Operational Theories and Categorical Quantum Mechanics

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Abstract

A central theme in current work in quantum information and quantum foundations is to see quantum mechanics as occupying one point in a space of possible theories, and to use this perspective to understand the special features and properties which single it out, and the possibilities for alternative theories. Two formalisms which have been used in this context are *operational theories*, and *categorical quantum mechanics*. The aim of the present paper is to establish strong connections between these two formalisms. We show how models of categorical quantum mechanics have representations as operational theories. We then show how *non-locality* can be formulated at this level of generality, and study a number of examples from this point of view, including Hilbert spaces, sets and relations, and stochastic maps. The local, quantum, and no-signalling models are characterized in these terms.

1 Introduction

A central theme in current work in quantum information and quantum foundations is to see quantum mechanics as occupying one point in a space of possible theories, and to use this perspective to understand the special features and properties which single it out, and the possibilities for alternative theories.

Two formalisms which have been used in this context are *operational theories* [47, 40, 51, 46], and *categorical quantum mechanics* [6, 7].

- Operational theories allow general formulations of results in quantum foundations and quantum information [11, 12, 10]. They also play a prominent rôle in current work on axiomatizations of quantum mechanics [35, 19, 48].
- Categorical quantum mechanics enables a high-level approach to quantum information and quantum foundations, which can be presented in terms of string-diagram representations of structures in monoidal categories [7].

This has proved very effective in providing a conceptually illuminating and technically powerful perspective on a range of topics, including quantum protocols [6], entanglement [24], measurement-based quantum computing [28], no-cloning [1], and non-locality [22].

The aim of the present paper is to establish strong connections between these two formalisms. We shall begin by reviewing operational theories. We then show how a proper formulation of *compound systems* within the operational framework leads to a view of operational theories as representations of monoidal categories of a particular form. We call these *operational representations*.

We then review some elements of categorical quantum mechanics, and show how *monoidal dagger categories*, equipped with a trace ideal, give rise to operational representations. Thus there is a general passage from categorical quantum mechanics to operational theories.

We go on to show how *non-locality* can be formulated at this level of generality, and study a number of examples from this point of view, including Hilbert spaces, sets and relations, and stochastic maps. The local, quantum, and no-signalling models are characterized in these terms.

We shall assume some familiarity with the linear-algebraic formalism of quantum mechanics, and with the first notions of category theory. To make the paper reasonably self-contained, we include an appendix which reviews the basic definitions of monoidal categories, functors and natural transformations.

We also include another appendix which proves a number of technical results on trace ideals. These are mathematically interesting, but would break up the flow of ideas in the main body of the paper.

2 Why operational theories?

Before proceeding to a formal description of operational theories, it may be useful to discuss the motivation for studying them.

As we see it, operational theories have the following attractions:

- Firstly, they focus on the empirical content of theories, and the means by which we can gain knowledge of the microphysical world. Any viable theory must account for this content.

- By focussing on this empirical and observational content, operational theories allow meaningful results to be formulated and proved about the 'space of theories' as a whole. At a stage in the development of physics where the next step is far from clear, this is a useful perspective, which may prove useful in finding 'deeper' theories.

- Indeed, the operational framework has proved fruitful as a basis for general results, *e.g.* on the information processing capabilities of theories under various assumptions [11, 12, 10]; and provides the setting for recent work on axiomatic reconstructions of quantum mechanics [35, 19, 48].

On the debit side, operational theories attract criticism on philosophical grounds. They are seen as linked to an 'instrumentalist' or 'epistemic' view of physics, as opposed to a 'realistic' approach. From our perspective, the fact that we study operational theories does not indicate any such philosophical commitment. Rather, they are pragmatically useful for the reasons already mentioned, and can be seen as expressing some irreducible minimum of empirical content, which will have to be accounted for by any presumptive 'deeper' theory.

3 Operational theories formalized

An operational theory is formulated in terms of directly accessible 'operations', which can be performed *e.g.* in a laboratory. We assume there are several different types of system, A, B, C, etc. For each system type A, the theory specifies the following:

- A set of *preparations* P_A which produce systems of that type.
- A set T_A of *transformations* which may be performed on systems of type A. More generally, we can consider transformations $T_{A,B}$ which can be performed on systems of type A to produce systems of type B.
- A set of *measurements* M_A which can be performed on systems of that type.

Each measurement has a set of possible *outcomes*. In this paper, we shall only consider 'finite-dimensional' theories, or parts of theories. This means that each measurement has only finitely many possible outcomes. For convenience, we shall assume a fixed *infinite* set of outcomes O, which will apply to all measurements. Any measurement with a finite set of outcomes $O' \subseteq O$ can be represented using O, where those outcomes outside O' have zero probability of occurring.

The empirical predictions of the theory are given by its *evaluation rule*, which is a function

$$v_A \colon P_A \times M_A \times O \to [0,1]$$

which assigns a probability $v_A(p,m,o)$ to the event that a system of type A, prepared by p, yields outcome o when measurement m is performed on it.

For each choice of p and m, the function $v_A(p,m,-)$ defines a probability distribution on outcomes. We shall use the function

$$d_A \colon P_A \times M_A \to \mathcal{D} \qquad d_A(p,m) \colon o \mapsto v_A(p,m,o)$$

where $\mathcal{D}$ is the set of probability distributions of finite support on O.

3.1 Compound systems

An important additional ingredient is to give an account of *compound systems*, *i.e.* putting systems, possibly space-like separated, together.

This leads to the following additional requirements.

- For each pair of system types A, B, a compound system type AB.
- Ways of combining preparations, measurements, etc. on A and B to yield corresponding operations on the compound system AB.

Moreover, these operations should be subject to axioms yielding a coherent mathematical structure on these notions.

Rather than trying to develop such 'meta-operations' and axioms from first principles, we see the essential elements as provided by *monoidal categories*, which have been developed extensively as a setting for quantum mechanics and quantum information in the categorical quantum mechanics programme [6, 7].

We shall therefore proceed by giving a precise formulation of operational theories with compound system structure as a certain class of representations of monoidal categories, which we call *operational representations*.

3.2 Operational representations: concrete description

Before giving the 'official' definition of operational representation, which is mathematically elegant but a little abstract, we shall give a more concrete account, which shows the naturalness of the ideas, and also indicates why guidance from category theory is helpful in finding the right structural axioms.

For each system type A, we can gather the relevant data provided by an operational theory into a single structure

$$(P_A, M_A, d_A \colon P_A \times M_A \to \mathcal{D}).$$

This immediately suggests the notion of *Chu space* [14, 20], which has received quite extensive development [53], and was applied to the modelling of physical systems in [2]. Indeed, it can be seen as a generalization of the notion of model of a physical system proposed by Mackey in his influential work on the foundations of quantum mechanics [47].

There is a natural equivalence relation on preparations: p is equivalent to p', where $p, p' \in P_A$, if for all $m \in M_A$:

$$d_A(p, m) = d_A(p', m).$$

This is exactly the notion of extensional equivalence in Chu spaces [2]. We can regard *states* operationally as equivalence classes of preparations [50].

In an entirely symmetric fashion, there is an equivalence relation on measurements. We define m to be equivalent to m', where $m, m' \in M_A$, if for all $p \in P_A$:

$$d_A(p, m) = d_A(p, m').$$

We can regard *observables* operationally as equivalence classes of measurements.

Quotienting an operational system (P_A, M_A, d_A) by these equivalences corresponds to the *biextensional collapse* of a Chu space [2].

Having identified operational systems with Chu spaces, we now turn to morphisms. A transformation in $T_{A,B}$ induces a map $f_* \colon P_A \to P_B$. That is, preparing a system of type A according to preparation procedure p, and then subjecting it to a transformation procedure t resulting in a system of type B, is itself a procedure for preparing a system of type B.

Such a transformation can also be seen as a procedure for converting measurements of type B into measurements of type A: given a measurement $m \in M_B$, to apply it to a state prepared by $p \in P_A$, we apply the transformation t to obtain a preparation of type B, to which m can be applied. Thus we can also associate a map $f^* \colon M_B \to M_A$ to the transformation t. The formal relationship that links the two maps f_* and f^* is that, whether we measure $f_*(p)$ with m, or p with $f^*(m)$, we should observe the same probability distribution on outcomes:

$$d_B(f_*(p), m) = d_A(p, f^*(m)). \tag{1}$$

This can be seen as an abstract form of the relationship between the Schrödinger and Heisenberg 'pictures' of quantum dynamics.

The equation (1) says exactly that the pair of maps (f_*, f^*) defines a morphism of Chu spaces

$$(f_*, f^*) \colon (P_A, M_A, d_A) \to (P_B, M_B, d_B).$$

Thus we see that in an entirely natural way, we can associate an operational theory with a sub-category of Chu spaces, more precisely of $\mathbf{Chu}(\mathbf{Set}, \mathcal{D})$ [53]. This sub-category will not in general be full, since not every Chu morphism will arise from a transformation in the theory.

However, this does not yet provide an account of compound systems. While Chu spaces have a standard monoidal structure, and indeed form $*$-autonomous categories [20], we should not in general expect that operational theories will give rise to *monoidal* sub-categories of Chu spaces. Rather, we should see the notion of compound system as an important degree of freedom, which is to be specified by the theory.

Thus given operational systems $A = (P_A, M_A, d_A)$ and $B = (P_B, M_B, d_B)$, we should be able to form a system $A \otimes B = (P_{A\otimes B}, M_{A\otimes B}, d_{A\otimes B})$.

What general properties should such a notion satisfy? One important requirement, which appears in one form or another in the various formulations of operational theories, is to have an *inclusion of pure tensors*. This is given by maps

$$\iota^{\mathsf{P}}_{A,B} \colon P_A \times P_B \to P_{A\otimes B}, \qquad \iota^{\mathsf{M}}_{A,B} \colon M_A \times M_B \to M_{A\otimes B}.$$

For readability, we shall write $p \otimes p'$ rather than $\iota^{\mathsf{P}}_{A,B}(p, p')$, and similarly for measurements.

The fundamental property which this inclusion must satisfy relates to the evaluation. For all $p \in P_A$, $p' \in P_B$, $m \in M_A$, $m' \in M_B$, we must have:

$$d_{A\otimes B}(p \otimes p', m \otimes m') = d_A(p, m) \cdot d_B(p', m'). \tag{2}$$

This expresses the probabilistic independence of pure tensors. Conceptually, pure tensors arise by preparing states or performing measurements independently on subsystems.

In addition, there are a number of coherence conditions which are needed to get a mathematically robust notion. Rather than writing these down in an ad hoc fashion, we shall now turn to a more systematic way of defining the categorical structure of operational theories, in which these conditions arise naturally from standard notions.

3.3 Operational representations: functorial formulation

We shall now take a different view, in which the structure of an operational theory arises from a symmetric monoidal category, which we think of as a *process category*. The operational theory will amount to a certain form of *representation* of this process category. The receiving category for the representation will be $(\mathbf{Set}, \times, \mathbf{1})$, viewed as a symmetric monoidal category.

Given a symmetric monoidal category $\mathbf{C}$, an operational representation of $\mathbf{C}$ is specified by the following data:

- A symmetric monoidal sub-category $\mathbf{C}_{\mathsf{t}}$ of $\mathbf{C}$. This will usually have the same objects as $\mathbf{C}$, and only those morphisms which correspond to admissible transformations.
- A symmetric monoidal functor $\mathsf{P} \colon \mathbf{C}_{\mathsf{t}} \to \mathbf{Set}$ which represents, for each object A of $\mathbf{C}_{\mathsf{t}}$, viewed as a type of system, the corresponding set of preparations or states.
- A contravariant symmetric monoidal functor $\mathsf{M} \colon \mathbf{C}_{\mathsf{t}}^{\mathrm{op}} \to \mathbf{Set}$ which for each A represents the measurements on A. Note that $\mathbf{C}_{\mathsf{t}}^{\mathrm{op}}$ is a symmetric monoidal category.
- A dinatural symmetric monoidal transformation

  $$\mathsf{d} \colon \mathsf{P} \times \mathsf{M} \stackrel{..}{\to} \mathrm{K}_{\mathcal{D}}$$

  which gives the evaluation rule of the theory. Here $\mathrm{K}_{\mathcal{D}}$ is the constant functor valued at $\mathcal{D}$. Note that a constant symmetric monoidal functor valued at a set M is just a commutative monoid $(M, \cdot, 1)$ in $\mathbf{Set}$. We take $\mathcal{D}$ to be a commutative monoid under pointwise multiplication.

We shall assume that the functors P, M are embeddings, *i.e.* injective on objects and faithful.

Let us now unpack this definition.

- The general point of view is that the structure of the operational theory is controlled by the 'abstract' category $\mathbf{C}$. The types of the theory are the objects of $\mathbf{C}_{\mathsf{t}}$.
- Rather than a single set of preparations, we have a *variable set* P, which for each type A gives us a set P_A. Moreover, this acts functorially on the admissible transformations $f \colon A \to B$ in $\mathbf{C}_{\mathsf{t}}$ to produce functions $f_* \colon \mathsf{P}_A \to \mathsf{P}_B$, where $f_* := \mathsf{P}(f)$. Thus these functions take preparations on A to preparations on B, as already discussed.

- Similarly, the functor M specifies a variable set M_A of measurements for each system type A. The contravariant action of this functor is again as expected from our previous discussion.

The first new ingredient which picks up the issue of monoidal structure is that P and M are required to be *monoidal* functors. The fact that P and M are monoidal means that there are natural transformations

$$\iota^{\mathsf{P}}_{A,B} \colon \mathsf{P}_A \times \mathsf{P}_B \to \mathsf{P}_{A\otimes B}, \qquad \iota^{\mathsf{M}}_{A,B} \colon \mathsf{M}_A \times \mathsf{M}_B \to \mathsf{M}_{A\otimes B}.$$

i.e. inclusions of pure tensors. Naturality means that the diagrams

$$\begin{array}{ccc} \mathsf{P}_A \times \mathsf{P}_B & \xrightarrow{\iota^{\mathsf{P}}_{A,B}} & \mathsf{P}_{A\otimes B} \\ {\scriptstyle f_* \times g_*}\downarrow & & \downarrow{\scriptstyle (f\otimes g)_*} \\ \mathsf{P}_{A'} \times \mathsf{P}_{B'} & \xrightarrow[\iota^{\mathsf{P}}_{A',B'}]{} & \mathsf{P}_{A'\otimes B'} \end{array} \qquad \begin{array}{ccc} \mathsf{M}_A \times \mathsf{M}_B & \xrightarrow{\iota^{\mathsf{M}}_{A,B}} & \mathsf{M}_{A\otimes B} \\ {\scriptstyle f^* \times g^*}\uparrow & & \uparrow{\scriptstyle (f\otimes g)^*} \\ \mathsf{M}_{A'} \times \mathsf{M}_{B'} & \xrightarrow[\iota^{\mathsf{M}}_{A',B'}]{} & \mathsf{M}_{A'\otimes B'} \end{array}$$

commute. The coherence conditions for monoidal natural transformations complete the required properties of pure tensors.

The dinatural transformation $\mathsf{d}_A \colon \mathsf{P}_A \times \mathsf{M}_A \to \mathcal{D}$ represents the evaluation function. Dinaturality says that for each admissible transformation $f \colon A \to B$:

$$\begin{array}{ccccc} & & \mathsf{P}_B \times \mathsf{M}_B & & \\ & {\scriptstyle f_* \times 1_B}\nearrow & & \searrow{\scriptstyle \mathsf{d}_B} & \\ \mathsf{P}_A \times \mathsf{M}_B & & & & \mathcal{D} \\ & {\scriptstyle 1_A \times f^*}\searrow & & \nearrow{\scriptstyle \mathsf{d}_A} & \\ & & \mathsf{P}_A \times \mathsf{M}_A & & \end{array}$$

Thus we see that dinaturality is exactly the Chu morphism condition (1). Monoidality of d is the equation (2).

3.4 Operational categories

If we are given an operational representation $(\mathbf{C}, \mathbf{C}_{\mathrm{t}}, \mathsf{P}, \mathsf{M}, \mathsf{d})$ we can construct from this a single category, recovering the picture given in Section 3.2.

For each object A of $\mathbf{C}$, we have the Chu space $(\mathsf{P}_A, \mathsf{M}_A, \mathsf{d}_A)$. By dinaturality of d, each morphism $f \colon A \to B$ gives rise to a Chu morphism

$$(f_*, f^*) \colon (\mathsf{P}_A, \mathsf{M}_A, \mathsf{d}_A) \to (\mathsf{P}_B, \mathsf{M}_B, \mathsf{d}_B).$$

By functoriality of P and M, we obtain a sub-category of Chu spaces.

Moreover, since P and M are embeddings, we can push the symmetric monoidal structure on $\mathbf{C}$ forward to this sub-category:

$$\mathsf{P}_A \otimes \mathsf{P}_B := \mathsf{P}_{A\otimes B}, \quad \mathsf{M}_A \otimes \mathsf{M}_B := \mathsf{M}_{A\otimes B}, \quad f_* \otimes f'_* := (f \otimes f')_*, \quad f^* \otimes f'^* := (f \otimes f')^*.$$

Thus we obtain a symmetric monoidal category, whose underlying category is a sub-category of Chu spaces. We call this the *operational category* arising from the operational representation.

3.5 Generalized representations

The structural properties of operational representations and categories are independent of the particular choice of the monoid $\mathcal{D}$ used in specifying the dinatural transformation d.

We shall define a *generalized operational representation with weights* $\mathcal{W}$, where $(\mathcal{W}, \cdot, 1)$ is a commutative monoid with a zero element, to be a tuple $(\mathbf{C}, \mathbf{C}_{\mathsf{t}}, \mathsf{P}, \mathsf{M}, \mathsf{d})$, where d now has the form

$$\mathsf{d} \colon \mathsf{P} \times \mathsf{M} \xrightarrow{..} \mathbf{K}_{\mathcal{W}}$$

and $\mathbf{K}_{\mathcal{W}}$ is the constant symmetric monoidal functor valued at $\mathcal{W}$. This yields the definition of operational representation given previously when $\mathcal{W} = \mathcal{D}$.

We now have a general scheme for representing symmetric monoidal categories as operational categories. So far, however, we have no examples. We shall now show how monoidal dagger categories give rise to operational representations in a canonical fashion, following the ideas of categorical quantum mechanics [7].

4 Monoidal dagger categories

Monoidal dagger categories are the basic structures used in categorical quantum mechanics [7]. We shall briefly review the definitions, and give a number of examples.

A *dagger category* is a category $\mathbf{C}$ equipped with an identity-on-objects, contravariant, strictly involutive functor. Concretely, for each arrow $f \colon A \to B$, there is an arrow $f^{\dagger} \colon B \to A$, and this assignment satisfies:

$$1^{\dagger} = 1, \qquad (g \circ f)^{\dagger} = f^{\dagger} \circ g^{\dagger}, \qquad f^{\dagger\dagger} = f\,.$$

We define an arrow $f \colon A \to B$ in a dagger category to be a *dagger-isomorphism* if:

$$f^{\dagger} \circ f = 1_A, \qquad f \circ f^{\dagger} = 1_B.$$

A *symmetric monoidal dagger category* is a dagger category with a symmetric monoidal structure $(\mathbf{C}, \otimes, I, \lambda, \rho, \alpha, \sigma)$ such that

$$(f \otimes g)^{\dagger} = f^{\dagger} \otimes g^{\dagger}$$

and moreover the natural isomorphisms λ, ρ, α, σ are componentwise dagger-isos.

Examples

- The category **Hilb** of Hilbert spaces and bounded linear maps, and its (full) sub-category **FHilb** of finite-dimensional Hilbert spaces. Here the dagger is the adjoint, and the tensor product has its standard interpretation for Hilbert spaces. More generally, any symmetric monoidal C*-category is an example [32, 27]. This includes categories of (right) Hilbert C*-modules, which are Hilbert spaces whose inner product takes values in an arbitrary C*-algebra instead of $\mathbb{C}$.

- The category **Rel** of sets and relations. Here the dagger is relational converse, while the monoidal structure is given by the cartesian product. This generalizes to relations valued in a commutative quantale [54], and to the category of relations for any regular category [18]. Small categories as objects and profunctors as morphisms behave very similarly to **Rel**, even though they only form a bicategory [16].

- A common generalization of **FHilb** and **FRel**, the category of finite sets and relations, is obtained by forming the category $\mathbf{FMat}(S)$, where S is a commutative semiring with involution. $\mathbf{FMat}(S)$ has finite sets as objects, and maps $X \times Y \to S$ as morphisms, which we think of as 'X times Y matrices'. Composition is by matrix multiplication, while the dagger is conjugate transpose, where conjugation of a matrix means elementwise application of the involution on S. The tensor product of X and Y is given by $X \times Y$, with the action on matrices given by componentwise multiplication. (This corresponds to the 'Kronecker product' of matrices). If we take $S = \mathbb{C}$, this yields a category equivalent to **FHilb**, while if we take S to be the Boolean semiring $\{0, 1\}$ (with trivial involution), we get **FRel**.

- An infinitary generalization of $\mathbf{FMat}(\mathbb{C})$ is given by **LMat**. This category has arbitrary sets as objects, and as morphisms matrices $M \colon X \times Y \to \mathbb{C}$ such that for each $x \in X$, the family $\{M(x, y)\}_{y \in Y}$ is ℓ_2-summable; and for each $y \in Y$, the family $\{M(x, y)\}_{x \in X}$ is ℓ_2-summable. **Hilb** is equivalent to a (non-full) sub-category of **LMat**.

- If **C** and **D** are symmetric monoidal dagger categories, then so is the category $[\mathbf{C}, \mathbf{D}]$ of functors $F \colon \mathbf{C} \to \mathbf{D}$ that preserve the dagger. Morphisms are natural transformations. This accounts for several interesting models. For example, setting $\mathbf{D} = \mathbf{FHilb}$ and letting **C** be a group, we obtain the category of unitary representations. Any topological or conformal quantum field theory is a sub-category of the case where $\mathbf{D} = \mathbf{FHilb}$ and **C** is the category of cobordisms [44, 8, 55]. Letting **C** be the discrete category $\mathbb{N}$, and letting **D** be either **FHilb** or **FRel**, we recover $\mathbf{FMat}(\mathbf{D}(I, I))$.

The doubling construction All of the above examples are variations on the theme of matrix categories. Indeed, it seems hard to find natural examples which are not of this form. However, there is a construction which produces a symmetric monoidal dagger category from *any* symmetric monoidal category. Although the construction is formal, it is interesting in our context since it can be seen as a form of *quantization*; it converts classical process categories into a form in which quantum constructions are meaningful.

Given a category $\mathbf{C}$, we define a dagger category $\mathbf{C}_{\leftrightarrows}$ as follows. The objects are the same as those of $\mathbf{C}$, and a morphism $(f, g) \colon A \to B$ is a pair of $\mathbf{C}$-morphisms $f \colon A \to B$, $g \colon B \to A$. Composition is defined componentwise; while $(f, g)^{\dagger} = (g, f)$. This is in fact the object part of the right adjoint to the evident forgetful functor $\mathbf{DagCat} \to \mathbf{Cat}$; see [37, 3.1.17]. Thus for each dagger category $\mathbf{C}$, there is a dagger functor $\eta_{\mathbf{C}} \colon \mathbf{C} \to \mathbf{C}_{\leftrightarrows}$ which is the identity on objects, and sends f to $(f, f^{\dagger})$. This has the universal property with respect to dagger functors $\mathbf{C} \to \mathbf{D}_{\leftrightarrows}$ for categories $\mathbf{D}$.

This cofree construction of a dagger category lifts to the level of symmetric monoidal categories. If $\mathbf{C}$ is a symmetric monoidal category, then $\mathbf{C}_{\leftrightarrows}$ is a symmetric monoidal dagger category, with the monoidal structure defined componentwise: thus $(f, g) \otimes (h, k) := (f \otimes h, g \otimes k)$. Note in particular that the structural isos in $\mathbf{C}$ turn into *dagger* isos in $\mathbf{C}_{\leftrightarrows}$.

4.1 Additional structure

We shall require two further structural ingredients. The first is *zero morphisms*: for each pair of objects A, B, a morphism $0_{A,B} \colon A \to B$ such that, for all $f \colon C \to A$ and $g \colon B \to D$,

$$0_{A,B} \circ f = 0_{C,B}, \qquad g \circ 0_{A,B} = 0_{A,D}.$$

Note that if zero morphisms exist, they are unique.

In the context of symmetric monoidal dagger categories, we further require that

$$f \otimes 0 = 0 = 0 \otimes g, \qquad 0^{\dagger} = 0.$$

Examples All the examples of symmetric monoidal dagger categories given above have zero morphisms in an evident fashion. Functor categories have componentwise zero morphisms. Zero morphisms in $\mathbf{C}_{\leftrightarrows}$ are pairs of zero morphisms in $\mathbf{C}$. For more examples, see [38].

The final ingredient we shall require is a *trace ideal* in the sense of [4].[1] Firstly, we recall that in any monoidal category, the *scalars*, *i.e.* the endomorphisms of the tensor unit I, form a commutative monoid [43].

An *endomorphism ideal* in a symmetric monoidal category $\mathbf{C}$ is specified by a set $\mathcal{I}(A) \subseteq \mathrm{End}(A)$ for each object A, where $\mathrm{End}(A) = \mathbf{C}(A, A)$ is the set of endomorphisms on A. This is subject to the following closure conditions:

$$g \colon A \to B, f \in \mathcal{I}(A), h \colon B \to A \;\Rightarrow\; g \circ f \circ h \in \mathcal{I}(B)$$

[1] Strictly speaking, we are defining the more restricted notion of *global trace* of an endomorphism, rather than a *parameterized trace* as in [4]. This restricted notion is all we shall need.

$$f \in \mathcal{I}(A), g \in \mathcal{I}(B) \;\Rightarrow\; f \otimes g \in \mathcal{I}(A \otimes B), \qquad \mathcal{I}(I) = \mathrm{End}(I)$$
$$0 \in \mathcal{I}(A).$$

If **C** is a dagger category, $\mathcal{I}$ is a *dagger endomorphism ideal* when additionally

$$f \in \mathcal{I}(A) \;\Rightarrow\; f^\dagger \in \mathcal{I}(A),$$

but we will also call these endomorphism ideals for short. A *trace ideal* is an endomorphism ideal $\mathcal{I}$, together with a function

$$\mathrm{Tr}_A \colon \mathcal{I}(A) \to \mathrm{End}(I)$$

for each object A, subject to the following axioms:

$$\mathrm{Tr}_A(g \circ f) = \mathrm{Tr}_B(f \circ g) \qquad (f \colon A \to B, g \colon B \to A, g \circ f \in \mathcal{I}(A), f \circ g \in \mathcal{I}(B))$$
$$\mathrm{Tr}_{A \otimes B}(f \otimes g) = \mathrm{Tr}_A(f)\mathrm{Tr}_B(g), \qquad \mathrm{Tr}_I(s) = s.$$

A *dagger trace ideal* additionally satisfies

$$\mathrm{Tr}_A(f^\dagger) = \mathrm{Tr}_A(f)^\dagger,$$

but we will also call these trace ideal for short. We call a morphism $f \in \mathcal{I}(A)$ *trace class*.

Examples All of the examples given above have trace ideals. In the case of finite matrices, the usual matrix trace is a total operation. In the case of **Hilb**, we interpret trace class in the standard sense for Hilbert spaces, and similarly for **LMat**. Through the GNS-embedding [32, Proposition 1.14], this also provides a trace ideal for any C*-category.

In the case of relations, the summation over the diagonal becomes a supremum in a complete semilattice, which is always defined.

Any symmetric monoidal dagger sub-category of $[\mathbf{C}, \mathbf{D}]$ inherits endomorphism ideals and zero morphisms from **D** componentwise, and has a trace function $\mathrm{Tr}(\alpha) = \bigvee_A \mathrm{Tr}(\alpha_A)$ as soon as $\mathbf{D}(I, I)$ has an operation $\bigvee$ satisfying $\bigvee_A s_A^\dagger = (\bigvee_A s_A)^\dagger$, $\bigvee_A s = s$, and $(\bigvee_A s_A t_A) = (\bigvee_A s_A)(\bigvee_A t_A)$, where A ranges over the objects of **C**. This is the case when **C** is a finite group, as well as for topological quantum field theories.

The doubling construction turns trace ideals into dagger trace ideals. For $(f, g) \colon A \to A$, define $(f, g) \in \mathcal{I}(A)$ if and only if $f \in \mathcal{I}(A)$ and $g \in \mathcal{I}(A)$, and $\mathrm{Tr}_A(f, g) = (\mathrm{Tr}_A(f), \mathrm{Tr}_A(g))$. Thus if **C** is a symmetric monoidal category with zero morphisms and a trace ideal, $\mathbf{C}_{\leftrightarrows}$ is a dagger category with the same structure.

In Appendix B, we prove a number of results about trace ideals:

- We characterize when trace ideals exist, and to what extent they are unique.

- We show that we really need to restrict to ideals to consider traces: the category of Hilbert spaces does not support a trace on all morphisms.
- As a corollary, we derive that dual objects in the category of Hilbert spaces are necessarily finite-dimensional.
- Finally, we prove in some detail that the category of Hilbert spaces indeed has a trace ideal; the details turn out to be quite subtle.

This material would have unduly interrupted the main flow of the paper, but is of mathematical interest in its own right.

5 From categorical quantum mechanics to operational categories

Let **C** be a symmetric monoidal dagger category with zero morphisms and a trace ideal. We shall show that **C** gives rise to an operational representation and operational category in a canonical fashion, directly inspired by quantum mechanics.

5.1 Transformations

We take $\mathbf{C}_{\mathrm{t}}$ to be the sub-category with the same objects as **C**, and with dagger-isomorphisms as arrows. This is a groupoid, *i.e.* all morphisms are invertible.

It is easily seen to be a monoidal dagger sub-category of **C**.

5.2 States

A morphism $f \in \mathrm{End}(A)$ in a dagger category is *positive* if for some $g\colon A \to B$, $f = g^\dagger \circ g$. We define a *state* on A to be a positive morphism $f \in \mathrm{End}(A)$ which is trace class, and such that $\mathrm{Tr}_A(f) = 1$. We write P_A for the set of states on A.

In **Hilb**, this definition yields exactly the standard notion of *density operator* as used in quantum mechanics.

Pure states can also be defined in this setting. An arrow $\psi\colon I \to A$ has *unit norm* if $\psi^\dagger \circ \psi = 1$. Given such an arrow, $\psi \circ \psi^\dagger \in \mathsf{P}_A$. Indeed, this arrow is clearly positive, and

$$\mathrm{Tr}_A(\psi \circ \psi^\dagger) = \mathrm{Tr}_I(\psi^\dagger \circ \psi) = \mathrm{Tr}_I(1) = 1$$

using our assumption on ψ and the axioms for the trace.

Given a dagger isomorphism $f\colon A \to B$ in **C**, the function $f_*\colon \mathsf{P}_A \to \mathsf{P}_B$ is defined by

$$f_*\colon s \mapsto f \circ s \circ f^\dagger.$$

Functoriality holds, since

$$g_* \circ f_*(s) = g \circ (f \circ s \circ f^\dagger) \circ g^\dagger = (g \circ f) \circ s \circ (g \circ f)^\dagger = (g \circ f)_*(s).$$

Inclusion of pure tensors is given by

$$\iota^{\mathsf{P}}_{A,B} \colon (s,t) \mapsto s \otimes t.$$

It is straightforward to check the coherence conditions.

5.3 Measurements

A *dagger idempotent*, or *projector*, on A is an arrow $P \in \mathrm{End}(A)$ such that

$$P^2 = P, \qquad P = P^\dagger.$$

A family $\{f_i\}_{i \in I}$ of endomorphisms on A is:

- *Pairwise disjoint* if $f_i \circ f_j = 0$, $i \neq j$;
- *Jointly monic* if for all $g, h \colon B \to A$:

$$[\forall i \in I.\, f_i \circ g = f_i \circ h\,] \;\Rightarrow\; g = h.$$

A *projective measurement* on A with finite set of outcomes $O' \subseteq O$ is a family of dagger idempotents $\{P_o\}_{o \in O'}$ on A which is pairwise disjoint and jointly monic. We take M_A to be the set of projective measurements on A.

The functorial action of the measurement functor on dagger isomorphisms $f \colon A \to B$ in $\mathbf{C}$ is defined by

$$f^*(P_o) = f^\dagger \circ P_o \circ f.$$

It is easily verified that f^* preserves disjointness and joint monicity of families of projectors, and hence carries projective measurements to projective measurements. Functoriality is also easily verified.

Inclusion of tensors is defined pointwise on projectors:

$$\iota^{\mathsf{P}}_{A,B} \colon (P_o, P_{o'}) \mapsto P_o \otimes P_{o'}.$$

Note that the combined measurement will have a finite set of outcomes which, perhaps with some relabelling, can be regarded as a subset of O.

5.4 Evaluation

The transformation d is defined as follows, where $s \in \mathsf{P}_A$, and $m = \{P_o\}_{o \in O'} \in \mathsf{M}_A$:

$$\mathsf{d}_A(s,m)(o) \;:=\; \begin{cases} \mathrm{Tr}_A(s \circ P_o), & o \in O' \\ 0, & \text{otherwise.} \end{cases}$$

Note that d is valued in the commutative monoid of scalars $\mathcal{W} := \mathrm{End}(I)^O$. By the assumption of zero morphisms, this monoid has a zero element.

The dinaturality of this transformation, *i.e.* the Chu morphism condition, is just:

$$\mathrm{Tr}_B(f \circ s \circ f^\dagger \circ P_o) = \mathrm{Tr}_A(s \circ f^\dagger \circ P_o \circ f).$$

The monoidality of d is verified as follows:

$$\begin{aligned}\mathsf{d}_{A\otimes B}(s\otimes s', m\otimes m')(o,o') &= \mathrm{Tr}_{A\otimes B}(s\otimes s' \;\circ\; P_o\otimes P_{o'})\\ &= \mathrm{Tr}_{A\otimes B}(s\circ P_o \;\otimes\; s'\circ P_{o'})\\ &= \mathrm{Tr}_A(s\circ P_o)\mathrm{Tr}_B(s'\circ P_{o'})\\ &= \mathsf{d}_A(s,m)(o)\cdot \mathsf{d}_B(s',m')(o').\end{aligned}$$

5.5 The canonical operational representation

We collect the constructions described in this section together. Given a symmetric monoidal dagger category $\mathbf{C}$ with zero morphisms and a trace ideal, we have defined a sub-category $\mathbf{C}_{\mathsf{t}}$, monoidal functors P and M, and a dinatural transformation d.

Proposition 3. *The tuple* $(\mathbf{C}, \mathbf{C}_{\mathsf{t}}, \mathsf{P}, \mathsf{M}, \mathsf{d})$ *is an operational representation with weights* $\mathcal{W}$. *We call this the* canonical operational representation *of* $\mathbf{C}$*. The corresponding operational category is the* canonical operational category *for* $\mathbf{C}$. □

We say that the canonical representation is *distributional* if the monoid of scalars $\mathrm{End}(I)$ has an addition making it a commutative semiring, and for each state $s \in \mathsf{P}_A$ and measurement $m \in \mathsf{M}_A$:

$$\sum_{o\in O} \mathsf{d}_A(s,m)(o) \;=\; 1. \tag{4}$$

We say that it is *probabilistic* if moreover the image of d embeds into the semiring of non-negative reals.

6 Examples of operational categories

We shall now examine the operational categories arising from various examples of symmetric monoidal dagger categories.

6.1 Hilbert spaces

The definitions of states, measurements and evaluation are directly inspired by those used in the standard Hilbert-space formulation of quantum mechanics. Thus it is immediate that the states in the canonical representation for **Hilb** are the density matrices, while the dagger-isomorphisms are the unitary transformations.

For measurements, we have the following result.

Proposition 5. *Measurements in* **Hilb** *have exactly their standard meaning. More precisely, observables with finite discrete spectra correspond exactly to the interpretation in* **Hilb** *of the abstract notion of measurements as defined in Section 5.3 for dagger categories.*

Proof. We think of the outcomes as labelling the eigenvalues of the observable; then the family $\{P_o\}_{o\in O'}$ should correspond to the *spectral decomposition* of the observable. Clearly, dagger idempotents correspond exactly to projectors in **Hilb**, and so does the notion of a pairwise disjoint family of projectors. It remains to show that the joint monicity condition captures the fact that a pairwise disjoint family of projectors $\{P_i\}_{i\in I}$ yields a *resolution of the identity*, *i.e.*

$$\sum_{i\in I} P_i = 1_A.$$

Indeed, if $\sum_{i\in I} P_i = 1_A$ and $P_i \circ g = P_i \circ h$ for all i, then

$$g = 1_A \circ g = (\sum_{i\in I} P_i) \circ g = \sum_{i\in I} P_i \circ g = \sum_{i\in I} P_i \circ h = (\sum_{i\in I} P_i) \circ h = 1_A \circ h = h.$$

For the converse, suppose that $\sum_{i\in I} P_i \neq 1_A$. This implies that for some non-zero vector ψ, $P_i(\psi) = 0$ for all i. Then for $f : \mathbb{C} \to A$ given by $1 \mapsto \psi$, we have $P_i \circ f = P_i \circ 0$ for all i, so the family is not jointly monic. □

Finally, the definition of d matches the standard statistical algorithm of quantum mechanics. Thus we obtain the standard interpretations of states, transformations, (projective) measurements, and probabilities of measurement outcomes.

The operational category arising from **Hilb** is of course probabilistic.

The same analysis holds for C*-categories through their GNS-construction, and for subcategories of $[\mathbf{C}, \mathbf{Hilb}]$ such as topological quantum field theories. States and measurements in such categories are just natural transformations whose components are states or measurements respectively. Because the tensor unit in such categories is the constant functor K_I, they have the same scalars as **Hilb**. Therefore the induced operational categories are probabilistic.

6.2 Relations

We shall now give a general analysis of the operational representation for locale-valued relations. This level of generality will be useful when we go on look at non-locality in operational categories.

We recall that a *locale* [41] (also known as a *frame* or *complete Heyting algebra*) is a complete lattice Ω such that the following distributive law holds:

$$a \wedge \bigvee_{i\in I} b_i \;=\; \bigvee_{i\in I} a \wedge b_i.$$

The category $\mathbf{Rel}(\Omega)$ has sets as objects, while the morphisms $R : X \to Y$ are Ω-valued relations (or matrices) $R : X \times Y \to \Omega$. We write $[\![xRy]\!] = \omega$ for $R(x, y) = \omega$. Composition is relational composition (or matrix multiplication) evaluated in Ω. If $R : X \to Y$ and $S : Y \to Z$, then:

$$[\![x(S \circ R)z]\!] \;:=\; \bigvee_{y\in Y} [\![xRy]\!] \wedge [\![ySz]\!].$$

Clearly, **Rel** is the special case that Ω is the Boolean semiring $\{\bot, \top\}$, where we identify $\bot$, the bottom element of the lattice, with 0, and $\top$, the top element, with 1. Note that the full subcategory $\mathbf{FRel}(\Omega)$ of finite sets is identical to $\mathbf{FMat}(\Omega)$, where we regard Ω as a semiring with idempotent addition and multiplication. Indeed, in the finite case, completeness of Ω need not be assumed, and we are simply in the case of matrices over idempotent semirings.

We shall take the tensor unit in $\mathbf{Rel}(\Omega)$ to be $I = \{\bullet\}$.

By an Ω-subset of a set X, we mean a function $X \to \Omega$. Any family $\{S_i\}$ of Ω-subsets of X has a 'union' $\bigvee_i S_i$ given by $x \mapsto \bigvee_i S_i(x)$, and an 'intersection' $\bigwedge_i S_i$ given by $x \mapsto \bigwedge_i S_i(x)$. In particular, we write $\top_X$ for the Ω-subset of X given by $x \mapsto \top$, and $\bot_X$ for the Ω-subset of X given by $x \mapsto \bot$. Given a set X, we say that a family $\{S_i\}_{i\in I}$ of Ω-subsets of X is a *disjoint cover* of X if:

$$S_i \wedge S_j = \bot_X \ \ (i \neq j), \qquad \bigvee_{i\in I} S_i = \top_X.$$

Given a Ω-subset S of X, we define a Ω-relation $\Delta_S \colon X \to X$ by

$$[\![x\Delta_S y]\!] = \begin{cases} S(x) & \text{if } x = y, \\ \bot & \text{if } x \neq y. \end{cases}$$

Note that

$$\Delta_S \circ \Delta_T = \bot_{X\times X} \iff S \wedge T = \bot_X, \qquad \bigvee_{i\in I} \Delta_{S_i} = 1_A \iff \bigvee_{i\in I} S_i = \top_X. \quad (6)$$

Proposition 7. *Projective measurements on X in $\mathbf{Rel}(\Omega)$ consist of families of relations $\{\Delta_{S_i}\}_{i\in I}$, where $\{S_i\}_{i\in I}$ is a disjoint cover of X.*

Proof. Clearly any family of relations of this form is a projective measurement. For the converse, suppose we have a projective measurement $\{P_i\}_{i\in I}$ on X. The fact that P_i is a projector in $\mathbf{Rel}(\Omega)$ means that $[\![xP_iy]\!] = [\![yP_ix]\!]$ and $[\![xPz]\!] = \bigvee_y [\![xPy]\!] \wedge [\![yPz]\!]$, which implies that $[\![xP_ix]\!] \geq [\![xP_iy]\!]$. Suppose for a contradiction that $[\![xP_iy]\!] = \omega > \bot$ where $x \neq y$. Define $R, S \colon I \to X$ by $[\![\bullet Rx]\!] = \omega = [\![\bullet Sy]\!]$, and $[\![\bullet Rz]\!] = \bot = [\![\bullet Sz]\!]$ for other z. Then $[\![\bullet(P_i \circ R)x]\!] = \bigvee_z [\![\bullet Rz]\!] \wedge [\![zP_ix]\!] = \omega \wedge [\![xP_ix]\!] = \omega$ since $[\![xP_ix]\!] \geq [\![yP_ix]\!] = \omega$, and also $[\![\bullet(P_i \circ S)x]\!] = \omega$. Similarly $[\![\bullet(P_i \circ R)y]\!] = \omega = [\![\bullet(P_i \circ S)y]\!]$, and $[\![\bullet(P_i \circ R)z]\!] = \bot = [\![\bullet(P_i \circ S)z]\!]$ for other z. Hence $P_i \circ R = P_i \circ S$. Moreover, $P_j \circ R = P_j \circ S = \bot$ for any $j \neq i$, by disjointness of the family, since *e.g.* $\bot < [\![xP_jz]\!] \leq [\![xP_jx]\!]$ implies $P_i \circ P_j \neq \bot$. Thus $P_k \circ R = P_k \circ S$ for all $k \in I$, contradicting joint monicity. Hence P_i must have the form $P_i = \Delta_{S_i}$ for some $S_i \subseteq X$. The fact that the family $\{S_i\}_{i\in I}$ is a disjoint cover of X now follows from (6). □

Next we analyze states in $\mathbf{Rel}(\Omega)$. Firstly, we give an explicit description of the trace. If $R \colon X \to X$ is an Ω-valued relation,

$$[\![\bullet \mathrm{Tr}_X(R) \bullet]\!] = \bigvee_x [\![xRx]\!].$$

Thus the trace can be viewed as a predicate on endo-relations, which is satisfied to the extent that the relation has a ‘fixpoint’, *i.e.* a reflexive element.

Note that Ω-valued relations $R\colon I \to X$ of unit norm correspond to Ω-subsets S of X satisfying

$$\bigvee_x S(x) = \top.$$

The corresponding pure state is P_S, defined by $[\![xP_Sy]\!] = S(x) \wedge S(y)$.

We say that states s, t on X are *equivalent* if for all Ω-subsets S of X:

$$\mathrm{Tr}_X(s \circ \Delta_S) = \mathrm{Tr}_X(t \circ \Delta_S).$$

Proposition 8. *Every state in* $\mathbf{Rel}(\Omega)$ *is equivalent to a pure state.*

Proof. If s is a state on X, then it satisfies $\top = \bigvee_x [\![xsx]\!]$, and for some relation R,

$$[\![xsy]\!] = \bigvee_z [\![xRz]\!] \wedge [\![yRz]\!].$$

Define an Ω-subset $S = \mathrm{dom}(s)$ of X by $x \mapsto [\![xsx]\!]$. We claim that s is equivalent to P_S. Indeed, for any Ω-subset T of X,

$$\begin{aligned}
\mathrm{Tr}_X(s \circ \Delta_T) &= \bigvee_x [x(s \circ \Delta_T)x] \\
&= \bigvee_{x,y} [\![x\Delta_T y]\!] \wedge [\![ysx]\!] \\
&= \bigvee_x T(x) \wedge [\![xsx]\!] \\
&= \bigvee_x T(x) \wedge S(x) \\
&= \bigvee_{x,y} [\![yP_Sx]\!] \wedge [\![x\Delta_T y]\!] \\
&= \mathrm{Tr}_X(P_S \circ \Delta_T).
\end{aligned}$$

□

Finally, we consider evaluation. The scalars in $\mathbf{Rel}(\Omega)$ can be identified with the locale Ω. Because states correspond to Ω-subsets S satisfying $\bigvee_x S(x) = \top$, and measurements to disjoint covers, we see that equation (4) is satisfied. Thus we have the following result.

Proposition 9. *The operational category arising from* $\mathbf{Rel}(\Omega)$ *is distributional.*

Proof. Let Δ_S be a state, and m be a measurement given by a disjoint cover

$\{S_o\}$ of X. Then

$$\begin{aligned}\sum_o \mathsf{d}_A(\Delta_S, m)(o) &= \bigvee_o \mathrm{Tr}_X(\Delta_S \circ \Delta_{S_o}) \\ &= \bigvee_{o,x,y} [\![x\Delta_S y]\!] \wedge [\![y\Delta_{S_o} x]\!] \\ &= \bigvee_{o,x} S(x) \wedge S_o(x) \\ &= \bigvee_x S(x) \wedge (\bigvee_o S_o(x)) \\ &= \bigvee_x S(x) \\ &= \top. \end{aligned}$$

□

Discussion These results highlight two important differences between **Rel**(Ω) and **Hilb** as operational categories. In **Hilb**, every projector can appear as part of a projective measurement, while in **Rel**(Ω) the collective conditions of disjointness and joint monicity impose the constraint that projectors have to be sub-identities Δ_S. Moreover, in **Rel**(Ω) the distinction between *superpositions* of pure states, and *convex combinations* to form mixed states, is lost, so that every state is equivalent to a pure one. The relevance of this will become apparent when we discuss non-locality in **Rel**(Ω) in Section 9.2.

7 Classical operational categories

The construction of operational representations on monoidal dagger categories is directly inspired by quantum mechanics. However, operational theories should also include classical physics — or its discrete operational residue. Our notion of operational representation is indeed broad enough for this, as we shall now show.

The basic classical setting we shall consider is the category **Stoch**. The objects are finite sets, and the morphisms $M \colon X \to Y$ are the $X \times Y$-matrices valued in $[0, 1]$ which are row-stochastic. Thus for each $x \in X$, we have a probability distribution on Y.

An alternative description of **Stoch** is as the Kleisli category for the monad of discrete probability distributions; see [39].

The monoidal structure is defined as for **FMat**(S). Note that **Stoch** is not closed under matrix transposition. Indeed, we have the following result.

Proposition 10. *There is no dagger structure on* **Stoch**.

Proof. Note that if a category **C** has a dagger structure, it is in particular self-dual, *i.e.* equivalent to $\mathbf{C}^{\mathrm{op}}$. However, the one-element set is terminal but not initial in **Stoch**, which is thus not self-dual. □

It follows that we cannot directly apply the construction of Section 5. One might consider using the formal doubling construction on **Stoch** to obtain a dagger symmetric monoidal category with a dagger trace ideal. But this would not yield the expected result; for example, the dagger would not be given by transpose of (bi-stochastic) matrices. However, it is easy to give a direct definition of an operational representation, as follows.

- The sub-category $\mathbf{Stoch}_{\mathsf{t}}$ is defined by restricting to the functions (deterministic transformations), represented as matrices by their characteristic maps. Thus if $f\colon X \to Y$ is a function, for each $x \in X$ the corresponding probability distribution is $\delta_{f(x)}$.
- A state on X is a morphism $I \to X$ in **Stoch**, or equivalently a probability distribution on X. This is the classical notion of mixed state. The functorial action of states is described as follows. Given $f\colon X \to Y$, we define
$$f_*(s)(y) \;=\; \sum_{f(x)=y} s(x).$$
- A measurement on X is a function $m\colon X \to O$ with finite image $O' \subseteq O$. This is just a discrete random variable. The functorial action on $f\colon X \to Y$ is just
$$m \mapsto m \circ f.$$
- The evaluation is defined by:
$$\mathsf{d}_X(s,m)(o) \;=\; \sum_{m(x)=o} s(x).$$

The following result is easily verified.

Proposition 11. *The above data specifies a probabilistic operational representation of* **Stoch**. □

Various generalizations of this construction are possible:

- We can generalize to 'distributions' over an arbitrary commutative semiring, as in [39]. This will still yield a distributional operational representation.
- We can generalize to probability measures over general measure spaces. This amounts to using the Kleisli category of the Giry monad [33].

8 Non-locality in operational categories

Having set up a general framework for operational categories, we shall now investigate an important foundational notion in this general setting; namely *non-locality*.

Throughout this section, we fix a distributional operational representation $(\mathbf{C}, \mathbf{C}_{\mathsf{t}}, \mathsf{P}, \mathsf{M}, \mathsf{d})$ on a monoidal category $\mathbf{C}$.

8.1 Empirical models

We shall begin by showing how probability models of the form commonly studied in quantum information and quantum foundations can be interpreted in the corresponding operational category. In these models, there are n agents or sites, each of which has the choice of one of several measurement settings; and each measurement has a number of distinct outcomes. For each choice of a measurement setting by each of the agents, we have a probability distribution on the joint outcomes of the measurements.

We shall associate objects $A_1, \ldots, A_n$ with the n sites. We define $A := A_1 \otimes \cdots \otimes A_n$. We fix a state $s \in \mathsf{P}_A$. For each combination of measurements $(m_1, \ldots, m_n)$, where $m_i \in \mathsf{M}_{A_i}$ for $i = 1, \ldots, n$, we obtain the measurement $m := m_1 \otimes \cdots \otimes m_n$ by inclusion of pure tensors. Now the probability of obtaining a joint outcome $o := (o_1, \ldots, o_n)$ for m is given by

$$p(o|m) \;:=\; \mathsf{d}_A(s, m)(o).$$

We can regard these models as observational 'windows' on the operational theory. They represent the directly accessible information predicted by the theory, and provide the empirical yardstick by which it is judged.

8.2 Non-locality

We now define what it means for an empirical model of the kind described in the previous sub-section to exhibit non-locality. We shall follow the traditional route of using hidden variables explicitly, although we could equivalently, and perhaps more elegantly, formulate non-locality in terms of the (non-)existence of a joint distribution [30, 5].

We are assuming a fixed distributional model, with a semiring of weights $\mathcal{W}$. A $\mathcal{W}$*-distribution* on a set X is a function $d : X \to \mathcal{W}$ of finite support, such that

$$\sum_{x \in X} d(x) \;=\; 1.$$

A hidden-variable model for an empirical model is defined using a set Λ of hidden variables, with a fixed distribution d.[2] For each $\lambda \in \Lambda$, the model specifies a distribution $q^{\lambda}(o|m)$ on outcomes o for each choice of measurements m. The required condition for the hidden variable model to realize the empirical model p is that, for all m and o:

$$p(o|m) \;=\; \sum_{\lambda \in \Lambda} q^{\lambda}(o|m) \cdot d(\lambda).$$

That is, we recover the empirical probabilities by averaging over the hidden variables.

[2]The assumption of a fixed distribution d is technically the condition of 'λ-independence' [25].

We say that the hidden-variable model is *local* if, for all $\lambda \in \Lambda$, $m = (m_1, \ldots, m_n)$, and $o := (o_1, \ldots, o_n)$:

$$q^\lambda(o|m) \;=\; \prod_{i=1}^{n} q^\lambda(o_i|m_i).$$

Here $q^\lambda(o_i|m_i)$ is the marginal:

$$q^\lambda(o_i|m_i) \;=\; \sum_{o'_i = o_i, m'_i = m_i} q^\lambda(o'|m').$$

We say that the empirical model p is *local* if it is realized by some local hidden-variable model; and *non-local* otherwise.

Note that the definition of non-locality makes sense for any distributional operational category. Thus we can lift these ideas to the general level of operational categories. We say that an operational category exhibits non-locality if it gives rise to a non-local empirical model. Ultimately, we have a criterion for ascribing non-locality to monoidal process categories themselves, relative to a given distributional operational representation.

9 Examples of non-locality

We shall now investigate non-locality in a number of examples.

9.1 Hilbert spaces

As expected, the operational category arising from **Hilb**, which is essentially the finite-dimensional part of standard quantum mechanics, does exhibit non-locality.

As a standard example — essentially the one used by Bell in his original proof of Bell's theorem — consider the following table.

	$(0,0)$	$(1,0)$	$(0,1)$	$(1,1)$
(a,b)	$1/2$	0	0	$1/2$
(a,b')	$3/8$	$1/8$	$1/8$	$3/8$
(a',b)	$3/8$	$1/8$	$1/8$	$3/8$
(a',b')	$1/8$	$3/8$	$3/8$	$1/8$

It lists the probabilities that one of two outcomes (0 or 1) occurs when simultaneously measured with one of two measurements at two sites (a or a' at the first site, and b or b' at the second). This table can be realized in quantum mechanics, *e.g.* by a Bell state, written in the Z basis as

$$\frac{|\uparrow\uparrow\rangle \,+\, |\downarrow\downarrow\rangle}{\sqrt{2}},$$

subjected to spin measurements in the XY-plane of the Bloch sphere, at a relative angle of $\pi/3$.

A standard argument (see *e.g.* [15, 5]) shows that this table cannot be realized by a local hidden-variable model.

The same reasoning applies to C*-categories and subcategories of $[\mathbf{C}, \mathbf{Hilb}]$, taking the hidden variables componentwise. The constant functor valued e.g. at the model described above then still shows that such operational categories are non-local.

9.2 Relations

Suppose we are given an empirical model in the distributional operational category obtained from $\mathbf{Rel}(\Omega)$. The types are sets $X_1, \ldots, X_n$, there is a state $s = \Delta_S$ for a Ω-subset S of $X := \prod_i X_i$ satisfying $\bigvee_x S(x) = \top$, and measurements $m_i = \{\Delta_{S^i_o}\}_{o \in O'}$, where $\{S^i_o\}$ is a disjoint cover of X_i. For each combination of measurements m and outcomes o, we have:

$$p(o|m) = \begin{cases} \bigvee_x S(x) \wedge S^i_o(x) & \text{if } o \in O', \\ 0 & \text{otherwise.} \end{cases}$$

We shall now construct a local hidden-variable model which realizes this empirical model, using the elements of X as the hidden variables. We define the distribution d_s on X as $x \mapsto S(x)$. Note that we are working over Ω (the locale of scalars in $\mathbf{Rel}(\Omega)$), so this is a well-defined distribution, which sums to 1.

We define $p^x(o|m) \equiv \bigwedge_i S^i_{o_i}(x_i)$, so this hidden-variable model is local by construction.

We must verify that this model agrees with the empirical model. This comes down to the following calculation for $o \in O'$:

$$p(o|m) = \bigvee_x S(x) \wedge S^i_o(x) = \bigvee_x S(x) \wedge \bigwedge_i S^i_{o_i}(x) = \bigvee_x p^x(o|m) \wedge d_s(x).$$

We conclude from this that $\mathbf{Rel}(\Omega)$, despite being a 'quantum-like' monoidal dagger-category, does *not* admit non-local behaviour. This stands in interesting counter-point to the fact that, as shown extensively in [3], relational models can be used to give 'logical' proofs of non-locality and contextuality, in the style of 'Bell's theorem without inequalities' [34]. The key point is that these logical proofs are based on showing the non-existence of global sections compatible with a given empirical model; while here we are looking at empirical models generated by *states* in $\mathbf{Rel}(\Omega)$, which are exactly sets of global elements.

The key feature of quantum mechanics, by contrast, is that quantum states under suitable measurements *are* able to realize families of probability distributions which have no global sections.

Bearing in mind that finite-dimensional quantum mechanics corresponds to the operational category arising from $\mathbf{FMat}(\mathbb{C})$, while $\mathbf{FRel}(\Omega)$ is $\mathbf{FMat}(\Omega)$, this shows that *idempotence of the scalars implies that only local behaviour can be realized*; thus non-locality can only arise in non-idempotent situations.

9.3 Classical stochastic maps

We now consider the case of classical stochastic maps, as discussed in Section 7. This is in fact quite similar to the case for **Rel**. Given an empirical model realized by sets $X_1, \ldots, X_n$, a state s which is a probability distribution on $X := \prod_i X_i$, and measurements $m_i \colon X_i \to O$, we again take the hidden variables to be the elements of X. We can write s as a convex combination

$$s = \sum_{x \in X} \mu_x \delta_x.$$

Note that μ is a probability distribution on X. We can define $p^x(o|m) := \delta_o(m(x))$. Clearly $p^x(o|m) = \prod_i p^x(o_i|m_i)$, so this hidden-variable model is local.

It is straightforward to verify that the probabilities $p(o|m)$ are recovered by averaging over the deterministic hidden variables.

Thus we conclude, as expected, that **Stoch** does not exhibit non-locality.

In fact, we can say more than this. We can calibrate the expressiveness of an operational theory in terms of which empirical models it realizes. We shall now show that **Stoch** realizes *exactly* those models which have local hidden-variable realizations.

To see this, suppose we are given sets of measurements $M_1, \ldots, M_n$. We define $M := \bigsqcup_i M_i$, the disjoint union of these sets of measurements, and $X := O^M$. Thus elements of X simultaneously assign outcomes to all measurements. For each $m = (m_1, \ldots, m_n) \in \prod_i M_i$, we define a map $\hat{m} \colon X \to O$ by

$$\hat{m} \colon x \mapsto (x(m_1), \ldots, x(m_n)).$$

For each m, we get the probability distribution on outcomes given by

$$d_m \colon o \mapsto \sum_{\hat{m}(x)=o} s(x).$$

This is the empirical model realized by the state x, viewed as a probability distribution on the hidden variables X; and as shown e.g. in [5], all local models are of this form.

9.4 Signed Stochastic Maps

We shall now consider a variant of **Stoch** which has much greater expressive power in terms of the empirical models it realizes. This is the category **SStoch** of *signed* stochastic maps; real matrices such that each row sums to 1. Thus for each input, there is a 'signed probability measure' on outputs, which may include 'negative probabilities' [60, 26, 49, 29]. An operational representation can be defined for **SStoch** in the same fashion as for **Stoch**; it is still distributional.

The following result can be extracted from [5, Theorem 5.9], using the same encoding of empirical models which we employed in the previous sub-section. The reader should refer to [5, Theorem 5.9] for the details, which are non-triviai.

Proposition 12. *The class of empirical models which are realized by the operational category obtained from* **SStoch** *are exactly the no-signalling models; thus they properly contain the quantum models.*

This says that the operational category obtained from **SStoch** is *more* expressive, in terms of the empirical models it realizes, than the canonical operational category derived from **Hilb**, which corresponds to quantum mechanics.

Example We consider the bipartite system with two measurements at each site, each with outcomes $\{0, 1\}$. Thus the disjoint union M of the two sets of measurements has four elements, and $X = \{0, 1\}^M$ has 16 elements. Now consider the following state:

$$x := [1/2, 0, 0, 0, -1/2, 0, 1/2, 0, -1/2, 1/2, 0, 0, 1/2, 0, 0, 0].$$

The distributions it generates for the various measurement combinations can be listed in the following table.

	$(0,0)$	$(1,0)$	$(0,1)$	$(1,1)$
(a,b)	$1/2$	0	0	$1/2$
(a',b)	$1/2$	0	0	$1/2$
(a,b')	$1/2$	0	0	$1/2$
(a',b')	0	$1/2$	$1/2$	0

This can be recognized as the *Popescu-Rohrlich box* [52], which achieves super-quantum correlations.

The state x can be obtained from the PR-box specification by solving a system of linear equations; see [5] for details.

10 Final remarks

This paper makes a first precise connection between monoidal categories, and the categorical quantum mechanics framework, on the one hand, and operational theories on the other. Clearly, this can be taken much further. We note a number of directions which it would be interesting to pursue.

- We have used our framework of operational categories to study non-locality in a general setting. In particular, we have a clear definition of whether a model of categorical quantum mechanics exhibits non-locality or not, as explained at the end of Section 8. As we saw, while Hilbert-space quantum mechanics does, the category of sets and relations, which forms a very useful 'foil' model for quantum mechanics in many respects [59, 22], does not. An important further direction is to apply a similar analysis to *contextuality*, which can be seen as a broader phenomenon, of which non-locality is a special case. In [5], a general setting is developed allowing a unified treatment of contextuality and non-locality. We would like to extend the present account to this setting, in which *compatibility* of measurements is explicitly represented, leading to a natural sheaf-theoretic structure.

- Such a development would also lead to a more satisfactory treatment of outcomes, in place of the somewhat clumsy device used in the present paper.
- It would also be interesting to interpret some of the general results which have been proved for operational theories, relating *e.g.* to no-broadcasting [11], teleportation [12], and information causality [10], in our categorical framework, and ultimately to obtain such results for classes of monoidal process categories.
- We would also like to examine the issue of axiomatization or 'reconstruction' of quantum mechanics from the categorical point of view.
- There are various constructions for turning a monoidal category of 'pure' states into one of 'mixed' states [56, 23]. It would be interesting to relate these constructions to our canonical operational categories. Similarly, there is a category embodying Spekkens' toy theory [59, 21]. It would be of interest to study the associated operational category.

Regarding related work, we note that in [13], the structure of the concrete category of convex operational theories is investigated.

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A First notions from category theory

We shall review some basic notions from category theory. For more detailed background, see [9].

A *category* $\mathbf{C}$ has a collection of objects $A, B, C, \ldots$, and arrows $f, g, h, \ldots$. Each arrow has specified *domain* and *codomain* objects: notation is $f\colon A \to B$ for an arrow f with domain A and codomain B. The collection of all arrows with domain A and codomain B is denoted as $\mathbf{C}(A, B)$. Given arrows $f\colon A \to B$ and $g\colon B \to C$, we can form the *composition* $g \circ f\colon A \to C$. Composition is associative, and there are identity arrows $1_A\colon A \to A$ for each object A, with $f \circ 1_A = f$, $1_A \circ g = g$, for every $f\colon A \to B$ and $g\colon C \to A$. An arrow $f\colon A \to B$ is called an *iso(morphism)* when $f \circ f^{-1} = 1_B$ and $f^{-1} \circ f = 1_A$ for some arrow $f^{-1}\colon B \to A$. An arrow $f\colon A \to B$ is *split monic* when $g \circ f = 1_A$ for some $g\colon B \to A$, and it is *split epic* when $f \circ g = 1_A$ for some $g\colon B \to A$; by abuse of notation, we will write $g = f^{-1}$ in both cases.

If $\mathbf{C}$ is a category, we write $\mathbf{C}^{\mathrm{op}}$ for the opposite category, with the same objects as $\mathbf{C}$, and arrows $A \to B$ corresponding to arrows $B \to A$ in $\mathbf{C}$.

If $\mathbf{C}$ and $\mathbf{D}$ are categories, a *functor* $F\colon \mathbf{C} \to \mathbf{D}$ assigns an object FA of $\mathbf{D}$ to each object A of $\mathbf{C}$; and an arrow $Ff\colon FA \to FB$ of $\mathbf{D}$ to every arrow $f\colon A \to B$ of $\mathbf{C}$. These assignments must preserve composition and identities: $F(g \circ f) = F(g) \circ F(f)$, and $F(1_A) = 1_{FA}$.

Given functors $F, G\colon \mathbf{C} \to \mathbf{D}$, a *natural transformation* $t\colon F \stackrel{\cdot}{\to} G$ is a family of arrows $\{t_A\colon FA \to GA\}$ indexed by the objects of $\mathbf{C}$, such that, for every $f\colon A \to B$ in $\mathbf{C}$, the following naturality diagram commutes:

$$\begin{array}{ccc} FA & \xrightarrow{t_A} & GA \\ {\scriptstyle Ff}\downarrow & & \downarrow{\scriptstyle Gf} \\ FB & \xrightarrow[t_B]{} & GB \end{array}$$

A *natural isomorphism* is a natural transformation whose components are isomorphisms. An *equivalence of categories* is a pair of functors $F\colon \mathbf{C} \to \mathbf{D}$ and $G\colon \mathbf{D} \to \mathbf{C}$ such that there are natural isomorphisms $F \circ G \cong 1_{\mathbf{D}}$ and $G \circ F \cong 1_{\mathbf{C}}$.

A *symmetric monoidal category* is a structure $(\mathbf{C}, \otimes, I, \alpha, \lambda, \rho, \sigma)$ where:

- $\mathbf{C}$ is a category;
- $\otimes\colon \mathbf{C} \times \mathbf{C} \to \mathbf{C}$ is a functor (*tensor*);
- I is a distinguished object of $\mathbf{C}$ (*unit*);
- α, λ, ρ, σ are natural isomorphisms (*structural isos*) with components

$$\alpha_{A,B,C}\colon A \otimes (B \otimes C) \to (A \otimes B) \otimes C$$

$$\lambda_A\colon I \otimes A \to A \qquad \rho_A\colon A \otimes I \to A$$

$$\sigma_{A,B}\colon A \otimes B \to B \otimes A$$

  such that certain coherence diagrams commute.

Products are a classical example of symmetric monoidal structure; the category is then called *Cartesian*. The symmetric monoidal structure can also support entanglement; the category is then called *compact* [7].

Let $\mathbf{C}$ and $\mathbf{D}$ be symmetric monoidal categories. A symmetric monoidal functor

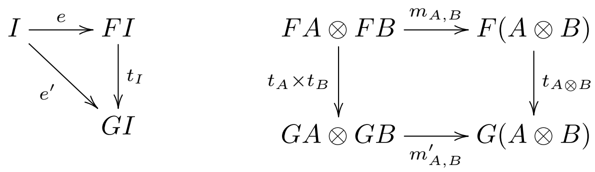
$$(F, e, m)\colon \mathbf{C} \to \mathbf{D}$$

comprises

- a functor $F\colon \mathbf{C} \to \mathbf{D}$,
- an arrow $e\colon I_{\mathbf{D}} \to FI_{\mathbf{C}}$,
- a natural transformation $m_{A,B}\colon FA \otimes FB \to F(A \otimes B)$,

subject to coherence conditions with the structural isomorphisms. The symmetric monoidal functor is called *strong* when m is a natural isomorphism.

Let $(F, e, m), (G, e', m') \colon \mathbf{C} \to \mathbf{D}$ be symmetric monoidal functors. A *monoidal natural transformation* between them is a natural transformation $t \colon F \stackrel{\cdot}{\to} G$ such that the following diagrams commute.



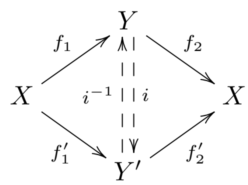
B Trace ideals

This appendix further studies the notion of trace ideal, introduced in Section 4.1. It presents several technical results that are mathematically interesting, but would break up the flow of the main text. For example, we characterize when trace ideals exist, and to what extent they are unique. Also, we show that we really need to restrict to ideals to consider traces: the category of Hilbert spaces does not support a trace on all morphisms. As a conceptually satisfying corollary, we derive that dual objects in the category of Hilbert spaces are necessarily finite-dimensional. Finally, we prove in some detail that the category of Hilbert spaces indeed has a trace ideal; this was claimed in Section 4.1, but the details are quite subtle.

B.1 Existence

The question whether a category allows a trace ideal at all can be answered as follows.

A subcategory $\mathbf{D}$ of $\mathbf{C}$ is called *tracial* when endomorphisms in $\mathbf{C}$ factoring through $\mathbf{D}$ can only do so in a way unique up to isomorphism. More precisely: if $f_1 \colon X \to Y$, $f_2 \colon Y \to X$, $f_1' \colon X \to Y'$, $f_2' \colon Y' \to X$ are morphisms of $\mathbf{C}$, and Y and Y' are objects of $\mathbf{D}$, and $f_2 \circ f_1 = f_2' \circ f_1'$, then there is a morphism $i \colon Y \to Y'$ in $\mathbf{D}$ that is either split monic or split epic, such that $f_1' = i \circ f_1$ and $f_2' = f_2 \circ i^{-1}$.



The category $\mathbf{C}$ is called *traceable* when the full subcategory consisting of the monoidal unit I is tracial. Notice that traceability generalizes the fact, holding in any monoidal category, that the scalars are commutative.

Proposition 13. *Any dagger monoidal tracial subcategory* $\mathbf{D}$ *of* $\mathbf{C}$ *with a trace ideal induces a trace ideal*

$$\mathcal{I}(X) = \{f \in \mathbf{C}(X,X) \mid f = f_2 \circ f_1 \text{ with } f_1 \colon X \to Y, f_2 \colon Y \to X \text{ and } Y \text{ in } \mathbf{D}, f_1 \circ f_2 \in \mathcal{I}_{\mathbf{D}}(Y)\}$$
$$\mathrm{Tr}(f) = \mathrm{Tr}_{\mathbf{D}}(f_1 \circ f_2)$$

on $\mathbf{C}$.

Proof. One directly checks that $\mathcal{I}(X)$ is an endomorphism ideal; in particular $\mathcal{I}(I) = \mathbf{D}(I,I) = \mathbf{C}(I,I)$. Because $\mathbf{D}$ is tracial, Tr is well-defined. The axioms for the trace function are also readily verified. □

Theorem 14. *A dagger monoidal category has a unique minimal trace ideal*

$$\mathcal{I}(X) = \{f \colon X \to X \mid f \text{ factors through } I\}$$
$$\mathrm{Tr}(f) = b \circ a, \text{ when } f = a \circ b \text{ with } a \colon I \to X \text{ and } b \colon X \to I$$

and hence has any trace ideal whatsoever, if and only if it is traceable.

Proof. That the given data form a trace ideal follows from the previous proposition, because the full subcategory consisting of just the monoidal unit I is certainly (totally) traced. To see that this trace ideal is minimal, *i.e.* that any trace ideal must contain this one, follows from the first and third axioms of endomorphism ideal. □

As a consequence of the previous theorem, the evaluation of measurements on pure states is completely determined by the structure of the category, independent of the trace ideal. If $s = \psi \circ \psi^\dagger$ is a pure state on X, and $\{P_o\}$ a measurement, then for every outcome o:

$$\mathrm{Tr}(s \circ P_o) = \mathrm{Tr}(\psi \circ \psi^\dagger \circ P_o) = \mathrm{Tr}(\psi^\dagger \circ P_o \circ \psi) = \psi^\dagger \circ P_o \circ \psi.$$

Therefore, the only possible freedom the choice of a trace ideal brings comes out in behaviour on mixed states.

B.2 Uniqueness

We now consider uniqueness of trace ideals. The following proposition proves that trace ideals are a categorical invariant, in the sense that they are preserved under equivalence. A dagger monoidal equivalence is a pair of functors $F \colon \mathbf{C} \to \mathbf{D}$ and $G \colon \mathbf{D} \to \mathbf{C}$ that form an equivalence of categories, such that $F(f^\dagger) = F(f)^\dagger$ and $G(f^\dagger) = G(f)^\dagger$, and there are natural isomorphisms $F(I) \cong I$, $G(I) \cong I$, $F(X \otimes Y) \cong F(X) \otimes F(Y)$ and $G(X \otimes Y) \cong G(X) \otimes G(Y)$ that interact with the coherence isomorphisms in the appropriate way.

Proposition 15. *Trace ideals are preserved under dagger monoidal equivalence: if* $F \colon \mathbf{C} \to \mathbf{D}$ *and* $G \colon \mathbf{D} \to \mathbf{C}$ *are strong monoidal functors that preserve daggers and form an equivalence of categories, and* $(\mathcal{I}, \mathrm{Tr}^{\mathcal{I}})$ *is a trace ideal in* $\mathbf{C}$*, then*

$$\mathcal{J}(X) = G^{-1}(\mathcal{I}(G(X))) = \{g \in \mathbf{D}(X,X) \mid G(g) \in \mathcal{I}(G(X))\},$$
$$\mathrm{Tr}^{\mathcal{J}}_X(g) = F(\mathrm{Tr}^{\mathcal{I}}_{G(X)}(G(g))),$$

form a trace ideal in **D**.

Proof. First, observe that if $f \in \mathcal{I}(X)$, and $g\colon X \to Y$ is an isomorphism with inverse h, then $\mathrm{Tr}(f) = \mathrm{Tr}(gfh)$. Then, to verify that $\mathcal{J}$ is an endomorphism ideal, the first requirement follows from functoriality of G; the second from the fact that G is monoidal; and the third from fullness of G together with monoidality of G. It is a dagger endomorphism ideal because G preserves daggers. Verifying that $\mathrm{Tr}^{\mathcal{J}}$ satisfies the requirements is completely analogous, except that the last condition additionally uses $F(G(s)) \cong s$. □

However, trace ideals need not be unique. In fact, there may even be more than one trace function making a fixed endomorphism ideal into a trace ideal, as the following example shows.

Example 16. A *tracial state* on a C*-algebra A is a linear map $\tau\colon A \to \mathbb{C}$ satisfying $\tau(a^*a) \geq 0$, $\tau(1) = 1$, and $\tau(ab) = \tau(ba)$. There exists a unital C*-algebra A with distinct tracial states $\tau \neq \tau'\colon A \to \mathbb{C}$ [45].

Make a category **C** as follows. Objects are natural numbers. There are only endomorphisms. Morphisms $0 \to 0$ are complex numbers; the identity is 0, and composition is addition. For $n \geq 1$, morphisms $n \to n$ are elements of the n-fold direct sum $A \oplus A \oplus \cdots \oplus A$; the identity is $(1, 1, \ldots, 1)$, and composition is pointwise multiplication.

We give this category a monoidal structure by letting the tensor product of objects n and m be $n + m$. If one of n or m is 0, the action on morphisms is by scalar multiplication. For $n, m \geq 1$, the action on morphisms is clear. The monoidal unit is the object 0.

Taking $\mathcal{I}(X)$ to be all endomorphisms on X certainly gives an endomorphism ideal. Define $\mathrm{Tr}_0(z) = z$, and $\mathrm{Tr}_n(a_1, \ldots, a_n) = \sum_{i=1}^{n} \tau(a_i)$ for $n \geq 1$. This satisfies all the conditions needed to make $\mathcal{I}$ into a trace ideal. But the very same construction with τ' gives a different trace function.

The previous example is in stark contrast to Cartesian categories or compact categories, where traces are unique; see [58] and [36], respectively. The counterexample above is somewhat artificial, because all morphisms are endomorphisms. It remains unclear whether trace ideals on, for example, compact categories, are unique.

B.3 The need for trace ideals

We will now show that in the category **Hilb**, there exists no trace ideal consisting of all morphisms. More precisely, we will show that **Hilb** is not an instance of the established notion of *traced monoidal category* [42]. This notion asks not just for traces of all endomorphisms, but requires a 'partial trace' of morphisms $f\colon X \otimes U \to Y \otimes U$, resulting in a morphism $\mathrm{Tr}^U(f)\colon X \to Y$. There are then several additional axioms, such as the following naturality:

$$\mathrm{Tr}^U(f) \circ g = \mathrm{Tr}^U(f \circ (g \otimes 1_U)) \quad \text{for } f\colon X \otimes U \to Y \otimes U, g\colon X' \to X.$$

We will now show that the monoidal category $(\mathbf{Hilb}, \otimes)$ cannot be traced monoidal. Subsequently, we will show that it *does* have a trace ideal. This justifies working with trace ideals in monoidal categories instead of traced monoidal categories. We are indebted to Peter Selinger for the following proof.

Lemma 17. *Suppose* $(\mathbf{Hilb}, \otimes)$ *is traced monoidal. Then* $\mathrm{Tr}(f+g) = \mathrm{Tr}(f) + \mathrm{Tr}(g)$ *for all endomorphisms* $f, g \colon H \to H$*.*

Proof. Choose an orthonormal basis $\{|0\rangle, |1\rangle\}$ for $\mathbb{C}^2$, and write $|+\rangle = |0\rangle + |1\rangle$. Recall that $\mathbb{C}^2 \otimes H \cong H \oplus H$. Define $F \colon \mathbb{C}^2 \otimes H \to H$ via the block matrix $\begin{pmatrix} f & g \end{pmatrix}$. Hence $F \circ (|0\rangle \otimes 1_H) = f$ and $F \circ (|1\rangle \otimes 1_H) = g$. Now:

$$\begin{aligned}
\mathrm{Tr}(f+g) &= \mathrm{Tr}(F \circ (|+\rangle \otimes 1_H)) \\
&= \mathrm{Tr}(F) \circ |+\rangle && \text{(by naturality)} \\
&= (\mathrm{Tr}(F) \circ |0\rangle) + (\mathrm{Tr}(F) \circ |1\rangle) \\
&= \mathrm{Tr}(F \circ (|0\rangle \otimes 1_H)) + \mathrm{Tr}(F \circ (|1\rangle \otimes 1_H) && \text{(by naturality)} \\
&= \mathrm{Tr}(f) + \mathrm{Tr}(g).
\end{aligned}$$

The third equality uses that composition is bilinear. □

Theorem 18. *The monoidal category* $(\mathbf{Hilb}, \otimes)$ *is not traced monoidal.*

Proof. Suppose $(\mathbf{Hilb}, \otimes)$ was traced monoidal. Let H be an infinite-dimensional Hilbert space. Then there exist isomorphisms $\varphi \colon H \oplus \mathbb{C} \xrightarrow{\cong} H$ and $\psi \colon H \xrightarrow{\cong} \mathbb{C} \oplus H$. Write them in block matrix form as $\varphi = \begin{pmatrix} \varphi_1 & \varphi_2 \end{pmatrix}$ and $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$. Consider the morphisms $f_1, f_2, f_3 \colon H \oplus \mathbb{C} \oplus H \to H \oplus \mathbb{C} \oplus H$ given by the following block matrices.

$$f_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad f_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad f_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Let $g = \varphi \oplus \psi \colon (H \oplus \mathbb{C}) \oplus H \to H \oplus (\mathbb{C} \oplus H)$. Then

$$\begin{aligned}
g \circ f_2 &= \begin{pmatrix} \varphi_1 & \varphi_2 & 0 \\ 0 & 0 & \psi_1 \\ 0 & 0 & \psi_2 \end{pmatrix} \circ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \varphi_1 & \varphi_2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \circ \begin{pmatrix} \varphi_1 & \varphi_2 & 0 \\ 0 & 0 & \psi_1 \\ 0 & 0 & \psi_2 \end{pmatrix} = f_1 \circ g.
\end{aligned}$$

Hence

$$\mathrm{Tr}(f_1) = \mathrm{Tr}(f_1 \circ g \circ g^{-1}) = \mathrm{Tr}(g \circ f_2 \circ g^{-1}) = \mathrm{Tr}(f_2 \circ g^{-1} \circ g) = \mathrm{Tr}(f_2).$$

But $\mathrm{Tr}(f_2) = \mathrm{Tr}(f_1 + f_3) = \mathrm{Tr}(f_1) + \mathrm{Tr}(f_3)$ by Lemma 17. And because f_3 has finite rank, we know that $\mathrm{Tr}(f_3) = \mathrm{Tr}(1_{\mathbb{C}}) = 1$. Thus $\mathrm{Tr}(f_2) = \mathrm{Tr}(f_2) + 1$, which is a contradiction. □

B.4 Dual objects in Hilb are finite-dimensional

The previous theorem allows an interesting corollary. Recall that the main characteristic of compact categories is that objects have duals: objects L, R in a monoidal category are called *dual* when there are maps $\eta \colon I \to R \otimes L$ and $\varepsilon \colon L \otimes R \to I$ making the following two composites identities.

$$L \cong L \otimes I \xrightarrow{1 \otimes \eta} L \otimes (R \otimes L) \cong (L \otimes R) \otimes L \xrightarrow{\varepsilon \otimes 1} I \otimes L \cong L$$
$$R \cong I \otimes R \xrightarrow{\eta \otimes 1} (R \otimes L) \otimes R \cong R \otimes (L \otimes R) \xrightarrow{1 \otimes \varepsilon} R \otimes I \cong R$$

It is well-known that if $H \in \mathbf{Hilb}$ is finite-dimensional, then H and H^* are dual objects by $\eta(1) = \sum_{i=1}^{n} |i\rangle \otimes \langle i|$ and $\varepsilon(|i\rangle) = 1$, for any choice of orthonormal basis $\{|i\rangle\}_{i=1,\ldots,n}$ for H; see [43, 42, 7]. This recipe does not work when H is infinite-dimensional, because $\sum_i |i\rangle$ does not converge in that case. However, this does not exclude the possibility that there might be other H^*, η, ε making H into a dual object. No rigorous proof that infinite-dimensional Hilbert spaces cannot have duals has been published, as far as we know.

Corollary 19. *Objects in* $(\mathbf{Hilb}, \otimes)$ *with duals are precisely finite-dimensional Hilbert spaces.*

Proof. Let H be an infinite-dimensional Hilbert space. Suppose H has a dual object H^*. For $f \colon H \to H$, define $\mathrm{Tr}^H(f)$ as the following composite.

$$I \xrightarrow{\eta} H^* \otimes H \cong H \otimes H^* \xrightarrow{f \otimes 1_{H^*}} H \otimes H^* \xrightarrow{\varepsilon} I$$

This satisfies all equations for a trace function, as far as these make sense 'locally', for just one object H. In **Hilb**, the object $\mathbb{C}$ always has a dual, and if H and K have duals, then so does $H \oplus K$. Now, notice that the proof of Theorem 18 only uses the trace properties 'locally', *i.e.* for the objects $\mathbb{C}, H, \mathbb{C}^2 \otimes H \cong H \oplus H, H \oplus \mathbb{C}, H \oplus \mathbb{C} \oplus H$. Hence the contradiction it results in holds here, too. □

In fact, in any monoidal category with biproducts, one can show that if $A \cong A \oplus I$, then $\mathrm{Tr}^A(1_A) = \mathrm{Tr}^A(1_A) + 1$. We thank Jamie Vicary for this observation.

B.5 Trace class maps form a trace ideal in Hilb

To show that the usual trace of continuous linear maps between Hilbert spaces does in fact give a trace ideal requires some work, as virtually all textbooks only consider endomorphisms, whereas the defining conditions of trace ideals also involve morphisms between different objects.

We need to recall some terminology; for any unexplained terms, we refer to [17]. Other good references are [31, 57]. A linear map $f \colon H \to K$ between Hilbert spaces is *Hilbert-Schmidt* when $\sum_n \|f(e_n)\|_K^2 < \infty$ for an orthonormal basis (e_n) of H. A positive continuous linear map $f \colon H \to H$ is *trace class* when $\sum_n \left|\langle e_n \mid f(e_n)\rangle\right| < \infty$ for an orthonormal basis (e_n) of H. An arbitrary continuous linear map $f\colon H \to H$ is trace class when its absolute value $|f|\colon H \to H$ is trace class. Both definitions are independent of the choice of basis (e_n). If f is trace class, then $\langle e_n \mid f(e_n)\rangle$ is absolutely summable, and hence the following *trace property* holds:

$$\mathrm{Tr}(f) = \sum_n \langle e_n \mid f(e_n)\rangle$$

is a well-defined complex number. The *Cauchy-Schwarz inequality* states that

$$\big|\langle x \mid y\rangle\big| \leq \big(\|x\|^2 \cdot \|y\|^2\big)^{1/2}$$

for any two elements x, y of a Hilbert space. The *Hölder inequality* states that

$$\sum_n |x_n \cdot y_n| \leq \big(\sum_n |x_n|^2\big)^{1/2} \cdot \big(\sum_n |y_n|^2\big)^{1/2}$$

for any two sequences (x_n) and (y_n) of complex numbers with $\sum_n |x_n|^2 < \infty$ and $\sum_n |y_n|^2 < \infty$.

Lemma 20. *Let* $H \underset{g}{\overset{f}{\rightleftarrows}} K$ *be morphisms in* **Hilb**. *Then* $g \circ f$ *is trace class if and only if* f *and* g *are Hilbert-Schmidt.*

Proof. By polar decomposition, there is a unique partial isometry $w\colon H \to K$ satisfying $g \circ f = w \circ |g \circ f|$ and $\ker(w) = \ker(g \circ f)$. It follows that $|g \circ f| = w^\dagger \circ g \circ f$. Hence, for an orthonormal basis (e_n) of H,

$$\begin{aligned}
\sum_n \big|\langle e_n \mid |g \circ f|(e_n)\rangle\big| &= \sum_n \big|\langle e_n \mid w^\dagger \circ g \circ f(e_n)\rangle\big| \\
&= \sum_n \big|\langle g^\dagger \circ w(e_n) \mid f(e_n)\rangle\big| \\
&\leq \sum_n \big(\|g^\dagger \circ w(e_n)\|^2 \cdot \|f(e_n)\|^2\big)^{1/2} && \text{(by Cauchy-Schwarz)} \\
&= \sum_n \big|\|g^\dagger \circ w(e_n)\| \cdot \|f(e_n)\|\big| \\
&\leq \big(\sum_n \|g^\dagger \circ w(e_n)\|^2\big)^{1/2} \cdot \big(\sum_n \|f(e_n)\|^2\big)^{1/2}. && \text{(by Hölder)}
\end{aligned}$$

Therefore gf is trace class if and only if $\sum_n \|f(e_n)\|^2 < \infty$ and $\sum_n \|g^\dagger \circ w(e_n)\|^2 < \infty$. Because w is a partial isometry, the latter inequality holds if and only if $\sum_n \|g(e_n)\|^2 < \infty$. That is, $g \circ f$ is trace class if and only if f and g are Hilbert-Schmidt. □

Proposition 21. *The category* **Hilb** *has a dagger trace ideal consisting of the usual trace class maps and the usual trace function.*

Proof. That the trace class maps on a Hilbert space H are closed under adjoint and tensor products is easily seen. Also, any morphism $\mathbb{C} \to \mathbb{C}$ is trivially trace class. Now suppose that $f\colon H \to H$ is trace class. By the previous lemma, we can write $f = f_2 \circ f_1$ for Hilbert-Schmidt maps f_i. If $g\colon H \to K$ and $h\colon K \to H$ are arbitrary morphisms, then $g \circ f_2$ and $f_1 \circ h$ are again Hilbert-Schmidt. Therefore, by the previous lemma again, $g \circ f \circ h = (g \circ f_2) \circ (f_1 \circ h)$ is trace class. Thus trace class maps indeed form an endomorphism ideal.

One easily sees from the trace property that trace is the identity on scalars, is multiplicative on tensor products, and preserves daggers. To prove that $\mathrm{Tr}(g \circ f) = \mathrm{Tr}(f \circ g)$ for $f\colon H \to K$ and $g\colon K \to H$ with both $f \circ g$ and $g \circ f$ trace class, we rely on *Lidskii's trace formula* for separable H: if h is trace class, then ($\sum_n \lambda_n(h)$ is absolutely convergent and) $\mathrm{Tr}(h) = \sum_n \lambda_n(h)$, where $\lambda_n(h)$ are the eigenvalues counted up to algebraic multiplicity [57, Theorem 3.7]. But $g \circ f$ and $f \circ g$ have precisely the same spectrum, so that $\mathrm{Tr}(g \circ f) = \sum_n \lambda_n(g \circ f) = \sum_n \lambda_n(f \circ g) = \mathrm{Tr}(f \circ g)$.

Finally, we claim that for positive, trace class functions $h\colon H \to H$ on any (possibly nonseparable) Hilbert space H, Lidskii's formula still holds, which finishes the proof that trace class operators form a trace ideal, because we may then replace $g \circ f$ and $f \circ g$ above by their absolute value. Pick an orthonormal basis $\{e_i\}$ for H. Since h is trace class, $\sum_i \langle e_i \mid h(e_i)\rangle = \sum_i \|\sqrt{h}(e_i)\|$ is summable. Hence $\ker(h)^\perp = \ker(\sqrt{h})^\perp$ can only contain countably many e_i. Because h is positive, its range is $\ker(h^\dagger)^\perp = \ker(h)^\perp$. Thus $h\colon H \to H$ restricts to a function $h\colon \ker(h)^\perp \to \ker(h)^\perp$ on a separable space. □

We have written the above example out in more detail than the reader might have thought necessary, because it is easy to overlook subtleties. For example, it is not true that if $f\colon H \to K$ and $g\colon K \to H$ are morphisms such that $g \circ f$ is trace class, then $f \circ g$ is trace class, too. For a counterexample, let $H = K = \ell^2(\mathbb{N})$, and define $f(x,y) = (0,x)$ and $g(x,y) = (x,0)$. Then certainly $g \circ f = 0$ is trace class. But it is easy to see that $f^\dagger(x,y) = (y,0)$, that $g = g^\dagger = g^\dagger \circ g$, and hence that $g = g^\dagger \circ g = (f \circ g)^\dagger \circ (f \circ g) \geq 0$. Therefore $|f \circ g| = g$, and

$$\mathrm{Tr}(f \circ g) = \sum_{m,n} \langle |f \circ g|(e_m, e_n) \mid (e_m, e_n)\rangle = \sum_{m,n} \langle e_m \mid e_m\rangle + \langle 0 \mid e_n\rangle = \dim(H) = \infty,$$

so that $f \circ g$ is not trace class.

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