarrow \mathcal{S}A(H)$ of positive operators is a module over the non-negative reals $\mathbb{R}_{\geq 0}$, for which there is a natural isomorphism in $\mathcal{M}od_{\mathbb{R}_{\geq 0}}$:

$$\mathcal{P}os(H) \xrightarrow{\text{hs}_{\mathcal{P}os}} \mathcal{P}os(H)^\ast = \mathcal{P}os(H) \rightarrow \mathbb{R}_{\geq 0} \text{ by } \text{hs}_{\mathcal{P}os}(A)(B) = \text{tr}(AB). \tag{7}$$

This isomorphism gives rise to a map of adjunctions:

$$\begin{array}{cc}
\mathcal{F}d\mathcal{H}ilb & \mathcal{F}d\mathcal{H}ilb^{\text{op}} \\
\mathcal{P}os & \downarrow \text{---} & \mathcal{P}os^{\text{op}} \\
\mathcal{M}od_{\mathbb{R}_{\geq 0}} & \downarrow \text{---} & \mathcal{M}od_{\mathbb{R}_{\geq 0}}^{\text{op}} \\
\mathcal{P}os \quad & \mathcal{P}os^{\text{op}} \\
\end{array}$$

**Proof.** We first have to check that $\text{tr}(AB) \geq 0$, for $A, B \in \mathcal{P}os(H)$, so that indeed $\text{tr}(A -)$ has type $\mathcal{P}os(H) \rightarrow \mathbb{R}_{\geq 0}$. We do so by first writing the spectral decomposition as $A = \sum_j \lambda_j |j\rangle\langle j|$, with $\lambda_j \geq 0$. Then:

$$\text{tr}(AB) = \sum_j \lambda_j \text{tr}(|j\rangle\langle j|B) = \sum_j \lambda_j \text{tr}(\langle j|B|j\rangle) = \sum_j \lambda_j \langle Bj|j\rangle$$

$$\geq 0, \quad \text{since } \langle Bj|j\rangle \geq 0.$$
These maps \( h_{\mathcal{P}H} = \text{tr}(A-) \) clearly preserve the module structure: additions and scalar multiplication (with a non-negative real number). Next, assume we have a linear map \( f : \mathcal{P}H \to \mathbb{R}_{\geq 0} \) in \( \text{Mod}_{\mathbb{R}_{\geq 0}} \). Like before, we wish to extend it, this time to a map \( f' : \mathcal{S}H \to \mathbb{R} \). If we have an arbitrary self-adjoint operator \( B \in \mathcal{S}H \) we can write it as difference \( B = B_p - B_n \) of its positive and negative parts \( B_p, B_n \in \mathcal{P}H \). One way to do it is to write \( B = \sum \lambda_j |j\rangle \langle j| \) as spectral decomposition, and to separate the (real-valued) eigenvalues \( \lambda_j \) into negative and non-negative ones. Then take:

\[
B_p = \sum_{\lambda_j \geq 0} \lambda_j |j\rangle \langle j| \quad \text{and} \quad B_n = \sum_{\lambda_j < 0} -\lambda_j |j\rangle \langle j|.
\]

(8)

Now we can define \( f'(B) = f(B_p) - f(B_n) \in \mathbb{R} \). This outcome is independent of the choice of \( B_p, B_n \), since if \( C, D \in \mathcal{P}H \) also satisfy \( B = C - D \), then \( B_p + D = C + B_n \), so that by linearity:

\[
f(B_p) + f(D) = f(B_p + D) = f(C + B_n) = f(C) + f(B_n),
\]

and thus:

\[
f'(B) = f(B_p) - f(B_n) = f(C) - f(D).
\]

It is not hard to see that the resulting function \( f' : \mathcal{S}H \to \mathbb{R} \) is linear (in \( \text{Vect}_{\mathbb{R}} \)). Hence by Proposition 2 there is a unique \( A = h_{\mathcal{S}H}^{-1}(f') \in \mathcal{S}H \) with \( f' = h_{\mathcal{S}H}(A) = \text{tr}(A-) : \mathcal{S}H \to \mathbb{R} \). For a positive operator \( B \in \mathcal{P}H \) we then get \( \text{tr}(AB) = f'(B) = f(B) \geq 0 \), since \( B = B_p \) for such a positive \( B \).

We now write \( A = A_p - A_n \) as in (8), where \( A_n = \sum_{\lambda_j < 0} -\lambda_j |j\rangle \langle j| \).

Projection operators of the form \( |j\rangle \langle j| \) are positive, so that we get for each \( j \) with \( \lambda_j < 0 \)

\[
0 \leq \text{tr}(A|j\rangle \langle j|) = \text{tr}(A_p|j\rangle \langle j|) - \text{tr}(A_n|j\rangle \langle j|) = 0 - (-\lambda_j) = \lambda_j.
\]

But this is impossible, since we assumed \( \lambda_j < 0 \). Hence \( A_n = 0 \), and \( A = A_p \) is a positive operator. Thus we have \( f = \text{tr}(A-) : \mathcal{P}H \to \mathbb{R}_{\geq 0} \), as required, so that we can take \( h_{\mathcal{P}H}^{-1}(f) = h_{\mathcal{S}H}^{-1}(f') \).

We briefly check uniqueness: if \( C \in \mathcal{P}H \) also satisfies \( f = \text{tr}(C-) \), then for an arbitrary \( B \in \mathcal{S}H \),

\[
f'(B) = f(B_p) - f(B_n) = \text{tr}(CB_p) - \text{tr}(CB_n) = \text{tr}(C(B_p - B_n)) = \text{tr}(CB).
\]

But then \( C = A \) by the uniqueness from Proposition 2.

This concludes our description of the spaces of operators \( \mathcal{B}H \leftrightarrow \mathcal{S}H \leftrightarrow \mathcal{P}H \) on a (finite-dimensional) Hilbert space \( H \), as naturally self-dual modules. Before we proceed to density operators \( \mathcal{D}M(H) \) and effects \( \mathcal{E}f(H) \)
on $H$ we wish to explore and exploit the similarities between these modules (over $\mathbb{C}$, $\mathbb{R}$, and $\mathbb{R}_{\geq 0}$) in terms of algebras of a monad.

§3. Categories of modules as algebras. We recall that a semiring [20] is like a ring but without an additive inverse. Modules are vector spaces except that the scalars need only be a ring, and not a field. Here we generalise further and will also consider modules over a semiring. In fact we have already done in the previous section, when we talked about positive operators forming a module over the non-negative reals $\mathbb{R}_{\geq 0}$. As we now proceed more systematically, we shall see that such a module over a semiring consists of a commutative monoid of vectors, with scalar multiplication by elements of the semiring. It will be captured as algebra of the multiset monad.

In this section we thus start with the standard description of categories of modules, over a semiring $S$, as categories of algebras of a monad, namely of the multiset monad $\mathcal{M}_S$ associated with $S$. We shall be especially interested in the examples $S = \mathbb{R}_{\geq 0}, \mathbb{R}, \mathbb{C}$ giving us a uniform description of the categories of modules in which the spaces of operators $\mathcal{P}(H), \mathcal{S}(H), \mathcal{B}(H)$ on a Hilbert space $H$ live. The general theory of monads—see e.g. [34, 5, 35, 7]—gives us certain structure for free, see Theorem 4 below.

The main result in this section, Theorem 6, relates the three spaces of operators $\mathcal{P}(H), \mathcal{S}(H), \mathcal{B}(H)$ via free constructions between categories of modules.

To start, let $S$ be a semiring, consisting of a commutative additive monoid $(S, +, 0)$ and a multiplicative monoid $(S, \cdot, 1)$, where multiplication distributes over addition. One can define a “multiset” functor $\mathcal{M}_S : \text{Sets} \to \text{Sets}$ by:

$$\mathcal{M}_S(X) = \{\varphi : X \to S \mid \text{supp(}\varphi\text{) is finite}\},$$

where $\text{supp}(\varphi) = \{x \in X \mid \varphi(x) \neq 0\}$ is the support of $\varphi$. For a function $f : X \to Y$ one defines $\mathcal{M}_S(f) : \mathcal{M}_S(X) \to \mathcal{M}_S(Y)$ by:

$$\mathcal{M}_S(f)(\varphi)(y) = \sum_{x \in f^{-1}(y)} \varphi(x).$$

Such a (finite) multiset $\varphi \in \mathcal{M}_S(X)$ may be written as formal sum $s_1|x_1\rangle + \cdots + s_k|x_k\rangle$ where $\text{supp}(\varphi) = \{x_1, \ldots, x_k\}$ and $s_i = \varphi(x_i) \in S$ describes the “multiplicity” of the element $x_i$. The ket notation $|x_i\rangle$ is justified because these elements are vectors, and useful, because it distinguishes $x$ as element of $X$ and as vector in $\mathcal{M}_S(X)$. These formal sum are quotiented by the usual commutativity and associativity relations. Also, the same element $x \in X$ may be counted multiple times, so that $s_1|x\rangle + s_2|x\rangle$ is considered to be the same as $(s_1 + s_2)|x\rangle$. With this formal sum notation one can write the application of $\mathcal{M}_S$ on a map $f$ as $\mathcal{M}_S(f)(\sum_i s_i |x_i\rangle) = \sum_i s_i f(x_i)\rangle$.

This multiset functor is a monad, whose unit $\eta : X \to \mathcal{M}_S(X)$ is $\eta(x) = 1|x\rangle$, and multiplication $\mu : \mathcal{M}_S(\mathcal{M}_S(X)) \to \mathcal{M}_S(X)$ is $\mu(\sum_i s_i |\varphi_i\rangle)(x) = \sum_i s_i \cdot \varphi_i(x)$, where $\cdot$ is multiplication in $S$. 

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In order to emphasise that elements of $\mathcal{M}_S(X)$ are finite multisets, one may call $\mathcal{M}_S$ the finitary multiset monad. In order to include non-finite multisets, one has to assume that suitable infinite sums exist in the underlying semiring $S$. This is less natural.

For the semiring $S = \mathbb{N}$ one gets the free commutative monoid $\mathcal{M}_\mathbb{N}(X)$ on a set $X$. The monad $\mathcal{M}_\mathbb{N}$ is also known as the ‘bag’ monad, containing ordinary ($\mathbb{N}$-valued) multisets. If $S = \mathbb{Z}$ one obtains the free Abelian group $\mathcal{M}_\mathbb{Z}(X)$ on $X$. The Boolean semiring $2 = \{0, 1\}$ yields the finite powerset monad $\mathcal{P}_{\text{fin}} = \mathcal{M}_2$. Here we shall be mostly interested in the cases where $S$ is $\mathbb{R}_{\geq 0}$, $\mathbb{R}$, or $\mathbb{C}$.

An (Eilenberg-Moore) algebra $\alpha : \mathcal{M}_S(X) \to X$ for the multiset monad corresponds to a monoid structure on $X$—given by $x + y = \alpha(1 | x ) + 1 | y )$—together with a scalar multiplication $\cdot : S \times X \to X$ given by $s \cdot x = \alpha(s | x )$. It preserves the additive structure (of $S$ and of $X$) in each coordinate separately. This makes $X$ a module, for the semiring $S$. Conversely, such an $S$-module structure on a commutative monoid $M$ yields an algebra $\mathcal{M}_S(M) \to M$ by $\sum_i s_i | x_i ) \mapsto \sum_i s_i \cdot x_i$. Thus the category of algebras $\text{Alg}(\mathcal{M}_S)$ is equivalent to the category $\text{Mod}_S$ of $S$-modules. When $S$ happens to be a field, this category $\text{Mod}_S$ is the category $\text{Vect}_S$ of vector spaces over $S$. Thus we have a uniform description of the three categories of relevance in the previous section, namely:

$$\text{Alg}(\mathcal{M}_{\mathbb{R}_{\geq 0}}) = \text{Mod}_{\mathbb{R}_{\geq 0}}$$

$$\text{Alg}(\mathcal{M}_\mathbb{R}) = \text{Mod}_\mathbb{R} = \text{Vect}_\mathbb{R}$$

$$\text{Alg}(\mathcal{M}_\mathbb{C}) = \text{Mod}_\mathbb{C} = \text{Vect}_\mathbb{C}.$$  

We continue this section with a basic result in the theory of monads, which is stated without proof, but with a few subsequent pointers.

**Theorem 4.** Let $A$ be a symmetric monoidal category, which is both complete and cocomplete, and let $T : A \to A$ be a monad on $A$. The category $\text{Alg}(T)$ of algebras is:

(a) also complete, with limits as in $A$;
(b) cocomplete as soon as certain special colimits exist in $\text{Alg}(T)$, namely colimits of reflexive pairs;
(c) symmetric monoidal closed in case these colimits exist and the monad $T$ is symmetric monoidal (commutative), where the free algebra functor $F : A \to \text{Alg}(T)$ preserves the monoidal structure (i.e. is strong monoidal).

A category of algebras is always “as complete” as its underlying category, see e.g. [35, 5]. Cocompleteness always holds for algebras over $\text{Sets}$ and follows from a result of Linton’s, see [5, § 9.3, Prop. 4] using the existence of coequalisers of reflexive pairs in $\text{Sets}$. We shall mostly use this result for $A = \text{Sets}$, so that we don’t have to worry about these special colimits: the monoidal structure on the underlying category $\text{Sets}$ is thus cartesian. Monoidal structure $(I, \otimes)$ in categories of algebras goes back to [33] (see also [23]). The tensor unit

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I is simply $F(1)$, for the free algebra functor $F : \text{Sets} \to \text{Alg}(T)$ and the final (singleton) set 1. The tensor $\otimes$ is obtained as a suitable coequaliser of algebras. Algebra maps $X \otimes Y \to Z$ then correspond to bi-homomorphisms $UX \times UY \to UZ$. In particular, there is a universal bi-homomorphism $\otimes : UX \times UY \to U(X \otimes Y)$. The free functor preserves these tensors.

The multiset monad $\mathcal{M}_S$ is symmetric monoidal if $S$ is a (multiplicatively) commutative semiring. In that case categories $\text{Mod}_S$ are monoidal closed, with $S \cong \mathcal{M}_S(1)$ as tensor unit. Maps $M \otimes N \to K$ in $\text{Mod}_S$ correspond to bilinear maps $M \times N \to K$ (linear in each argument separately). The associated exponent is written as $-\circ$, like before.

For modules $M, N \in \text{Mod}_S$ there are obvious correspondences:

\[
\begin{align*}
M \otimes N &\to S \\
N \otimes M &\to S
\end{align*}
\]

This means that there are adjunctions:

\[
\text{Mod}_S \xleftarrow{(-) \to S} \quad \Downarrow \quad \text{Mod}_S^{\text{op}}
\]

as used in the previous section.

In summary, we have a sequence of categories of algebras of monads:

\[
\begin{array}{ccc}
\text{Alg}(\mathcal{M}_\mathbb{R}_{\geq 0}) & \leftarrow & \text{Alg}(\mathcal{M}_\mathbb{R}) & \leftarrow & \text{Alg}(\mathcal{M}_\mathbb{C}) \\
\text{Mod}_\mathbb{R}_{\geq 0} & \cong & \text{Vect}_\mathbb{R} & \cong & \text{Vect}_\mathbb{C}
\end{array}
\]

where the maps between them can be understood as arising from maps of monads in the other direction:

$\mathcal{M}_\mathbb{R}_{\geq 0} \Rightarrow \mathcal{M}_\mathbb{R} \Rightarrow \mathcal{M}_\mathbb{C}$ via semiring inclusions $\mathbb{R}_{\geq 0} \hookrightarrow \mathbb{R} \hookrightarrow \mathbb{C}$.

This follows from the following general result.

**Proposition 5.** A homomorphism of semirings $f : S \to S'$, preserving both the additive and multiplicative monoid structures, gives rise to a map of monads $\mathcal{M}_S \Rightarrow \mathcal{M}_{S'}$, by $\left(\sum_j s_j | x_j\right) \mapsto \left(\sum_j f(s_j) | x_j\right)$, and thus to a functor $\text{Alg}(\mathcal{M}_{S'}) \to \text{Alg}(\mathcal{M}_S)$, by $(\mathcal{M}_{S'}(X) \to X) \mapsto (\mathcal{M}_S(X) \to \mathcal{M}_{S'}(X) \to X)$. This functor always has a left adjoint.

The left adjoint exists because categories of modules $\text{Alg}(\mathcal{M}_S) = \text{Mod}_S$ are cocomplete; it can be constructed via a coequaliser, see e.g. [23, 29]. Thus, modules over their semirings have the structure of a bifibration [24].
The different spaces of operators $B(H)$, $SA(H)$, $Pos(H)$ on a Hilbert space $H$ turn out to be related via free constructions. This was used implicitly in the proofs of Propositions 2 and 3 in the previous section, and also in [8].

**Theorem 6.** Write the left adjoints to the two forgetful functors in (11) as:

$$\begin{array}{ccc}
\text{Mod}_{R \geq 0} & \xrightarrow{\mathcal{R}} & \text{Vect}_R \\
& & \xrightarrow{\mathcal{C}} \text{Vect}_C.
\end{array}$$

(12)

For a finite-dimensional Hilbert space $H$, the canonical inclusion morphisms $\mathcal{Pos}(H) \hookrightarrow SA(H)$ in $\text{Mod}_{R \geq 0}$, and $SA(H) \hookrightarrow B(H)$ in $\text{Vect}_R$ yield via these adjunctions (transposed) maps that turn out to be isomorphisms:

$$\mathcal{R}(\mathcal{Pos}(H)) \xrightarrow{\sim} SA(H) \quad \text{and} \quad \mathcal{C}(SA(H)) \xrightarrow{\sim} B(H).$$

Thus we have the following situation of triangles commuting up-to-isomorphism.

![Diagram](https://doi.org/10.1017/CBO9781139519687.008 Published online by Cambridge University Press)

**Proof.** The proof uses explicit constructions of the left adjoints $\mathcal{R}$ and $\mathcal{C}$ in (12). A module $X$ over $R_{\geq 0}$ can be turned into a vector space over $R$ via the same construction that turns a commutative monoid into a commutative group

$$\mathcal{R}(X) = (X \times X)/\sim \quad \text{where} \quad (x_1, x_2) \sim (y_1, y_2) \iff \exists z. x_1 + y_2 + z = y_1 + x_2 + z.$$

Addition is done componentwise: $[x_1, x_2] + [y_1, y_2] = [x_1 + y_1, x_2 + y_2]$, minus by reversal: $-[x_1, x_2] = [x_2, x_1]$, and scalar multiplication $\bullet : R \times \mathcal{R}(X) \to \mathcal{R}(X)$ via:

$$r \bullet [x_1, x_2] = \begin{cases} [r \bullet x_1, r \bullet x_2] & \text{if } r \geq 0 \\ [(-r) \bullet x_2, (-r) \bullet x_1] & \text{if } r < 0 \end{cases}$$

(Notice the reversal of the $x_i$ in the second case.)

A vector space $X$ over $\mathbb{R}$ can be turned into a vector space over $\mathbb{C}$, simply via $C(X) = X \times X$. The additive structure is obtained pointwise, and scalar multiplication $\bullet : \mathbb{C} \times C(X) \to C(X)$ is done as follows.

$$(a + ib) \bullet (x_1, x_2) = (a \bullet x_1 - b \bullet x_2, b \bullet x_1 + a \bullet x_2).$$

The inclusion morphism $\mathcal{Pos}(H) \hookrightarrow SA(H)$ in $\text{Mod}_{R \geq 0}$ yields as transpose the map $\varphi : \mathcal{R}(\mathcal{Pos}(H)) \to SA(H)$ in $\text{Vect}_R$ given by $\varphi([B_1, B_2]) = B_1 - B_2$. It is surjective since each $A \in SA(H)$ can be written as $A = A_p - A_n$ for $A_p, A_n \in Pos(H)$ as in (8). Thus $A = \varphi([A_p, A_n])$.

Similarly, the inclusion $SA(H) \hookrightarrow B(H)$ in $\text{Vect}_R$ gives rise to a transpose $\psi : \mathcal{C}(SA(H)) \to B(H)$ in $\text{Vect}_C$, given by $\psi(B_1, B_2) = B_1 + iB_2$. Also
this map is surjective since each $A \in \mathcal{B}(H)$ can be written as $A = \frac{1}{2}(A + A^\dagger) + \frac{i}{2}(-iA + iA^\dagger)$, where $A + A^\dagger$ and $-iA + iA^\dagger$ are self-adjoints. Hence $A = \psi\left(\frac{1}{2}(A + A^\dagger), \frac{i}{2}(-iA + iA^\dagger)\right)$.

§4. Convex sets and effect modules. In the previous section we have seen how the spaces of operators $\mathcal{P}\text{os}(H)$, $\mathcal{S}\text{A}(H)$, $\mathcal{B}(H)$ fit in the context of modules. The spaces $\mathcal{D}\mathcal{M}(H)$ of density operators (states) and $\mathcal{E}\text{f}(H)$ of effects (statements/predicates) require more subtle structures that will be introduced in this section, namely convex sets and effect modules. We show that they are related by a dual adjunction, and that there exists a map of adjunctions from Hilbert spaces, like in Section 2.

First we recall the definition of the two sets of operators that are relevant in this section.

$$\mathcal{D}\mathcal{M}(H) = \{ A \in \mathcal{P}\text{os}(H) \mid \text{tr}(A) = 1 \}$$
$$\mathcal{E}\text{f}(H) = \{ A \in \mathcal{P}\text{os}(H) \mid A \leq I \},$$

where $I$ is the identity map $H \rightarrow H$ and $\leq$ is the Löwner order (described before Proposition 3). A further subset of $\mathcal{E}\text{f}(H)$ is the set of projections, given as:

$$\mathcal{P}\text{r}(H) = \{ A \in \mathcal{B}(H) \mid A^\dagger = A = AA \}.$$ 

For a projection $A \in \mathcal{P}\text{r}(H)$ there is an orthosupplement $A^\perp \in \mathcal{P}\text{r}(H)$ with $A + A^\perp = I$. This shows $A \leq I$, since $I - A = A^\perp$ is positive.

Before we investigate the algebraic structure of these sets of operators we briefly mention the following alternative formulation of effects. It is used for instance in [11], where these effects $A$ are called predicates: they give a “quantum expectation value” $\text{tr}(AB)$ for a density matrix $B$ (see the map $\eta_\mathcal{E}\text{f}$ in Theorem 14 below, elaborated in Remark 15).

**Lemma 7.** A positive operator $A \in \mathcal{P}\text{os}(H)$ is an effect if and only if all of its eigenvalues are in $[0, 1]$. 

**Proof.** Suppose $A$ is an effect with spectral decomposition $A = \sum_j \lambda_j |j\rangle\langle j|$, where we may assume that the eigenvectors $|j\rangle$ form an orthonormal basis. The eigenvalues $\lambda_j$ are necessarily real and positive. They satisfy:

$$\lambda_j = \lambda_j \langle j | j \rangle = \langle j | \lambda_j | j \rangle = \langle j | A | j \rangle \leq \langle j | I | j \rangle = \langle j | j \rangle = 1.$$ 

Conversely, assume a positive operator $A$ with spectral decomposition $A = \sum_j \lambda_j |j\rangle\langle j|$ where the $|j\rangle$ form an orthonormal basis and $\lambda_j \in [0, 1]$. Then:

$$A = \sum_j \lambda_j |j\rangle\langle j| \leq \sum_j |j\rangle\langle j| = I.$$ 

**4.1. Convex sets.** We start with convex sets, and (conveniently) describe them via a monad, so that we can benefit from general results like in Theorem 4. Analogously to the multiset monad one defines the distribution monad
\( D : \text{Sets} \to \text{Sets} \) as:

\[
D(X) = \{ \varphi : X \to [0, 1] \mid \text{supp}(\varphi) \text{ is finite and } \sum_{x \in X} \varphi(x) = 1 \}. \tag{13}
\]

Elements of \( D(X) \) are convex combinations \( s_1 | x_1 \rangle + \cdots + s_k | x_k \rangle \), where the probabilities \( s_i \in [0, 1] \) satisfy \( \sum_i s_i = 1 \). Unit and multiplication making \( D \) a monad can be defined as for the multiset monad \( M_S \). This multiplication \( \mu \) is well-defined since:

\[
\sum_x \mu \left( \sum_i s_i \varphi_i \right)(x) = \sum_x \sum_i s_i \varphi_i(x) = \sum_i s_i \cdot \left( \sum_x \varphi_i(x) \right) = \sum_i s_i = 1.
\]

The distribution monad \( D \) is always symmetric monoidal (commutative). Here it is defined for probabilities in the unit interval \([0, 1]\), but the more general structure of an “effect monoid” may be used instead, see [26].

The following result goes back to [39], see also [32, 13, 25].

**Theorem 8.** The category \( \text{Alg}(D) \) of algebras of the monad \( D \) is the category \( \text{Conv} \) of convex sets with affine maps between them.

Here we shall identify such a convex set simply with an algebra \( a : D(X) \to X \) of the monad \( D \). It thus consists of a set \( X \) in which there is an interpretation \( a(\sum_j s_j | x_j \rangle) \in X \) for each formal convex combination \( \sum_j s_j | x_j \rangle \in D(X) \). In particular, for each \( r \in [0, 1] \) and \( x, y \in X \) there is an interpretation of the convex sum \( r x + (r - 1)y \), namely as \( a(r | x \rangle + (1 - r) | y \rangle) \in X \). The unit interval \([0, 1]\) of real numbers is an obvious example of a convex set. Actually, it is a free one since \([0, 1] \cong D(\{0, 1\}) \). Affine maps preserve such interpretations of convex combinations. We recall that in the present context all such convex combinations involve only finitely many elements \( x_j \).

**Lemma 9.** Let \( \text{FdHilb}_{\text{Un}} \) be the category of finite-dimensional Hilbert spaces with unitary maps between them. Taking density operators yields a functor \( \text{DM} : \text{FdHilb}_{\text{Un}} \to \text{Conv} = \text{Alg}(D) \).

**Proof.** As is well-known, the set \( \text{DM}(H) \) of density operators is convex: given finitely many \( A_j \in \text{DM}(H) \) and \( r_j \in [0, 1] \) with \( \sum_j r_j = 1 \), the operator \( A = \sum_j r_j A_j \) is positive and has trace 1, since:

\[
\text{tr}(A) = \text{tr} \left( \sum_j r_j A_j \right) = \sum_j r_j \text{tr}(A_j) = \sum_j r_j = 1.
\]

Moreover, if \( U : H \to K \) is unitary—i.e. \( U U^\dagger = I \) and (thus) \( U^\dagger U = I \), so that \( U^\dagger = U^{-1} \)—then \( \text{DM}(U)(A) = UAU^\dagger : K \to K \) is in \( \text{DM}(K) \), if \( A \in \text{DM}(H) \), since:

\[
\text{tr} \left( \text{DM}(U)(A) \right) = \text{tr}(UAU^\dagger) = \text{tr}(U^\dagger UA) = \text{tr}(IA) = \text{tr}(A) = 1.
\]

The three example categories \( \text{Alg}(M_S) \) of interest here—that arise from multiset monads \( M_S \) for \( S = \mathbb{R}_{\geq 0}, \mathbb{R}, \mathbb{C} \)—are different from the category \( \text{Alg}(D) \) of convex sets in at least three aspects:
These categories $\text{Alg} (\mathcal{M}_S)$ are dually self-adjoint via the functor $(-) \mapsto S$ as in (10).

- They have biproducts, because the monads $\mathcal{M}_S$ are ‘additive’, see [10].
- The tensor unit in $\text{Alg} (D) = \text{Conv}$ is the singleton set $1$, since $D(1) \cong 1$, so that tensors $\otimes$ in $\text{Conv}$ have projections (see [23]).

The mapping $X \mapsto \text{Conv} (X, [0, 1])$, for $X$ a convex set, does not yield an adjunction as in (10), but does lead to an interesting dual adjunction with a category of ‘effect modules’. This will be described in the next subsection.

But first we conclude this part on convex sets with an observation like in Theorem 6. There is an obvious map of monads $\mathcal{D} \Rightarrow \mathcal{M}_{\mathbb{R}_{\geq 0}}$, that gives rise to an inclusion functor $\mathcal{Mod}_{\mathbb{R}_{\geq 0}} = \text{Alg} (\mathcal{M}_{\mathbb{R}_{\geq 0}}) \rightarrow \text{Alg} (D) = \text{Conv}$, saying that modules over non-negative reals are convex sets—in a trivial manner. For general reasons, this functor has a left adjoint, that can be described explicitly in terms of a representation construction that goes back to [38] (see also [25]).

This left adjoint $S: \text{Conv} \rightarrow \mathcal{Mod}_{\mathbb{R}_{\geq 0}}$ is given on $X \in \text{Conv}$ by:

$$S(X) = \{0\} + \mathbb{R}_{\geq 0} \times X,$$

with addition for $u, v \in S(X)$, in trivial cases given by $u + 0 = u = 0 + u$ and:

$$(s, x) + (t, y) = (s + t, \frac{s}{s + t} x + \frac{t}{s + t} y).$$

A scalar multiplication $\cdot: \mathbb{R}_{\geq 0} \times S(X) \rightarrow S(X)$ is defined as:

$$s \cdot u = \begin{cases} 0 & \text{if } u = 0 \text{ or } s = 0 \\ (s \cdot t, x) & \text{if } u = (t, x) \text{ and } s \neq 0. \end{cases}$$

This makes $S(X)$ a module over $\mathbb{R}_{\geq 0}$.

**Theorem 10.** For a finite-dimensional Hilbert space $H$, transposing the inclusion $\mathcal{D} \mathcal{M}(H) \hookrightarrow \mathcal{P} \mathcal{O} \mathcal{S}(H)$ in $\text{Conv}$ gives an isomorphism $S(\mathcal{D} \mathcal{M}(H)) \cong \mathcal{P} \mathcal{O} \mathcal{S}(H)$ in $\mathcal{Mod}_{\mathbb{R}_{\geq 0}}$. In this way one obtains a triangle commuting up-to-isomorphism:

$$\begin{array}{ccc} \mathcal{F} \mathcal{D} \mathcal{H} \mathcal{I} \mathcal{B} \mathcal{U} \mathcal{N} & \mathcal{D} \mathcal{M} & \mathcal{P} \mathcal{O} \mathcal{S} \\ \downarrow & \downarrow & \downarrow \\ \text{Alg}(\mathcal{D}) = \text{Conv} & \overset{\text{free}}{S} & \mathcal{M}_{\mathbb{R}_{\geq 0}} = \text{Alg}(\mathcal{M}_{\mathbb{R}_{\geq 0}}) \end{array}$$

**Proof.** The induced map $S(\mathcal{D} \mathcal{M}(H)) = \{0\} + \mathbb{R}_{\geq 0} \times \mathcal{D} \mathcal{M}(H) \overset{\varphi}{\rightarrow} \mathcal{P} \mathcal{O} \mathcal{S}(H)$ is given by $0 \mapsto 0$ and $(r, A) \mapsto rA$. It is injective, since if $rA = sB$ for $A, B \in \mathcal{D} \mathcal{M}(H)$, then $r = r \cdot \text{tr}(A) = \text{tr}(rA) = \text{tr}(sB) = s \cdot \text{tr}(B) = s$, and thus $A = B$. It is also surjective: since each non-zero $B \in \mathcal{P} \mathcal{O} \mathcal{S}(H)$ can be written as $B = \text{tr}(B)(\frac{B}{\text{tr}(B)}) = \varphi(\text{tr}(B), \frac{B}{\text{tr}(B)})$, where the operator $\frac{B}{\text{tr}(B)}$ has trace 1 by construction.

$\square$
By combining this result with Theorem 6 we see that each of the spaces of operators \( B(H) \), \( SA(H) \), and \( Pos(H) \) can be obtained from the space \( DM(H) \) of density operators via free constructions. As we will see in Theorem 14 below, density matrices and effects can be translated back and forth: \( \mathcal{E}f(H) \cong \text{Conv}(DM(H), [0,1]) \) and \( DM(H) \cong \text{EMod}(\mathcal{E}f(H), [0,1]) \). Hence these density operators and effects are in a sense most fundamental among the operators on a Hilbert space.

4.2. Effect modules. Effect modules are structurally like modules over a semiring. But instead of a semiring of scalars one uses an effect monoid, such as the unit interval \([0,1]\). Such an effect monoid is a monoid in the category of effect algebras, just like a semiring is a monoid in the category of commutative monoids. Thus, in order to define an effect module, we need the notion of effect algebra and of monoid in effect algebras. This will be introduced first.

But in order to define an effect algebra, we need the notion of partial commutative monoid (PCM). Before reading the definition of PCM, think of the unit interval \([0,1]\) with addition \(+\). This \(+\) is obviously only a partial operation, which is commutative and associative in a suitable sense. This will be formalised next.

A partial commutative monoid (PCM) consists of a set \( M \) with a zero element \( 0 \in M \) and a partial binary operation \( \odot : M \times M \to M \) satisfying the three requirements below. They involve the notation \( x \perp y \) for: \( x \odot y \) is defined; in that case \( x, y \) are called orthogonal.

1. Commutativity: \( x \perp y \) implies \( y \perp x \) and \( x \odot y = y \odot x \);
2. Associativity: \( y \perp z \) and \( x \perp (y \odot z) \) implies \( x \perp y \) and \( (x \odot y) \perp z \) and also \( x \odot (y \odot z) = (x \odot y) \odot z \);
3. Zero: \( 0 \perp x \) and \( 0 \odot x = x \);

For each set \( X \) the lift \( \{0\} + X \) of \( X \), obtained by adjoining a new element 0, is an example of a PCM, with \( u \odot 0 = u = 0 \odot u \), and \( \odot \) undefined otherwise. Such structures are also studied under the name ‘partially additive monoid’, see [3].

The notion of effect algebra is due to [18], see also [14] for an overview.

**Definition 11.** An effect algebra is a PCM \((E, 0, \odot)\) with an orthosupplement. The latter is a unary operation \((-)\perp : E \to E\) satisfying:

1. \( x\perp \in E \) is the unique element in \( E \) with \( x \odot x\perp = 1 \), where \( 1 = 0\perp \);
2. \( x \perp 1 \Rightarrow x = 0 \).

A homomorphism \( E \to D \) of effect algebras is given by a function \( f : E \to D \) between the underlying sets satisfying \( f(1) = 1 \), and if \( x \perp x' \) in \( E \) then both \( f(x) \perp f(x') \) in \( D \) and \( f(x \odot x') = f(x) \odot f(x') \).

Effect algebras and their homomorphisms form a category, called \( \mathcal{EA} \).

The unit interval \([0,1]\) is a PCM with sum of \( r, s \in [0,1] \) defined if \( r + s \leq 1 \), and in that case \( r \odot s = r + s \). The unit interval is also an effect algebra with \( r\perp = 1 - r \). Each orthomodular lattice is an effect algebra, see [14, 17] for more

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information and examples. In particular, the projections \( \mathcal{P}r(H) \) of a Hilbert space form an effect algebra, with \( P \perp Q \) iff \( P \leq Q_{\perp} \). In [26] a notion of ‘convex category’ is introduced in which homsets \( \text{Hom}(X, 2) \) are effect algebras (where \( 2 = 1 + 1 \) and \( 1 \) is final). Most importantly in the current setting, the set of effects \( \mathcal{E}f(H) \), consisting of positive operators \( A \leq I \) is an effect algebra, with \( A \perp B \) iff \( A + B \leq I \), and in that case \( A \otimes B = A + B \); further, \( A_{\perp} = I - A \). This yields a functor \( \mathcal{E}f : \text{FdHilb}_{\mathbb{U}} \rightarrow \mathcal{E}A \).

In [28] it is shown that the category \( \mathcal{E}A \) is symmetric monoidal, where morphisms \( E \otimes D \rightarrow C \) in \( \mathcal{E}A \) correspond to ‘bimorphisms’ \( f : E \times D \rightarrow C \), satisfying \( f(1, 1) = 1 \), and for all \( x, x' \in E \) and \( y, y' \in D \),

\[
\begin{align*}
 x \perp x' &\implies f(x, y) \perp f(x', y) \quad \text{and} \quad f(x \otimes x', y) = f(x, y) \otimes f(x', y) \\
y \perp y' &\implies f(x, y) \perp f(x, y') \quad \text{and} \quad f(x, y \otimes y') = f(x, y) \otimes f(x, y').
\end{align*}
\]

The tensor unit is the two-element effect algebra \( 2 = \{0, 1\} \). Since \( 2 \) is at the same time initial in \( \mathcal{E}A \) we have a ‘tensor with coprojections’ (see [23] for ‘tensors with projections’). One can think of elements of the tensor \( E \otimes D \) as finite sums \( \bigotimes_j x_j \otimes y_j \), where one identifies:

\[
0 \otimes y = 0 \quad \quad \quad \quad \quad x \otimes 0 = 0
\]

\[
(x \otimes x') \otimes y = (x \otimes y) \otimes (x' \otimes y) \quad \quad x \otimes (y \otimes y') = (x \otimes y) \otimes (x \otimes y'),
\]

when \( x \perp x' \) and \( y \perp y' \).

**Example 12.** For an arbitrary set \( X \) the powerset \( \mathcal{P}(X) \) is a Boolean algebra, and so an orthomodular lattice, and thus an effect algebra. For \( U, V \in \mathcal{P}(X) \) one has \( U \perp V \) iff \( U \cap V = \emptyset \) and in that case \( U \cup V = U \cup V \). The tensor product \( [0, 1] \otimes \mathcal{P}(X) \) of effect algebras is then given by the set of step functions \( f : X \rightarrow [0, 1] \); such functions have only finitely many output values. When \( X \) is a finite set, say with \( n \) elements, then \( [0, 1] \otimes \mathcal{P}(X) \cong [0, 1]^n \), see [21].

As special case we have \([0, 1] \otimes \{0, 1\} \cong [0, 1], \) since \( \{0, 1\} \) is the tensor unit. One writes \( \text{MO}(n) \) for the orthomodular lattice with \( 2n + 2 \) elements, namely \( 0, 1, i, i^\perp \), for \( 1 \leq i \leq n \), with only minimal equations. Thus \( \text{MO}(0) = \{0, 1\} \) and \( \text{MO}(1) \cong \mathcal{P}(\{0, 1\}) \), so that \([0, 1] \otimes \text{MO}(1) \cong [0, 1]^2 \). It can be shown that \([0, 1] \otimes \text{MO}(2) \) is an octahedron.

Using this symmetric monoidal structure \( (\otimes, 2) \) on \( \mathcal{E}A \) we can consider, in a standard way, the category \( \text{Mon}(\mathcal{E}A) \) of monoids in the category \( \mathcal{E}A \) of effect algebras. Such monoids are similar to semirings, which are monoids in the category of commutative monoids, i.e. objects of \( \text{Mon}(\text{CMon}) \). A monoid \( S \in \text{Mon}(\mathcal{E}A) \) consists of a set \( S \) carrying effect algebra structure \((0, \otimes, (-)_{\perp})\) and a monoid structure, written multiplicatively, as in: \( S \otimes S \rightarrow S \leftarrow 2 \). Since \( 2 \) is initial, the latter map \( S \leftarrow 2 \) does not add any structure. The monoid structure on \( S \) is thus determined by a bimorphism \( \cdot : S \times S \rightarrow S \) that preserves \( \otimes \) in each variable separately and satisfies \( 1 \cdot x = x = x \cdot 1 \).
For such a monoid $S \in \text{Mon}(EA)$ we can consider the category $\text{Act}_S(EA) = \text{EMod}_S$ of $S$-monoid actions (scalar multiplications), or ‘effect modules’ over $S$ (see [34, VII, §4]). Again this is similar to the situation in Section 3 where the category $\text{Mod}_S$ of modules over a semiring $S$ may be described as the category $\text{Act}_S(\text{CMon})$ of commutative monoids with $S$-scalar multiplication.

In this section an effect module $X \in \text{Act}_S(EA)$ thus consists of an effect algebra $X$ together with an action (or scalar multiplication) $\bullet : S \otimes X \to X$, corresponding to a bimorphism $S \times X \to X$. A homomorphism of effect modules $X \to Y$ consists of a map of effect algebras $f : X \to Y$ preserving scalar multiplication $f(s \bullet x) = s \bullet f(x)$ for all $s \in S$ and $x \in X$.

By completely general reasoning the forgetful functor $\text{EMod}_S \to EA$ has a left adjoint, given by tensoring with $S$, as in:

\begin{equation}
\text{EMod}_S = \text{Act}_S(EA)
\end{equation}

\begin{equation}
S \otimes (-) \Downarrow \rightleftharpoons \Downarrow \text{EA}
\end{equation}

See [34, VII, §4] for details.

The main example of a (commutative) monoid in $EA$ is the unit interval $[0, 1] \in EA$ via ordinary multiplication. If $r_1 + r_2 \leq 1$, then we have the familiar distributivity in each variable, as in:

\[ s \cdot (r_1 \circ r_2) = s \cdot (r_1 + r_2) = (s \cdot r_1) + (s \cdot r_2) = (s \cdot r_1) \otimes (s \cdot r_2). \]

We shall be most interested in the associated category $\text{EMod}_{[0,1]} = \text{Act}_{[0,1]}(EA)$. In the sequel ‘effect module’ will mean ‘effect module over $[0, 1]$’. In particular, we shall write $\text{EMod}$ for $\text{EMod}_{[0,1]}$. These effect modules have been studied earlier under the name ‘convex effect algebras’, see [36]. We prefer the name ‘effect module’ to emphasise the similarity with ordinary modules.

The effects $\mathcal{E}f(H)$ of a Hilbert space form an example of an effect module, with the usual scalar multiplication $[0, 1] \times \mathcal{E}f(H) \to \mathcal{E}f(H)$. It is not hard to see that this mapping $H \mapsto \mathcal{E}f(H)$ yields a functor $\text{FdHilb}_{\text{Un}} \to \text{EMod}$.

A (dual) adjunction between convex sets and effect algebras is described in [25]. Here it is strengthened to an adjunction between convex sets and effect modules.

**Proposition 13.** By “homming into $[0, 1]$” one obtains an adjunction:

\[ \text{Conv} \simeq \Downarrow \text{EMod} \]

**Proof.** Given a convex set, the homset $\text{Conv}(X, [0, 1])$ of affine maps is an effect module, with $f \perp g$ iff $\forall x \in X. f(x) + g(x) \leq 1$. In that case one defines $f \otimes g = \lambda x \in X. f(x) + g(x)$. It is easy to see that this is again an affine function. Similarly, the pointwise scalar product $r \bullet f = \ldots$

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\(\lambda x \in X. r \cdot f(x)\) yields an affine function. This mapping \(X \mapsto \text{Conv}(X, [0, 1])\) gives a contravariant functor since for \(h: X \to X'\) in \(\text{Conv}\) pre-composition with \(h\) yields a map \((-) \circ h: \text{Conv}(X', [0, 1]) \to \text{Conv}(X, [0, 1])\) of effect modules.

In the other direction, given an effect module \(Y\), the homset \(\text{EMod}(Y; [0, 1])\) of effect module maps yields a convex set: for a formal convex sum \(\sum_j r_j \cdot f_j\), where \(f_j: Y \to [0, 1]\) in \(\text{EMod}\), we can define an actual sum \(f: Y \to [0, 1]\) by \(f(y) = \sum_j r_j \cdot f_j(y)\). This \(f\) forms a map of effect modules. Again, functoriality is obtained via pre-composition.

The dual adjunction between \(\text{Conv}\) and \(\text{EMod}\) involves a bijective correspondence that is obtained by swapping arguments, like in (10). For \(X \in \text{Conv}\) and \(Y \in \text{EMod}\), we have:

\[
\begin{align*}
X & \xrightarrow{f} \text{EMod}(Y, [0, 1]) & \text{in Conv} \\
Y & \xrightarrow{g} \text{Conv}(X, [0, 1]) & \text{in EMod}
\end{align*}
\]

What needs to be checked is that for a map \(f\) of convex sets as indicated, the swapped version \(\hat{f} = \lambda y \in Y. \lambda x \in X. f(x)(y): Y \to \text{Conv}(X, [0, 1])\) is a map of effect modules—and similarly for \(g\). This is straightforward. \(\dashv\)

With this adjunction in place we can give a clearer picture of density matrices and effects, forming a map of adjunctions (like in Section 2. The isomorphisms involved are well-known, see e.g. [8], but the framing of the relevant structure in terms of maps of adjunctions is new.

**Theorem 14.** There is a ‘dual adjunction’ between convex sets and effect modules as in the lower part of the diagram below. Further, there are natural isomorphisms:

\[
\begin{align*}
\mathcal{E}f(H) & \xrightarrow{\text{hs}_\mathcal{E}f} \text{Conv}(\mathcal{D}M(H), [0, 1]) \\
A & \xrightarrow{\text{tr}(A \cdot^{-})} B \xrightarrow{\text{tr}(B \cdot^{-})}
\end{align*}
\]

that give rise to a map of adjunctions given by states \(\mathcal{D}M\) and statements (effects) \(\mathcal{E}f\) in:

\[
\begin{align*}
\text{FdHilb}_{\text{Un}} & \xrightarrow{(-)\dagger} \text{FdHilb}_{\text{Un}}^{\text{op}} \\
\mathcal{D}M & \xrightarrow{\text{Conv}(-, [0, 1])} \text{EMod}^{\text{op}}
\end{align*}
\]

**Proof.** This map of adjunctions involves natural isomorphisms (15), in the categories \(\text{EMod}\) and \(\text{Conv}\). We start with the first one, labeled \(\text{hs}_{\mathcal{E}f}\) in (15),
and note that it is well-defined: for $A \in \mathcal{E}_f(H)$ and $B \in \mathcal{DM}(H)$ one has:

$$h_{\mathcal{E}_f}(A)(B) = \text{tr}(AB) \leq \text{tr}(IB) = \text{tr}(B) = 1.$$  

Injectivity of $h_{\mathcal{E}_f}$ is obtained as follows. Assume $A_1, A_2 \in \mathcal{E}_f(H)$ satisfy $h_{\mathcal{E}_f}(A_1) = h_{\mathcal{E}_f}(A_2)$, i.e. $\text{tr}(A_1 - A_2) = \text{tr}(A_2 - A_1) : \mathcal{DM}(H) \to [0, 1]$. For an arbitrary non-zero element $x \in H$ there is a density matrix $B_x = \frac{|x\rangle \langle x|}{|x|^2} : H \to H$. Thus $\text{tr}(A_1 B_x) = \text{tr}(A_2 B_x)$. Then:

$$\langle (A_1 - A_2)x | x \rangle = \langle x | A_1 x \rangle - \langle x | A_2 x \rangle$$

$$= \text{tr}(\langle x | A_1 | x \rangle) - \text{tr}(\langle x | A_2 | x \rangle)$$

$$= \text{tr}(A_1 | x \rangle \langle x |) - \text{tr}(A_2 | x \rangle \langle x |)$$

$$= |x|^2 \left( \text{tr}(A_1 B_x) - \text{tr}(A_2 B_x) \right)$$

$$= 0.$$  

Since this equation holds for all $x \in H$, including $x = 0$, we get $A_1 - A_2 \geq 0$, and thus $A_2 \leq A_1$. Similarly $A_1 \leq A_2$, and thus $A_1 = A_2$.

For surjectivity of $h_{\mathcal{E}_f}$ assume a morphism of convex sets $h : \mathcal{DM}(H) \to [0, 1]$. We turn it into a linear map $h' : \mathcal{Pos}(H) \to \mathbb{R}_{\geq 0}$ in the category $\text{Mod}_{\mathbb{R}_{\geq 0}}$ of modules over $\mathbb{R}_{\geq 0}$ via:

$$h'(B) = \begin{cases} 
0 & \text{if } B = 0, \text{ or equivalently, } \text{tr}(B) = 0 \\
\text{tr}(B) \cdot h\left( \frac{B}{\text{tr}(B)} \right) & \text{otherwise}. 
\end{cases}$$

This is well-defined since $\frac{\text{tr}(B)}{\text{tr}(B)} = \frac{\text{tr}(B)}{\text{tr}(B)} = 1$. We check linearity of $h'$. It is easy to see that $h'(rB) = rh'(B)$, for $r \in \mathbb{R}_{\geq 0}$, and for non-zero $B, C \in \mathcal{Pos}(H)$ we have:

$$h'(B) + h'(C)$$

$$= \text{tr}(B) \cdot h\left( \frac{B}{\text{tr}(B)} \right) + \text{tr}(C) \cdot h\left( \frac{C}{\text{tr}(C)} \right)$$

$$= \text{tr}(B + C) \cdot \left( \frac{\text{tr}(B)}{\text{tr}(B + C)} \cdot h\left( \frac{B}{\text{tr}(B)} \right) + \frac{\text{tr}(C)}{\text{tr}(B + C)} \cdot h\left( \frac{C}{\text{tr}(C)} \right) \right)$$

since $h$ preserves convex sums and:

$$\frac{\text{tr}(B)}{\text{tr}(B + C)} + \frac{\text{tr}(C)}{\text{tr}(B + C)} = \frac{\text{tr}(B)}{\text{tr}(B) + \text{tr}(C)} + \frac{\text{tr}(C)}{\text{tr}(B) + \text{tr}(C)} = 1$$

$$= \text{tr}(B + C) \cdot h\left( \frac{B + C}{\text{tr}(B + C)} \right)$$

$$= h'(B + C).$$

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By Proposition 3 there is a unique \( A = \eta_h \phi_{\rho_B}^{-1}(h') \in \mathcal{P}os(H) \) with \( h' = \text{tr}(A) : \mathcal{P}os(H) \to \mathbb{R}_{\geq 0} \). For a density operator \( B \in \mathcal{D}M(H) \) we get \( \text{tr}(AB) = h'(B) = h(B) \in [0, 1] \). We claim that \( A \) is an effect, i.e. is in \( \mathcal{E}f(H) \), Write \( A = \sum_j \lambda_j | j \rangle \langle j | \) as spectral decomposition, where \(| j \rangle \) form an orthonormal basis. By Lemma 7 we need to prove \( \lambda_j \leq 1 \). Each operator \(| j \rangle \langle j | \) is a density matrix, and thus \( \lambda_j = \text{tr}(A| j \rangle \langle j |) = h'(| j \rangle \langle j |) = h(| j \rangle \langle j |) \leq 1 \).

We turn to the second map \( \eta_h \phi_{\mathcal{D}M} \) in (15). Injectivity is obtained like for \( \eta_h \phi_{\mathcal{E}f} \), using that each operator \(| x \rangle \langle x | \) is a projection and thus an effect. For surjectivity assume a map of effect modules \( g : \mathcal{E}f(H) \to [0, 1] \), we extend it to a linear map \( g' : \mathcal{P}os(H) \to \mathbb{R}_{\geq 0} \) by:

\[
g'(B) = n \cdot g \left( \frac{1}{n} B \right)
\]

where \( n \in \mathbb{N} \) is such that \( \frac{1}{n} B \in \mathcal{E}f(H) \). Such an \( n \) can be found in the following way. Take the spectral decomposition \( B = \sum_j \lambda_j | j \rangle \langle j | \), where \( \lambda_j \geq 0 \), because \( B \) is positive, and the \(| j \rangle \) form an orthonormal basis. We can find an \( n \in \mathbb{N} \) with \( \lambda_j \leq n \) for each \( j \). Then \( \frac{1}{n} B = \sum_j \frac{1}{n} \lambda_j | j \rangle \langle j | \) is an effect by Lemma 7. We also have to check that the definition of \( g' \) is independent of the choice of \( n \): if also \( \frac{1}{m} B \in \mathcal{E}f(H) \), assume, without loss of generality \( m \leq n \); then we use that \( g \) is a map of \([0, 1]\)-actions:

\[
n \cdot g \left( \frac{1}{n} B \right) = n \cdot g \left( \frac{m}{n} \cdot \frac{1}{m} B \right) = n \cdot \frac{m}{n} \cdot g \left( \frac{1}{m} B \right) = m \cdot g \left( \frac{1}{m} B \right).
\]

It is easy to see that the map \( g' \) is linear. Hence by Proposition 3 there is a (unique) \( B = \eta_h \phi_{\rho_B}^{-1}(g') \in \mathcal{P}os(H) \) with \( g' = \text{tr}(B') : \mathcal{P}os(H) \to \mathbb{R}_{\geq 0} \). Then for \( A \in \mathcal{E}f(H) \) we have \( g(A) = g'(A) = \text{tr}(BA) \in [0, 1] \). In particular \( 1 = g(I) = \text{tr}(BI) = \text{tr}(B) \), so that \( B \in \mathcal{D}M(H) \).

One of the equations that \( \eta_h \phi_{\mathcal{E}f} \) and \( \eta_h \phi_{\mathcal{D}M} \) should satisfy to ensure that we have a map of adjunctions is the following; the other one is similar and left to the reader.

\[
\mathcal{D}M(H) \xrightarrow{\eta_h \phi_{\mathcal{D}M}^{-1}} \mathcal{P}os(H) \xrightarrow{\text{tr}} \mathcal{P}os(H) \xrightarrow{\text{tr}} \mathcal{D}M(H)
\]

This triangle commutes since for \( B \in \mathcal{D}M(H) \),

\[
\left( \eta_h \phi_{\mathcal{D}M}^{-1} \circ \lambda \cdot \eta_h \phi_{\mathcal{E}f} \right)(B) = \eta_h \phi_{\mathcal{D}M}^{-1} \circ \eta(B) \circ \eta_h \phi_{\mathcal{E}f}
\]

\[
= \eta_h \phi_{\mathcal{D}M}^{-1} \circ \lambda \cdot A \cdot \eta(B) \circ \eta_h \phi_{\mathcal{E}f}(A)
\]

\[
= \eta_h \phi_{\mathcal{D}M}^{-1} \circ \lambda \cdot A \cdot \eta_h \phi_{\mathcal{E}f}(A)(B)
\]
Remark 15. In [11] a quantum weakest precondition calculus is developed using effects on a finite-dimensional Hilbert space as predicates and density matrices as states. The underlying duality can be made explicit in the current setting. Programs act on states and are thus modeled as “state transformer” maps $\mathcal{D}M(H) \to \mathcal{D}M(K)$. Here we ignore complete positivity aspects and simply consider these state transformers as affine maps, i.e. as maps in the category $\text{Conv}$. Corresponding to such programs there are “predicate transformers” $E f(K) \to E f(H)$ going in the opposite direction. Naturally we consider them to be maps of effect modules. The (dual) correspondence between state transformers and predicate transformers can then be derived using the adjunction $\text{Conv} \dashv \text{EMod}^{\text{op}}$ from Proposition 13 and the isomorphisms (15) from Theorem 14:

\[
\begin{align*}
\mathcal{D}M(H) & \longrightarrow \mathcal{D}M(K) \\
\mathcal{D}M(H) & \longrightarrow \text{EMod}(E f(K), [0, 1]) \\
E f(K) & \longrightarrow \text{Conv}(\mathcal{D}M(H), [0, 1]) \\
E f(K) & \longrightarrow E f(H)
\end{align*}
\]

(15) in $\text{Conv}$

(Prop. 13)

(15) in $\text{EMod}$

Such correspondences form the basis of Dijkstra’s seminal work on program correctness, see e.g. [12]. For a state transformer $f : \mathcal{D}M(H) \to \mathcal{D}M(K)$ the corresponding predicate transformer $wp(f, -) : E f(K) \to E f(H)$ is the “weakest precondition operation”. It is given by:

\[
wp(f, A) = \eta_{E f}^{-1}(\lambda B \in \mathcal{D}M(H). \eta_{\mathcal{D}M}(f(B))(A)) = \eta_{E f}^{-1}(\lambda B \in \mathcal{D}M(H). tr(f(B)A)),
\]

where we use the isomorphisms $\eta_{\mathcal{D}M} : \mathcal{D}M(K) \cong \text{EMod}(E f(K), [0, 1])$ and $\eta_{E f}^{-1} : \text{Conv}(\mathcal{D}M(H), [0, 1]) \cong E f(H)$ from (15). By elaborating the formulas for the matrix entries $wp(f, A)_{jk}$, the weakest precondition can be computed explicitly (for instance, by a computer algebra tool).

The dual adjunction $\text{Conv} \dashv \text{EMod}^{\text{op}}$ from Proposition 13 can be restricted to a (dual) equivalence of categories, giving a probabilistic version of Gelfand duality, see [29]. One obtains an equivalence $\text{CCH}_{\text{obs}} \simeq \text{BEMod}^{\text{op}}$ between ‘observable’ convex compact Hausdorff spaces and Banach effect modules. The latter are suitably complete with respect to a definable norm. The map of
adjunctions from Theorem 14 then restricts to a map of equivalences:

\[
\begin{array}{ccc}
FdHilb_{\text{Un}} & \overset{\sim}{\longrightarrow} & FdHilb_{\text{Un}}^{\text{op}} \\
\mathcal{D}M & \downarrow & \mathcal{E}f \\
CCH_{\text{obs}} & \overset{\sim}{\longrightarrow} & BE\text{Mod}^{\text{op}}
\end{array}
\]

We refer to [29] for further details. This equivalence leads to a reformulation of Gleason’s Theorem [19]. In original form it says that projections on a Hilbert space \( H \) (of dimension at least 3) correspond to measures:

\[
\mathcal{D}M(H) \cong EA(\mathcal{P}r(H), [0, 1])
\]

In [29] it is shown that Gleason’s theorem is equivalent to:

\[
\mathcal{E}f(H) \cong [0, 1] \otimes \mathcal{P}r(H).
\]

This says that effects form the free effect module on projections. We can now summarise how the whole edifice of operators on a Hilbert space \( H \) can be obtained from its projections \( \mathcal{P}r(H) \), see Table 1.

| Operators          | Formula                           | Description                  |
|--------------------|-----------------------------------|------------------------------|
| effects            | \( \mathcal{E}f(H) \cong [0, 1] \otimes \mathcal{P}r(H) \) | Gleason’s Theorem            |
| density matrices   | \( \mathcal{D}M(H) \cong E\text{Mod}(\mathcal{E}f(H), [0, 1]) \) | Theorem 14                   |
| positive operators | \( \mathcal{P}os(H) \cong S(\mathcal{D}M(H)) \) | Theorem 10                   |
| self-adjoint operators | \( \mathcal{S}A(H) \cong R(\mathcal{P}os(H)) \) | Theorem 6                    |
| bounded operators  | \( \mathcal{B}(H) \cong \mathcal{C}(\mathcal{S}A(H)) \) | Theorem 6                    |

This concludes our overview of the categorical structure of the various operators on a (finite dimensional) Hilbert space.

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