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Conditional quantum iteration from categorical traces

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Abstract

In order to describe conditional iteration in quantum systems, we consider categories where hom-sets have a partial summation based on an axiomatisation of uniform convergence. Such structures, similar to Haghverdi's Unique Decomposition Categories (UDCs), allow for a number of fundamental constructions including the *standard*, or *'particle-style'*, categorical trace.

We demonstrate that the category of continuous maps on Hilbert spaces falls within this fraqmework, and has a (partially defined) categorical trace based on iteration. This trace formula converges for unitary maps, but has no immediate physical interpretation. We then give a general construction that splits this trace into the composite of three maps: a canonical inclusion, a series of unitary operations, and a co-diagonal. We show that these unitary operations give a particle-style trace in a larger category (the convolution category), and demonstrate how the familiar (Elgot, Arbib-Manes) programming language interpretation of 'conditional loops' (via the standard trace over coproducts) gives a semantics of iteration conditioned on a purely quantum variable. Algorithms and physical interpretations are given.

1. Introduction

In this paper, we study conditional iteration in Hilbert spaces, in order to give a physically reasonable notion of conditional quantum iteration. This is not the "quantum data, classical code" paradigm (Selinger 2004(i)) — rather we seek a fully quantum, and hence unitary, system that allows for iteration conditioned on quantum variables, without measurement.

A natural first question is whether such a thing exists at all — indeed, the usual model of *While* loops (The Elgot Dagger, described in Section 10.1) is not even applicable to

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classical reversible computation. However, partial feedback – without measurement – is certainly a physical construction, and is a common feature of (for example) quantum optics experiments and quantum error-correction (Sarovar, Millburn 2005). Similarly, the original conception of a universal quantum Turing machine (Deutsch 1985) has a purely unitary evolution (We emphasise that it is the *evolution* of the quantum Turing machine that is purely unitary, not the Halting Scheme described in (Deutsch 1985). This is based on repeated observation of a subsystem, and we refer to (Myers 1997) and (Linden, Popescue 1998) for the problems associated with this approach), and hence a fully quantum control structure.

However, there are a number of well-established problems associated with a direct attempt to generalise iteration to the unitary setting: we refer to (Linden, Popescue 1998) for a general discussion, (Hagar, Korolev 2004) for a good discussion in terms of *halting problems*, and (Bernstein, Vazirani 1997) for an analysis of the restricted case, where all branches of a superposition reach a halting state after the same number of steps.

The approach we take is to investigate the structure of conditional iteration, using familiar categorical tools, but without assuming that it may fit into pre-existing programming language paradigms (such as 'While loops'). By generalising the Unique Decomposition Categories of (Haghverdi 2000; Haghverdi, Scott 2006) to cover categories of Hilbert spaces and linear maps, we give a description of conditional iteration in unitary systems. This is via the construction of an 'iterative' or 'particle-style' trace, and corresponds to physical experiments based on partial feedback. The particle-style trace is a description of 'eliminating a subspace by conditional iteration' that is applicable to classical reversible computation. We refer to (Abramsky 1996) for an overview of categorical traces, including interpretations as both iteration and fixed-point constructions, (Haghverdi 2000) for the formalisation of the particle-style trace in Unique Decomposition Categories and applications to reduction in linear logic, (Abramsky et. al. 2002) for examples of traces used in building models of linear logic and (untyped λ -calculus equivalent) combinatory algebra, (Hines 2003) for the particle-style trace as the semantics of reversible space-bounded Turing machines, and (Selinger 2004(i)) for applications to classical-control, quantum-data programming languages.

The particle-style trace is defined in terms of categories with additional structure which permits both formal sums of families of arrows, and matrix representations (the Unique Decomposition Categories of (Haghverdi 2000)). We generalise this notion to a setting that covers Hilbert and Banach spaces, and demonstrate that this more general setting also gives a categorical trace. Consideration of partial feedback in a simple linear-optics thought experiment also demonstrates that the iterative or 'particle-style' trace is a 3step process: a canonical inclusion, a reversible (and, in the appropriate setting unitary) process, and a codiagonal. Further, the central reversible (or unitary) part of this is itself a categorical trace in a larger category.

Finally, we consider computational interpretations. Given a classical reversible function f computed by an algorithm based on conditional iteration, we demonstrate how we may produce a quantum-mechanical analogue F. This reproduces the behaviour of this

classical algorithm on the computational-basis (i.e. $F(|x\rangle) = |f(x)\rangle$ for basis vectors $|x\rangle$), and is superposition-preserving, so $F(\alpha(|m\rangle) + \beta|n\rangle) = \alpha|f(m)\rangle + \beta|f(n)\rangle$.

2. Categorical Preliminaries

We assume the reader is familiar with the basic language of category theory. We refer to (MacLane 1998) for the definitions, together with the notions of *naturality*, *functors*, *natural transformations* and *adjoints* (see also (Blute, Scott 2004) for a basic survey).

Definition 2.1. Symmetric Monoidal Categories

A monoidal (or tensored) category $(\mathcal{C}, I, \otimes, \alpha, \ell, r)$ is a category \mathcal{C} , with functor $\otimes : \mathcal{C} \times \mathcal{C} \to \mathcal{C}$, unit object $I \in ob(\mathcal{C})$, and specified isos:

$$\begin{array}{c} -- \alpha_{ABC} : (A \otimes B) \otimes C \xrightarrow{\cong} A \otimes (B \otimes C) \\ -- \ell_A : I \otimes A \xrightarrow{\cong} A \\ -- r_A : A \otimes I \xrightarrow{\cong} A \end{array}$$

satisfying various naturality and coherence equations. A monoidal category is symmetric if there is a natural isomorphism (or "twist") $s_{AB} : A \otimes B \to B \otimes A$ satisfying $s_{B,A} \circ s_{A,B} = id_{A \otimes B}$ in addition to appropriate naturality and coherence equations.

Monoidal tensors satisfying additional conditions are of particular importance :

— (**Products**) If, for all objects $X_1, X_2 \in Ob(\mathcal{C})$ there exist arrows

$$X_1 \xleftarrow{\pi_1} X_1 \otimes X_2 \xrightarrow{\pi_2} X_2$$

such that, for all arrows $f_1 \in \mathcal{C}(Y, X_1)$ and $f_2 \in \mathcal{C}(Y, X_2)$ there exists a unique arrow $\langle f_1, f_2 \rangle \in \mathcal{C}(Y, X_1 \otimes X_2)$ making the following diagram commute :



then \otimes is called a **categorical product**, and often denoted \times . - (Coproducts) If, for all objects $X_1, X_2 \in Ob(\mathcal{C})$ there exist arrows

$$X_1 \xrightarrow{\iota_1} X_1 \otimes X_2 \xleftarrow{\iota_2} X_2$$

such that, for all arrows $f_1 \in \mathcal{C}(X_1, Y)$ and $f_2 \in \mathcal{C}(X_2, Y)$ there exists a unique arrow $[f_1, f_2] \in \mathcal{C}(Y, X_1 \otimes X_2)$ making the following diagram commute :



then \otimes is called a **categorical coproduct**, and often denoted II.

For numerous examples, we refer to the previously mentioned sources, as well as (Geroch 1985), a category-oriented text on mathematical physics. Particular important examples, to be described in Section 3 below, include categories of relations (**Rel**, \uplus) (sets and relations, with tensor being disjoint union), (**pFun**, \uplus) (sets and partial functions), (**Vec**_{fd}, \oplus) (finite dimensional vector spaces and linear maps, with monoidal tensor being the direct sum), and various categories of Banach and Hilbert Spaces.

Notation: We write our categories in **boldface**. Some authors adopt the convention of naming categories according to their objects — an equally common alternative convention is to name categories according to their arrows. Where possible we follow previously established conventions so, for example, we refer to the category **Vec** of vector spaces and linear maps, but the category **pInj** of partial injections, &c.

2.1. Traced Monoidal Categories

Traced monoidal categories, introduced by Joyal, Street, and Verity (Joyal et. al. 1996) for studies in knot theory and algebraic topology, turn out to provide a convenient framework for studying many areas of theoretical computer science, including iteration theories, parametrized feedback, fixed-points in computation, algebra of networks, state machines, and categorical aspects of Girard's Geometry of Interaction (GoI) program (Abramsky 1996; Hines 1997; Haghverdi 2000; Abramsky et. al. 2002; Hines 2003; Haghverdi, Scott 2006).

The following definition is equivalent to the original, in the case of a traced symmetric monoidal category.

Definition 2.2. A traced symmetric monoidal category is a symmetric monoidal category $(\mathcal{C}, \otimes, I, s)$ with a family of functions $Tr_{X,Y}^U : \mathcal{C}(X \otimes U, Y \otimes U) \longrightarrow \mathcal{C}(X,Y)$ called a trace, subject to the following conditions:

- 1 Natural in X, $Tr_{X,Y}^U(f)g = Tr_{X',Y}^U(f(g \otimes 1_U))$, where $f : X \otimes U \longrightarrow Y \otimes U$, $g : X' \longrightarrow X$,
- 2 Natural in Y, $gTr_{X,Y}^U(f) = Tr_{X,Y'}^U((g \otimes 1_U)f)$, where $f: X \otimes U \longrightarrow Y \otimes U$, $g: Y \longrightarrow Y'$,
- 3 **Dinatural** in U, $Tr_{X,Y}^U((1_Y \otimes g)f) = Tr_{X,Y}^{U'}(f(1_X \otimes g))$, where $f: X \otimes U \longrightarrow Y \otimes U'$, $g: U' \longrightarrow U$,
- 4 Vanishing I, $Tr_{X,Y}^{I}(f) = f$, for $f: X \otimes I \longrightarrow Y \otimes I$.
- 5 **Vanishing II**, $Tr_{X,Y}^{U\otimes V}(g) = Tr_{X,Y}^U(Tr_{X\otimes U,Y\otimes U}^V(g))$, for $g: X \otimes U \otimes V \longrightarrow Y \otimes U \otimes V$.
- 6 Superposing,

$$g \otimes Tr_{X,Y}^{\mathcal{O}}(f) = Tr_{W \otimes X, Z \otimes Y}^{\mathcal{O}}(g \otimes f)$$
for $f: X \otimes U \longrightarrow Y \otimes U$ and $q: W \longrightarrow Z$.

7 Yanking, $Tr_{U,U}^U(\sigma_{U,U}) = 1_U$.

The axioms of a traced monoidal category have a strongly geometric flavour, with an associated graphical calculus (Joyal et. al. 1996; Joyal,Street 1991; Abramsky et. al. 2002), all this being presaged by R. Penrose's graphical notation for tensor calculus (Penrose 1971). We also observe that (Joyal et. al. 1996) studies the braided and tortile monoidal cases, giving further close connections to braid closure in knot theory. However, categorical traces in symmetric monoidal categories have been shown to have important connections to computer science (Abramsky 1996; Abramsky et. al. 2002; Hines 2003).

3. Sets with notions of summation

In order to produce categorical traces that provide a notion of iteration, we will consider categories whose hom-sets have a notion of partial summation. We now introduce a very general notion of summation, motivated by *absolute convergence*.

We recall some standard notation. Let M be a fixed set. If I is a set, an I-indexed family of M is a function $x : I \to M$. We often denote such a family x by $\{x_i\}_{i \in I}$. In what follows we only consider countably indexed families. As we are considering *partial* summations, we also make heavy use of Kleene's notation for equality of partial functions as in (Freyd and Scedrov 1990): $u \simeq v$ means: one side is defined iff the other side is, and in that case they are equal. When we know that both sides exist, we use the usual symbol = for equality.

Definition 3.1. Partial commutative monoids, Weak partition-associativity

We define a **partial commutative monoid** or **PCM** to be a set M together with a partial function Σ from countably indexed families of M to elements of M that satisfies the following axioms, where we write $\sum_{i \in I} x_i$ for $\Sigma(x)$, when the operation Σ is defined:

- 1 The **Unary Sum axiom** Any family $\{x_i\}_{i \in I}$, where $I = \{i'\}$ is a singleton set, is summable, and $\sum_{i \in I} x_i = x_{i'}$.
- 2 The Weak Partition-Associativity Let $\{x_i\}_{i \in I}$ be a countably indexed summable family, and let $\{I_j\}_{j \in J}$ be a countable partition[†] of I. Then $\{x_i\}_{i \in I_j}$ is summable for every $j \in J$, and $\{\sum_{i \in I_j} x_i\}_{j \in J}$ is summable, and

$$\sum_{i \in I} x_i = \sum_{j \in J} \left(\sum_{i \in I_j} x_i \right)$$

We then say that (M, Σ) is a PCM.

We first need to show that the Σ operation of a PCM is well-defined — that is, the partial summation operation preserves "equivalent" families. For this, we define *equivalence of families* as follows: given families $x : I \to M$ and $y : J \to M$, two countably indexed families of elements of M, we write $x \cong y$ when there exists a bijection $\varphi : I \to J$ such that $y \circ \varphi = x$. This means, for all $i \in I$, $y_{\varphi(i)} = x_i$.

[†] Here, 'countable' means either finite or denumerable. Following (Manes, Arbib 1986), we allow countable many I_j to be empty.

Proposition 3.2 (Well-definedness of Σ). Suppose $x \cong y$ are two equivalent families of M. If $\Sigma(y)$ is well defined, then so is $\Sigma(x)$ and they are equal. That is, writing $x = \{x_i\}_{i \in I}$, and similarly for y, if $\Sigma_{j \in J} y_j$ exists, then so does $\Sigma_{i \in I} x_i$ and $\Sigma_{j \in J} y_j = \Sigma_{i \in I} x_i$. In particular, if $x \cong y$ then $\Sigma(x) \simeq \Sigma(y)$ (note the use of Kleene equality).

Proof. Suppose φ is a bijection, as above, so $x_i = y_{\varphi(i)}$, for all $i \in I$. Let $J_i = \{\varphi(i)\}$ be a singleton set; hence $\{J_i \mid i \in I\}$ is a partition of J. Then we have:

$$\begin{split} \Sigma_{j\in J} y_j &= \Sigma_{i\in I} \Sigma_{j\in J_i} y_j & \text{Weak partition associativity} \\ &= \Sigma_{i\in I} y_{\varphi(i)} & \text{Defn, and Unary sum axiom} \\ &= \Sigma_{i\in I} x_i & \text{Defn} \end{split}$$

If $\Sigma(x)$ is defined, where $x = \{x_i\}_{i \in I}$, we may write $\Sigma(x)$ (unambiguously) as $\sum_{i \in I} x_i$. For example, if $I = \{1, \ldots, n\}$, we write $\Sigma(x) = x_1 + x_2 + x_3 + \cdots + x_n$, and if $I = \mathbb{N}$, $\Sigma(x) = x_1 + x_2 + x_3 + \cdots + x_n + \cdots$. Notice that by Weak Partition Associativity, we may equate different partitions of a summable family x, for example:

$$x_1 + x_2 + x_3 + \dots = x_1 + (x_2 + x_3 + \dots + x_n + \dots)$$

= $(x_1 + x_2) + (x_3 + x_4) + \dots + (x_n + x_{n+1}) + \dots$

The terminology 'Weak Partition Associativity' comes from the Partition Associativity Axiom of Definition 3.4 (for example, as presented in (Manes, Arbib 1986)). We have weakened this to allow for analogues of negative elements in a summation, which are ruled out by the full partition-associativity axiom (see the Positivity Property of Proposition 3.5).

Proposition 3.3. Let (M, Σ) be a PCM. Then

- 1 (Summable Subfamilies) Let $\{x_i\}_{i \in I}$ be a summable family of M. Then any subfamily $\{x_i\}_{i \in K}$, where $K \subseteq I$, is also summable.
- 2 (Existence of Zero) The empty set is summable, and $x + \{\} = x = \{\} + x$ for all $x \in M$. Hence it is a zero for M, and we write $0 = \sum\{\}$.
- 3 (Sums of Zeros) For any index set I, let $0_I : I \to M$ denote the constantly zero family (so $O_I(i) = 0$, for all $i \in I$). Then 0_I is summable, and $\Sigma_I 0_I = 0$. More generally, for any element $x \in M$, $x + 0 + 0 + 0 + \cdots = x$ (where $0 + 0 + \cdots$ denotes (the sum of) either a finite or infinite sequence of 0's).

Proof. The proofs of (1) and (2) below are based on very similar proofs (for the special case of partially additive monoids – see below) presented in (Manes, Arbib 1986).

- 1 (Summable Subfamilies) Any subset $K \subseteq I$ defines a partition of I, namely $\{K, I \setminus K\}$. By Weak Partition Associativity, $\sum_{i \in K} x_i$ exists.
- 2 (Existence of Zero) As M is by definition non-empty, the unary sum axiom implies that the set of summable families is also non-empty. The empty family is a subfamily

of any summable family; hence letting $K = \emptyset$ in the partition above, we see that the empty family {} is summable. It is then immediate that \sum {} = 0 is a zero for the summation operation, and 0 + x = x = x + 0 exists for arbitrary $x \in M$.

3 (Sums of Zeros) Pick any partition of I whose first cell is I itself, and the remaining cells are empty (the number of empty cells is either finite or infinite, depending upon whether one wishes a finite (resp. infinite) sum of 0's. For example, write $I = I_1 \uplus (\uplus_{n>1}I_n)$, where $I_1 = I$, $I_i = \emptyset$, if i > 1. If $x = \{x_i\}_{i \in I}$ is an I-indexed summable family, then by Weak Partition Associativity we have: $\sum_{i \in I} x_i = \sum_{i \in I_1} x_i + \sum_{n>1} (\sum_{i \in I_n} x_i) = \sum_{i \in I_1} x_i + 0 + 0 + \cdots$. Now pick a singleton family $\{x\}$, so $\Sigma(x) = x$. The result follows.

We now present Σ -monoids, and *partially additive monoids*, as introduced in (Manes, Benson 1985), as special cases of PCMs :

Definition 3.4. (Σ -monoids, Partially additive monoids)

A PCM (M, Σ) is called a Σ -monoid when it satisfies the following additional axiom :

— The (full) Partition-Associativity Axiom. Let $\{x_i\}_{i\in I}$ be a countably indexed family, and let $\{I_j\}_{j\in J}$ be a countable partition of I. Then $\{x_i\}_{i\in I}$ is summable if and only if $\{x_i\}_{i\in I_j}$ is summable for every $j \in J$, and $\{\sum_{i\in I_j} x_i\}_{j\in J}$ is summable, in which case

$$\sum_{i \in I} x_i = \sum_{j \in J} \left(\sum_{i \in I_j} x_i \right)$$

Note that this is a special case of the *weak partition-associativity axiom*, with a two-way, instead of a one-way, implication.

We say a Σ -monoid is a **partially additive monoid** if it also satisfies the axiom :

— The **Limit Axiom.** If $\{x_i\}_{i \in I}$ is a countably indexed family, and $\{x_i\}_{i \in F}$ is summable for every finite $F \subseteq I$, then $\{x_i\}_{i \in I}$ is summable.

The limit axiom is a very strong condition that certainly is not satisfied by many forms of summation. When considering summation on the real line, finite sums always exist. However, the convergence of an infinite sum is certainly not implied by the (guaranteed) convergence of all finite sub-sums. An illustrative example of a summation satisfying the limit axiom is the set-theoretic union of partial functions. In Section 5, the distinction between 'analytic' and 'algebraic' notions of summation is explored in various contexts.

Partially additive monoids are used in the theory of program and flowchart semantics (Manes, Arbib 1986). The following results on Σ -monoids are given in this reference:

Proposition 3.5. Let (M, Σ) be a Σ -monoid. Then

- 1 (Summable Subfamilies) Let $\{x_i\}_{i \in I}$ be a summable family of M. Then any subfamily $\{x_i\}_{i \in K}$, where $K \subseteq I$ is also summable.
- 2 (Existence of Zero) The empty set is summable, and $x + \{\} = x = \{\} + x$ for all $x \in M$. Hence it is a zero for M, and we write $0 = \sum\{\}$.

3 (The Positivity Property) Let $X = \{x_i\}_{i \in I}$ be a summable family of M satisfying $\sum_{i \in I} x_i = 0$. Then $x_i = 0$ for all $i \in I$.

Proof. 1. and 2. follow immediately, since Σ -monoids are special cases of PCMs. It remains to prove 3., the positivity property:

Let $X = \{x_i\}_{i \in I}$ be a summable family satisfying $\sum_{i \in I} x_i = 0$. For some $i \in I$, we define $Y = \{x_j\}_{j \neq i \in I}$, so $x_i + \sum Y = 0 = \sum Y + x_i$ by weak partition associativity. Then by the full partition-associativity axiom,

$$x_{i} = x_{i} + 0 + 0 + 0 + \dots \text{ by Proposition 3.3}$$

= $x_{i} + (\sum Y + x_{i}) + (\sum Y + x_{i}) + (\sum Y + x_{i}) + \dots$
(by full partition associativity)
= $(x_{i} + \sum Y) + (x_{i} + \sum Y) + (x_{i} + \sum Y) + \dots$
= $0 + 0 + \dots = 0$, by Proposition 3.3

Hence $x_i = 0$. However, as i was chosen arbitrarily, $x_k = 0$ for all $k \in I$.

We emphasise that the above proof of positivity does *not* apply to general PCMs, as it depends on the two-way implication in the (full) partition-associativity axiom. In Section 6, we present examples of PCMs that do not satisfy the positivity property.

Remark Positivity and quantum computation

Categories that carry a Σ -monoid structure on their hom-sets (see Section 5) have long been known to have a close connection with models of conditional iteration (see, for example (Manes, Arbib 1986)) – however, we have gone to a great deal of trouble to find generalisations of Σ -monoids that do not satisfy the positivity property of Proposition 3.5. This is because positivity prevents Σ -monoids from being used to reason about negative or complex values.

Our eventual aim is quantum computation where both *constructive* and *destructive interference* play an important part in quantum algorithms. The importance of complex amplitudes in quantum computation is shown by the Gottesman-Knill Theorem (Gottesman 1999) (Knill et. al. 2001). This states that a system with the *controlled not* gate, computational-basis preparations and measurements, and classical control can be efficiently simulated by a classical computer, whereas a system with these features, and additionally, single-qubit $\pi/8$ phase shifts, is universal for quantum computation (up to a well-defined notion of approximation, see (Shi 2002)).

3.1. A group-like notion of summation

For completeness, we also consider Σ -groups – sets with a notion of summation similar to Σ -summability, where the failure of positivity is part of the definition. These were introduced, in slightly different terms, in (Wylie 1957) and by Denis Higgs in his theory of axiomatic integration theory. We follow the notations and conventions of (Higgs 1988), in particular because of the direct application to Banach and Hilbert spaces given in (Higgs 1989). The following definitions and notions are due to Higgs.

Definition 3.6. Σ -groups

A Σ -group is defined in (Higgs 1989) to be a set G, together with a partial summation $\Sigma : \mathcal{F}(G) \to G$, where $\mathcal{F}(G)$ is the set of arbitrarily indexed families of G. Then

- 1 Unary sum axiom Any family $\{g_i\}_{i \in I}$, where $I = \{i'\}$ is a singleton set, is summable, and $\sum_{i \in I} \{g_i\} = g_{i'}$.
- 2 Finite abelian group axiom The set G, together with the restriction of Σ to finite sets, is an abelian group, and hence all finite families are summable.
- 3 Weak Higgs axiom (I) Let $\{g_i\}_{i \in I}$ be a summable family, and let $\{I_j\}_{j \in J}$ be a partition of I into finite subsets. Then $\{g_i\}_{i \in I_j}$ is summable for every $j \in J$, and $\sum_{i \in I_i} g_i$ is summable for $j \in J$. Finally,

$$\sum_{i \in I} g_i = \sum_{j \in J} \left(\sum_{i \in I_j} g_i \right)$$

4 Weak Higgs axiom (II) Let $\{g_i\}_{i\in I}$ be an arbitrary family, and let $\{I_j\}_{j\in F}$ be a partition of I for some *finite* index set F. If $\{g_i\}_{i\in I_j}$ is summable for every $j\in J$, and $\sum_{i\in I_j} g_i$ is summable for $j\in J$, then $\{g_i\}_{i\in I}$ is summable and

$$\sum_{i \in I} g_i = \sum_{j \in J} \left(\sum_{i \in I_j} g_i \right)$$

Proposition 3.7. The following properties of Σ -groups are immediate from the definition:

- 1 A Σ -group G, together with the restriction of the summation to binary pairs $x + y = \sum \{x, y\}$ for all $x, y \in G$, gives an abelian group. Hence Σ -groups do not satisfy the positivity property.
- 2 Imposing the *limit axiom* (as in Definition 3.4) on a Σ -group results in *all series* being summable.

The Higgs axioms provided the motivation for the generalisation from Σ -monoids to the more general PCMs. Despite this, Σ -groups themselves are not PCMs : Σ -groups allow for *arbitrarily indexed* summable families, and the Weak Higgs axioms (I) and (II) are restricted to either *finite partitions*, or partitions into *finite subsets*. However, all the examples of Σ -groups we consider are also PCMs. Because of this, we make the following definition :

Definition 3.8. Strong Σ -groups

A strong Σ -group is defined to be a Σ -group that is also a PCM (with respect to the same summation operator). Examples will be presented in Section 6.3.

Terminology We also use the generic term "Sigma-structures" for any of the structures given in the above section.

4. The category of PCMs

As may be expected, we may form a category of partial commutative monoids :

Definition 4.1.

We define the category **PCM** as follows:

- The objects of **PCM** are partial commutative monoids.
- Given objects $(X, \Sigma), (Y, \Sigma') \in Ob(\mathbf{PCM})$, an arrow $f : (X, \Sigma) \to (Y, \Sigma')$ is a function from X to Y such that, for all countably indexed families $\{x_i\}_{i \in I}$ of X,

 $\{x_i\}_{i \in I}$ is summable $\Rightarrow \{f(x_i)\}_{i \in I}$ is summable

in which case

$$f\left(\sum_{i\in I} x_i\right) = \Sigma'_{i\in I} f(x_i)$$

Note that $f(0_X) = 0_Y$, for arbitrary $f \in \mathbf{PCM}(X, Y)$, since $0_X = \Sigma^{(X)}\{\}$, and so $0_Y = \Sigma^{(Y)}\{\} = f(\Sigma^{(X)}\{\}) = f(0_X).$

We may make similar definitions for PAMs, Σ -groups and Σ -monoids, to give the categories **PAM**, Σ **Grp**, Σ **Mon** respectively. Note that **PAM** and Σ **Mon** are subcategories of **PCM**; however Σ **Grp** is not because, as noted above, Σ -groups are not required to satisfy the weak partition-associativity axiom.

Proposition 4.2. The category **PCM** has products, coproducts, and equalizers.

Proof.

- (products) We first describe finite products. Given PCMs $A = (X, \Sigma^{(X)})$ and $B = (Y, \Sigma^{(Y)})$, their product $A \times B$ has, as underlying set the Cartesian product $Z = X \times Y$. A countably indexed family $\{z_i\}_{i \in I} = \{(x_i, y_i)\}_{i \in I}$ is defined to be summable exactly when either
 - 1 The sums $\sum_{i \in I}^{(X)} x_i$ and $\sum_{i \in I}^{(Y)} y_i$ exist, in which case $\sum_{i \in I}^{(Z)} z_i = \left(\sum_{i \in I} x_i, \sum_{i \in i} y_i\right)$
 - 2 *I* is the empty set, in which case $\Sigma^{(Z)}{} = (\Sigma^{(X)}{}, \Sigma^{(Y)}{})$, giving the zero element of $A \times B$.

It is easy to verify that $A \times B$ satisfies the axioms for a PCM and satisfies the required universal property for a categorical product.

Extension to arbitrary Λ -indexed products $\Pi_{\lambda \in \Lambda} A_{\lambda}$, where $A_{\lambda} = (X_{\lambda}, \Sigma^{(X_{\lambda})})$, is defined analogously to the finite case, with coordinate-wise Σ structure.

- (coproducts) Again, we start with finite coproducts. Given PCMs $A = (X, \Sigma^{(X)})$ and $B = (Y, \Sigma^{(Y)})$, their coproduct $A \amalg B$ has as underlying set the disjoint union $X \uplus Y = X \times \{0\} \cup Y \times \{1\}$. A countably indexed family $\{u_i\}_{i \in I}$ in $X \uplus Y$ is defined to be summable when either
 - 1 $\{u_i\}_{i\in I} = \{(x_i, 0)\}_{i\in I}$ and $\{x_i\}_{i\in I}$ is a summable family of A. In this case $\sum_{i\in I}^{(X \oplus Y)} u_i = \left(\sum_{i\in I}^{(X)} x_i, 0\right)$
 - 2 $\{u_i\}_{i \in I} = \{(y_i, 1)\}_{i \in I}$ and $\{y_i\}_{i \in I}$ is a summable family of B. In this case $\sum_{i \in I}^{(X \oplus Y)} u_i = \left(\sum_{i \in I}^{(Y)} y_i, 1\right)$
 - 3 *I* is the empty set, in which case $\Sigma^{(X \uplus Y)} \{\} = (\Sigma^{(X)} \{\}, 0) = (\Sigma^{(Y)} \{\}, 1)$ giving the zero element of $A \amalg B$.

It is again easy to verify that $X \amalg Y$ satisfies both the PCM axioms and the required universal property for a coproduct.

The case of Λ -indexed coproducts $\coprod_{\lambda \in \Lambda} A_{\lambda}$ is analogous: one forms the disjoint union of their underlying sets, and we declare a family $\{u_i\}_{i \in I}$ in the disjoint union to be summable if it arises as the injection of a summable family from a component (in which case, the sum is the appropriate injection of the sum in that component). More precisely, if $\{u_i\}_{i \in I}$ in the disjoint union is summable because it arises from a summable family $(x_i^{\alpha_0})$ in the α_0 -th component, then we define the sum $\sum_{i \in I}^{(\Pi_{\lambda \in \Lambda} X_{\lambda})} u_i = \left(\sum_{i \in I}^{(X_{\alpha_0})} x_i^{\alpha_0}, \alpha_0\right)$.

Finally, equalizers are constructed as in the category of sets, with the induced Σ -structure. That is, given morphisms $f, g : (X, \Sigma^{(X)}) \to (Y, \Sigma^{(Y)})$, we form the settheoretic equalizer $E = \{x \in X \mid f(x) = g(x)\}$. We declare a family to be summable in E iff it is already summable in X, in which case its sum is the sum in X. Notice this forces the inclusion map $E \hookrightarrow X$ to be a morphism. It is readily verified that the universal property is satisfied; in particular, this amounts to showing that the unique map in Sets making the appropriate diagram commute actually is a morphism in **PCM**. This follows from the induced Σ structure on E.

4.1. **PCM** as a closed category

We show that **PCM** is a closed category, without assuming it is *monoidal* closed; for the latter, see Section 7 below. We follow the treatment in Laplaza (Laplaza 1977). We demonstrate that hom-sets in **PCM** are themselves PCMs, i.e., there is a notion of internal hom satisfying appropriate naturality equations.

Lemma 1. Let A, B be PCMs with summations $\Sigma^{(A)}, \Sigma^{(B)}$, respectively. Define the internal hom $[A, B] = \mathbf{PCM}(A, B)$. Then [A, B] can be given a natural PCM structure.

Proof. Recall the definition of arrows in the category **PCM** : an arrow $f : A \to B$ is a function from A to B such that, for all countably indexed summable families $\{x_i\}_{i \in I}$ of A, the family $\{f(x_i)\}_{i \in I}$ in B is summable and

$$f\left(\Sigma_{i\in I}^{(A)}x_i\right) = \Sigma_{i\in I}^{(B)}f(x_i)$$

We say an indexed family of arrows $\{f_j\}_{j\in J}$ in [A, B] is summable when, for all summable families $\{x_k\}_{k\in K} \in A$, the doubly-indexed family $\{f_j(x_k)\}_{j\in J, k\in K}$ is summable in B: that is, if $\sum_{j\in J}\sum_{k\in K} f_j(x_k)$ exists.

In the case $\{f_j\}_{j \in J}$ in [A, B] is summable, we define its sum pointwise:

$$\left(\Sigma_{j\in J}^{[A,B]}f_j\right)(x) = \Sigma_{j\in J}^{(B)}f_j(x) \quad \text{for all } x\in A.$$

We now show $\Sigma^{[A,B]}$ satisfies the unary sum and partition-associativity axioms:

— (unary sum) Given a singleton family $\{f\}$, observe that, for all summable families $\{x_k\}_{k\in K}$, the family $\{f(x_k)\}_{k\in K}$ is summable, by definition of morphism.

— (weak partition-associativity) Consider a summable family $\{f_i \in [A, B]\}_{i \in I}$, and a partition $I = \biguplus_{j \in J} I_j$. Then for all $j \in J$ and $\{x_k\}_{k \in K} \in A$, the (sub)families $\{f_i(x_k)\}_{i \in I_j, k \in K}$ are summable (over I_j, K) by the weak partition-associativity axiom for $(B, \Sigma^{(B)})$, and hence so is the subfamily $\{f_i\}_{i \in I_j}$. Similarly, since $\{f_i\}_{i \in I}$ is summable, then for all $\{x_k\}_{k \in K} \in A$, the family of subsums

 $\{\sum_{i \in I_i} f_i(x_k)\}_{j \in J, k \in K}$ is itself summable.

Hence [A, B], with this summation, is a PCM.

We demonstrate functoriality of this operation :

Lemma 2. The map [,] above defines a functor from $\mathbf{PCM}^{op} \times \mathbf{PCM}$ to \mathbf{PCM} .

Proof.

- (on objects) [,] is as defined in Lemma 1 above.
- (on arrows) Given $f \in \mathbf{PCM}^{op}(A, B)$ and $g \in \mathbf{PCM}(C, D)$, we define $[f, g] \in \mathbf{PCM}([A, C], [B, D])$ as follows :

First note that $f \in \mathbf{PCM}^{op}(A, B)$ is specified by $f' \in \mathbf{PCM}(B, A)$ in the usual way. Then, given $p \in [A, C]$, we define $[f, g](p) \in [B, D]$ to be the morphism [f, g](p) = gpf' given by the diagram below

$$\begin{array}{c} A \xrightarrow{p} C \\ f' & \downarrow g \\ B \xrightarrow{[f,g](p)} D \end{array}$$

and functoriality follows by pasting together such commuting squares.

We now show that PCM has a unity object.

Lemma 3. There exists an object $I \in Ob(\mathbf{PCM})$ such that $[I, A] \cong A$, for all $A \in Ob(PCM)$.

Proof. We define I to be the PCM with two elements $\{*, 0\}$. Note that the summation $\Sigma^{(I)}$ on I is uniquely determined by the PCM axioms, so $\Sigma^{(I)}\{*\} = *$ and $\Sigma^{(I)}\{\} = 0$. The isomorphism $i_A : A \to [I, A]$ is then given by, for all $a \in A$,

$$i_A(a)(x) = \begin{cases} a & x = * \\ 0 & x = 0 \end{cases}$$

It is immediate that *i* is a bijection — we now demonstrate that it preserves summation. Let $\{a_i\}_{i \in I}$ be an indexed family of *A*. By definition, $\{i_A(a_i)\}_{i \in I}$ is summable in [I, A] exactly when $\{a_i\}_{i \in I}$ is summable in *A*, in which case

$$\left(\Sigma_{i\in I}^{[I,A]}i_A(a_i)\right)(x) = \begin{cases} \Sigma_{i\in I}^{(A)}a_i & x=*\\ 0 & x=0 \end{cases}$$

and hence $\sum_{i \in I}^{[I,A]} i_A(a_i) = i_A\left(\sum_{i \in I}^{(A)} a_i\right)$. Hence $i : A \to [I, A]$ is indeed an isomorphism of PCMs.

Corollary 4.3. This family of isomorphisms i_A , $A \in Ob(\mathbf{PCM})$ are natural in A, and so form the components of a natural isomorphism $Id_{\mathbf{PCM}} \xrightarrow{\cong} [I, _]$.

Definition 4.4. For all $A \in Ob(\mathbf{PCM})$, we define $j_A \in \mathbf{PCM}(I, [A, A])$ by

$$j_A(x) = \begin{cases} id_A \in \mathbf{PCM}(A, A) & x = * \\ 0_{AA} & x = 0 \end{cases}$$

and this almost trivially gives the components of a natural transformation (note that 0_{AA} exists, since [A, A] is a PCM, as shown in the first Lemma above).

Finally, following Laplaza, we require a natural map $L_{ABC} : [B, C] \to [[A, B], [A, C]]$, representing composition: $L(g)(f) = g \circ f$. We must show that this is a morphism.

Suppose $\{g_j\}_{j\in J}$ is summable in [B, C]. We claim the family $\{L(g_j)\}_{j\in J}$ is summable in [[A, B], [A, C]]. Hence we must show: if $\{f_i\}_{i\in I}$ is summable in [A, B] then $\{g_j \circ f_i\}_{j\in J, i\in I}$ is summable in [A, C], i.e. that $\sum_{j\in J} (\sum_{i\in I} g_j \circ f_i)$ exists. This latter means: for any summable family $\{x_k\}_{k\in K}$, the family $\{(g_j \circ f_i)(x_k)\}_{j\in J, i\in I, k\in K}$ is summable in C.

Let us break this down into steps. We introduce the notation $\sum_{J,I}(g_j \circ f_i)$ for $\sum_{i \in J} (\sum_{i \in I} g_j \circ f_i)$.

- 1 Let us show for each $j \in J$, $\sum_{i \in I} g_j \circ f_i$ exists (in [A, C]). So suppose $\{x_k\}_{k \in K}$ is summable in A, i.e. $\sum_k x_k$ exists. Then since $\{f_i\}_{i \in I}$ is summable, the sum $\sum_{I,K} f_i(x_k)$ exists. But g_j is a morphism, so $g_j(\sum_{I,K} f_i(x_k)) = \sum_{I,K} g_j(f_i(x_k))$ exists. Hence each sum $\sum_{i \in I} g_j \circ f_i$ exists, for any $j \in J$.
- 2 Consider the family of sums $\{\sum_{i\in I} g_j \circ f_i\}_{j\in J}$. We must show it is summable (over J). This means whenever $\{x_k\}_{k\in K}$ is summable in A, that we must show $\sum_{J,K} (\sum_I (g_j \circ f_i)(x_k)) = \sum_{J,K} (\sum_I (g_j (f_i(x_k))))$ exists. But since the families $\{f_i\}_{i\in I}$ and $\{g_j\}_{j\in J}$ are summable, then $\sum_{J,K} ((g_j (\sum_I f_i(x_k))))$ exists. But the g_j s are morphisms, so this equals $\sum_{J,K} (\sum_I (g_j (f_i(x_k))))$, which is what we want.

It is easy to verify the diagrams in Laplaza (Laplaza 1977) trivially commute (pointwise), thus we obtain what he calls a *formally closed category* structure. Finally, Laplaza defines a *closed category* in the sense of Eilenberg-Kelly as one for which the natural map $\mathbf{PCM}(A, B) \longrightarrow \mathbf{PCM}(I, [A, B])$ given by $f \mapsto [id_A, f] \circ j_A$ is an isomorphism. This is the case here; indeed, it is easily seen that $[id_A, f] \circ j_A = i_{[A,B]}(f)$, for any $f \in \mathbf{PCM}(A, B)$.

5. Categories carrying Σ -structures

Motivated by a definition of (Manes, Arbib 1986), p.75 for partially additive monoids, we consider categories where there is a partial summation on hom-sets, compatible with composition.

Definition 5.1. Let \mathcal{C} be a category. A **PCM-structure on** \mathcal{C} is an assignment, for all objects $X, Y \in Ob(\mathcal{C})$, of a partial summation $\Sigma^{(X,Y)}$ on indexed families of $\mathcal{C}(X,Y)$, such that $(\mathcal{C}(X,Y), \Sigma^{(X,Y)})$ is a PCM. This assignment is required to satisfy the left and right distributive laws :

— for all summable $\{g_j\} \subseteq \mathcal{C}(Y, Z)$ and $f \in \mathcal{C}(X, Y)$, then $\{g_j f\}_{j \in J}$ is summable and

$$\left(\sum_{j\in J}^{(Y,Z)} g_j\right) \circ f = \sum_{j\in J}^{(X,Z)} (g_j \circ f)$$

— for all summable $\{f_i\}_{i \in I} \subseteq \mathcal{C}(X, Y)$ and $g \in \mathcal{C}(Y, Z)$, then $\{gf_i\}_{i \in I}$ is summable, and

$$g \circ \left(\sum_{i \in I}^{(X,Y)} f_i\right) = \sum_{i \in I}^{(X,Z)} (g \circ f_i)$$

We say that C carries a PCM-structure, and make similar definitions for categories carrying various Σ -structures (e.g. Σ -groups, Σ -monoids, PAMs, &c.). Although the Σ structure assignment to the hom-sets need not be unique, in practice we do not consider distinct Σ -structures on the same hom-set. We also omit the superscripts on Σ for clarity and refer to the Σ -structure ($C(X, Y), \Sigma$).

Note that the above definition does not require an explicit description of the category of PCMs (or PAMs, Σ -monoids, &c.) or its monoidal structure. However, when a category S of Σ -structures has a suitable monoidal tensor, there is a close connection with the theory of categorical enrichment (Definition 7.1). We consider this further in Section 7.

We also consider functors between categories carrying PCM-structures, and monoidal tensors on such categories. This is in the general setting of the structure of the category of all categories carrying PCM-structures, and is postponed until Section 14.

6. Examples of categories carrying Σ -structures

We now give examples of various categories that carry Σ -structures (i.e. their homsets have the appropriate Σ -structure and composition distributes over summation as in Definition 5.1). We also indicate their consistency, or otherwise, with the various axioms from Section 3. In what follows, keeping with usual tradition of summation theory, we restrict ourselves to Σ structures with countably-indexed families.

Example 6.1. (Relations, Partial functions, partial injections)

- 1 The category of relations (**Rel**, \uplus) has sets as objects, relations between sets (with the usual relational composition) as arrows, and disjoint union as monoidal tensor. Any (countable or otherwise) set of arrows $\{R_i : X \to Y\}_{i \in I}$ has a sum, given by set-theoretic union, and basic set theory demonstrates that **Rel** carries a Partially Additive Monoid structure.
- 2 The subcategory of **Rel** of partial functions, (**pFun**, \uplus), has the same objects as **Rel**, partial functions as arrows, and again disjoint union as monoidal tensor. A family $\{f_i : X \to Y\}_{i \in I}$ is summable when $dom(f_i) \cap dom(f_j) = \emptyset$ for all $i \neq j$, in which case $(\sum_{i \in I} f_i)(x) = \begin{cases} f_j(x) & x \in dom(f_j) \\ \bot & \text{otherwise} \end{cases}$. We refer to (Manes, Arbib 1986) for a detailed study of this category, including the fact that it carries a Partially Additive Monoid structure.

- 3 An important subcategory of (**pFun**, \oplus) is the category **pInj** of partial injections. This again has sets as objects, with arrows restricted to partial functions that are injective on their domains. The monoidal tensor is once again disjoint union, and a family $\{f_i : X \to Y\}_{i \in I}$ is summable when $dom(f_i) \cap dom(f_j) = \emptyset = im(f_i) \cap im(f_j)$ for all $i \neq j$, in which case the sum is the same as for **pFun**. We refer to (Haghverdi 2000) for a proof that **pInj** carries a Σ -monoid structure, (Hines 1997) for a study of this category, and (Lawson 1998) for the algebraic theory of inverse semigroups – the endomorphism monoids of this category.
- 4 We may also consider the subcategory **Bij** of (**pInj**, \uplus) of global bijections between sets. However, in this case, the only summable families are the singleton sets, and hence it does *not* carry any Σ structure (as the empty set is not summable).

We now present a number of examples based on Banach and Hilbert spaces. Because of the required connection with matrix representations (see Section 8) we use the direct sum as monoidal tensor in each case.

Definition 6.2. (Banach spaces, direct sums, inner products, Hilbert Spaces)

Let I be a countable (i.e. finite or denumerable) index set. Let $\{B_i\}_{i\in I}$ be a family of *Banach spaces* (i.e. complete normed vector spaces). The *direct sum* of a countably indexed family of Banach spaces $\{B_i\}_{i\in I}$ is the vector space whose elements are functions $x: I \to \biguplus_{i\in I} B_i$ satisfying

$$\begin{array}{ccc} 1 & x(i) \in X_i \\ 2 & \sum \| x(i) \| \end{array}$$

 $2 \quad \sum_{i \in I} \|x(i)\|_{X_i} < \infty$

under componentwise addition and scalar multiplication, with norm given by 2. above. We refer to (Brown, Page 1970) for the theory of Banach Spaces. Categorically, finite direct sums are biproducts.

Given a vector space V over \mathbb{C} , an *inner product* is a Hermitian symmetric form (i.e. a map $\langle _|_\rangle : V \times V \to \mathbb{C}$ that is linear in the first variable and conjugate-linear in the second) satisfying $\langle x|x \rangle \geq 0$ and $\langle x|x \rangle = 0$ iff x = 0. A complex Hilbert Space is then a Banach space over \mathbb{C} whose norm is defined by an inner product, $||x|| = (\langle x|x \rangle)^{\frac{1}{2}}$.

By the Reisz representation theorem (Hartig 1983), for every bounded linear map $L: H \to K$ of Hilbert spaces, there exists a unique bounded linear map $L^*: K \to H$ such that, for all $k \in K$ and $h \in H$,

$$k|L(h)\rangle = \langle L^*(k)|h\rangle$$

This is called the **Hermitian adjoint** of L, and is often denoted by either L^{\dagger} (quantummechanical notation) or L^{H} (functional-analysis notation).

We refer to (Halmos 1958) for the abstract theory of Hilbert spaces, including the definition of the direct sum of an indexed family of Hilbert spaces : Given an indexed family of Hilbert spaces, $\{H_i\}_{i \in I}$, the direct sum $\bigoplus_{i \in I} H_i$ has elements given by functions $\alpha : I \to \biguplus_{i \in I} H_i$ such that $\alpha(i) \in H_i$, and $\sum_{i \in I} \|x_i\|_{H_i}^2 < \infty$. exists. The inner product of two elements $\alpha, \beta \in \bigoplus_{i \in I} H_i$ is then given by $\langle \alpha | \beta \rangle = \sum_{i \in I} \langle \alpha(i) | \beta(i) \rangle$.

When the index set I is the natural numbers, this implies that a member of $\oplus^{\omega} X$ may be written as (x_0, x_1, x_2, \ldots) where $\sum_{i=0}^{\infty} ||x_i||^2$ exists. By the triangle inequality,

 $\sum_{i=0}^{\infty} x_i$ exists, and this implies that Hilbert spaces with direct sum as monoidal tensor have *countable codiagonal* maps $\oplus^{\omega} X \to X$, given by $(x_0, x_1, \cdots) \mapsto \Sigma_i x_i$.

The following categories carry Σ -structures :

Example 6.3. (Analytic examples: Banach and Hilbert spaces)

We restrict ourselves to *separable* Banach and Hilbert spaces in all the following examples. We also take the direct sum \oplus as the monoidal tensor in each case.

- 1 The category **Ban** has Banach spaces as objects and bounded linear maps as arrows.
- 2 The subcategory **cBan** of **Ban** has the same objects, and *nonproper contraction maps* or *non-expansive maps* as arrows, i.e. linear maps L satisfying $||L(x)|| \le ||x||$.
- 3 The category **Hilb** has Hilbert spaces as objects and continuous (and hence bounded see (Brown, Page 1970)) linear maps as arrows.
- 4 The subcategory **cHilb** consists of Hilbert spaces and non-expansive contraction maps.
- 5 A partial isometry in **Hilb** is a linear map $L : X \to Y$ where $L^*L : X \to X$ and $LL^* : Y \to Y$ are projectors, called the *initial* and *terminal* projectors respectively. Given partial isometries $L : X \to Y$ and $M : Y \to Z$, it is well known (Erdelyi 1968) that the composite $ML \in \text{Hilb}(X, Z)$ is a partial isometry exactly when the terminal projector of L commutes with the initial projector of M. However, an associative composition on partial isometries is given in (Lawson 1998), and put into a categorical setting in (Braunstein, Hines 2007).

The category **pIsom** has the same objects as **cHilb**. An arrow $L \in \mathbf{cHilb}(X, Y)$ is an arrow of $\mathbf{pIsom}(X, Y)$ exactly when it is a partial isometry. The composition in **pIsom** is as follows:

Let $L : X \to Y$ and $M : Y \to Z$ be partial isometries with initial and terminal projectors E_L, F_L and E_M, F_M respectively. Their composite in **pIsom** is given by $M(E_M \wedge F_L)L$ where $E_M \wedge F_L$ is given by the 'infinite filter procedure' of (Shimony 1970) or (Jauch 1968) as $(E_M \wedge F_L) = \lim_{n\to\infty} (E_M F_L)^n$. By the properties of the meet in the lattice of projectors, $E_M \wedge F_L$ commutes with both E_M and F_L , as required. Note that when E_M commutes with F_L , this is exactly the usual composition of linear maps. We also refer to (Szymanski 1990) for a semigroup-theoretic perspective on partial isometries.

- 6 The category **uHilb** has Hilbert spaces as objects, and unitary maps (i.e. linear, innerproduct preserving isomorphisms) as arrows, with the usual composition. Unitary maps are trivially partial isometries, with (commuting) global identities as initial and terminal projectors, so **uHilb** is a subcategory of both **cHilb** and **pIsom**.
- 7 Another subcategory of both **pIsom** and **cHilb** is given by the image of Barr's ℓ_2 monoidal functor. Recall (Definition 6.1) the category **pInj** of sets and partial injections. This category is self-dual (**pInj**^{op} \cong **pInj**). In (Barr 1992) the following functor ℓ_2 : **pInj**^{op} \rightarrow **Hilb** is studied:
 - On objects: Given a set X, $\ell_2(X)$ is defined to be the set of all complex valued functions $a: X \to \mathbb{C}$ for which the sum $\sum_{x \in X} ||a(x)||^2$ is finite. It is immediate to verify

that this is a Hilbert space, with inner product given by $\langle b|a \rangle = \sum_{x \in X} b(x) \overline{a(x)}$ for all $a, b \in \ell_2(X)$.

— On arrows: Given a partial injection $f: X \to Y$ in **pInj**, then $l_2(f): \ell_2(Y) \to \ell_2(X)$ is defined by

$$\ell_2(f)(b)(x) = \begin{cases} b(f(x)) & x \in Dom(f) \\ 0 & \text{otherwise.} \end{cases}$$

— The monoidal tensor : Recall that the monoidal tensor of **pInj** is disjoint union. Note that the functor ℓ_2 satisfies, for objects X, Y,

$$\ell_2(X \uplus Y) = \ell_2(X) \oplus \ell_2(Y)$$

and for arrows $g: A \to B, C \to D$ in **pInj**,

$$\ell_2(f \uplus g) = \ell_2(f) \oplus \ell_2(g) \; .$$

This implies that $\ell_2(\mathbf{pInj}^{op})$ is a monoidal subcategory of **Hilb** and ℓ_2 is a monoidal functor. Observe that for arbitrary partial injections $f : X \to Y$ and $g : Y \to Z$, the images $\ell_2(f) : \ell_2(Y) \to \ell_2(X)$ and $\ell_2(g) : \ell_2(Z) \to \ell_2(Y)$ are partial isometries. However, as ℓ_2 is a faithful functor, the appropriate initial and terminal projectors commute, and so $\ell_2(\mathbf{pInj}^{op})$ is a subcategory of both **pIsom** and **cHilb**.

The category $\ell_2(\mathbf{pInj})$ is studied in (Haghverdi, Scott 2006) under the name **Hilb**₂ for its role in Geometry of Interaction, following Girard's original presentation of the Geometry of Interaction (Girard 1988). However, as this functor is faithful, the results of (Girard 1988) do not require C^* -algebras, and may be given entirely in terms of the algebra of partial injections on sets.

Finally, the ℓ_2 functor may also be applied to the subcategory **Bij** of global bijections between sets, yielding $\ell_2(\mathbf{Bij}^{op})$, as a subcategory of both **pIsom** and **uHilb**.

For all the spaces above, we may also consider the subcategories given by restricting the objects to **finite-dimensional** spaces. We denote these categories by a subscript $(-)_{\rm fd}$, for example $\operatorname{Vec}_{\rm fd}$, $\operatorname{Hilb}_{\rm fd}$, &c.

We may give the above inclusions (up to the isomorphism $\mathbf{pInj} \cong \mathbf{pInj}^{op}$) of subcategories diagrammatically:



Theorem 6.4.

- 1 The categories **Ban** and **Hilb** carry both strong Σ -group and PCM structures.
- 2 The categories **cHilb** and **cBan** carry PCM structures, but not strong Σ -group structures.

- 3 The categories $\ell_2(\mathbf{pInj})$ and \mathbf{pIsom} carry Σ -monoid structures.
- 4 The categories **uHilb** and $\ell_2(\mathbf{Bij})$ do not carry PCM structures.

Proof.

1 We present the proof for **Ban**; the proof for **Hilb** follows as a special case.

We first demonstrate that Banach spaces are PCMs. The proof that they are Σ -groups is found in (Higgs 1989) and we do not reproduce it here.

Let \mathcal{B} be a Banach space and, as in Definition 3.6, denote the set of arbitrarily indexed families of \mathcal{B} by $\mathcal{F}(\mathcal{B})$. We define a partial summation $\sum : \mathcal{F}(\mathcal{B}) \to \mathcal{B}$ by

- A countable family $\{x_i\}_{i \in I}$ is summable exactly when $\sum_{i \in I} ||x_i|| < \infty$ in \mathbb{R}^+
- Given that a family is summable, its sum in \mathcal{B} is the usual Banach space summation $\sum_{i \in I} x_i$.

It is trivial that the unary sum axiom holds. It is also almost immediate that \mathcal{B} is closed under this summation. For a summable family $\{x_i\}_{i\in I}$, the triangle inequality gives $\left\|\sum_{i\in I} x_i\right\| \leq \sum_{i\in I} \|x_i\|$. As Banach spaces are (by definition) complete, $\sum_{i\in I} \|x_i\| < \infty$ implies that $(\sum_{i\in I} x_i) \in \mathcal{B}$. Therefore the sum of any summable family is in \mathcal{B} . To show that this summation satisfies weak Partition-Associativity, we need to show that, for a countably indexed summable family $\{x_i\}_{i\in I}$ and partition $I = \{I_i\}_{i\in J}$:

- (a) $\{x_i\}_{i \in I_i}$ is summable for each $j \in J$
- (b) $\{\sum_{i \in I_j} x_i\}_{j \in J}$ is summable
- (c) $\sum_{i \in I} x_i = \sum_{j \in J} \left(\sum_{i \in I_j} x_i \right).$

We demonstrate these properties as follows:

- (a) As norms of elements of Banach spaces are non-negative reals, $\sum_{i \in I_j} ||x_i|| \leq \sum_{i \in I} ||x_i|| < \infty$ and so $\{x_i\}_{i \in I_j}$ is summable.
- (b)By the triangle inequality, $\left\|\sum_{i\in I_j} x_i\right\| \leq \sum_{i\in I_j} \|x_i\|$ and as J is a partition of I, we deduce that $\sum_{j\in J} \left(\sum_{i\in I_j} \|x_i\|\right) = \sum_{i\in I} \|x_i\|$, since all summands are non-negative real numbers. Therefore, $\sum_{j\in J} \left\|\sum_{i\in I_j} x_i\right\|$ is finite and so $\{\sum_{i\in I_J} x_i\}_{j\in J}$ is a summable family.
- (c) Given that both the left and right hand sides of this sum converge absolutely, and J is a partition of I, this is just the fact that absolutely convergent series may be reordered without affecting the result.

We have now shown that Banach spaces are PCMs. It is then a simple corollory that they also carry PCM structures :

A standard fact of linear algebra (as in (Brown, Page 1970)) is that the hom-set of linear maps $\{L : R \to S\}$ between Banach spaces R, S is itself a Banach space, with

norm given by the supremum norm

 $||L|| = \sup_{||r||=1} \{ ||L(r)|| \}$

We write this as $hom(R, S) \in Ob(Ban)$. This shows that hom(R, S) in **Ban** is a PCM. It is also immediate that composition of arrows distributes over summation, and our result follows.

2 We present the proof for **cBan**; the proof for **cHilb** again follows as a special case. Let \mathcal{B} be a Banach space, and let $Ball_{\mathcal{B}}$ denote the unit ball

$$Ball_{\mathcal{B}} = \{b \in \mathcal{B} : \|b\| \le 1\}$$

We define a partial summation $\sum : \mathcal{F}(Ball_{\mathcal{B}}) \to Ball_{\mathcal{B}}$ by

- A countable set $\{x_i\}_{i \in I}$ is summable exactly when $\sum_{i \in I} ||x_i|| \le 1$ in \mathbb{R}^+
- Given that a set is summable, its sum in $Ball_{\mathcal{B}}$ is the usual Banach space summation $\sum_{i \in I} x_i$.

To show that $Ball_{\mathcal{B}}$ is closed under this summation, note that for a summable family $\{x_i\}_{i\in I}$, the triangle inequality gives $\left\|\sum_{i\in I} x_i\right\| \leq \sum_{i\in I} \|x_i\|$, and the sum $\sum_{i\in I} x_i$ exists since Banach spaces are complete. However, by assumption, $\sum_{i\in I} \|x_i\| \leq 1$, so the sum of any summable family is in $Ball_{\mathcal{B}}$.

It is trivial that the unary sum axiom holds, since any $x \in Ball_{\mathcal{B}}$ satisfies $||x|| \leq 1$, so $\{x\}$ is summable, and $\sum\{x\} = x$. To show the weak (i.e. one-way) Partitionassociativity axiom holds, for a countable summable family $\{x_i\}_{i \in I}$ and partition $I = \{I_i\}_{i \in J}$, we need:

- (a) $\{x_i\}_{i \in I_i}$ is summable for each $j \in J$
- (b) $\{\sum_{i \in I_j} x_i\}_{j \in J}$ is summable
- (c) $\sum_{i \in I} x_i = \sum_{j \in J} \left(\sum_{i \in I_j} x_i \right).$

To show (a), the definition of summability gives that $\sum_{i \in I} ||x_i|| \le 1$, and as norms of elements of Banach spaces are non-negative reals,

$$I_j \subseteq I \Rightarrow \sum_{i \in I_j} \|x_i\| \le \sum_{i \in I} \|x_i\| \le 1$$

Hence $\{x_i\}_{i \in I_j}$ is summable. To show (b), note that by the triangle inequality,

$$\left|\sum_{i\in I_j} x_i\right| \leq \sum_{i\in I_j} \|x_i\|$$

and as J is a partition of I,

$$\sum_{j \in J} \left(\sum_{i \in I_j} \|x_i\| \right) = \sum_{i \in I} \|x_i\| \text{ since } \|b\| \in \mathbb{R}^+ \quad \forall \ b \in Ball_{\mathcal{B}}$$

Therefore,

$$\sum_{j \in J} \left\| \sum_{i \in I_j} x_i \right\| \leq \sum_{i \in I} \|x_i\| \leq 1$$

So the family $\{\sum_{i \in I_j} x_i\}_{j \in J}$ is summable. Part **c**) follows trivially, since the summability condition $\sum_{i \in I} ||x_i|| \leq 1$ implies uniform convergence in complete normed linear spaces. Hence $(Ball_{\mathcal{B}}, \sum)$ is a PCM.

Finally, recall from part 1. above that $hom(R, S) \in Ob(\mathbf{Ban})$. The unit ball on this space, $Ball_{hom(R,S)}$ is exactly the set of nonproper contraction maps, by definition of the supremum norm—and we have seen that unit balls are PCMs. This shows that hom(R, S) in **cBan** is a PCM. The distributivity of composition over summation also follows from part 1. above.

Note that neither **cHilb** nor **cBan** carry Σ -group structures; the definition of Σ groups calls for the summability of all finite families: as a counterexample, consider two identity maps $\{I_B, I_B\}$ on a Banach space. Then $||I_B + I_B|| = 2$, so $I_B + I_B$ is not a contraction!

3 The proof that $\ell_2(\mathbf{pInj}^{op})$ carries a Σ -monoid structure follows from the fact that ℓ_2 is an embedding of \mathbf{pInj}^{op} into **cHilb** — note that the condition for summability in \mathbf{pInj} , namely:

A family $\{f_i\}_{i \in I}$ is summable exactly when, for all $i \neq j$,

$$- dom(f_i) \cap dom(f_j) = \emptyset$$

$$- im(f_i) \cap im(f_j) = \emptyset$$

becomes the condition

- A family $\{L_i\}_{i \in I}$ is summable exactly when, for all $i \neq j$,
- The initial projectors E_i and E_j of L_i and L_j satisfy $E_i E_j = 0 = E_j E_i$
- The terminal projectors F_i and F_j of L_i and L_j satisfy $F_iF_j = 0 = F_jF_i$

A proof that **pIsom** carries a Σ -monoid structure is to be found in (Braunstein, Hines 2007). This relies on the fact that **pIsom** is an *inverse category* with zero arrows.

4 Any Σ -structure on hom-sets of a category implies the existence of zero arrows between objects (given by the summation of the empty set), and neither **uHilb** nor $\ell_2(\mathbf{Bij})$ admit zero arrows. Also, we cannot artifically adjoin zero elements; observe that doing this to $\ell_2(\mathbf{Bij})$ will generate the whole of $\ell_2(\mathbf{pInj})$, since every partial injection may be thought of as the direct sum of total bijections and zero arrows.

7. Categories carrying Σ -structures and categorical enrichment

The notion of a Σ -structure on a category, or (in our terminology) a category carrying a Σ -structure, is based on a construction of (Manes, Arbib 1986) for Partially Additive Monoids. In certain cases, there is a very close connection with the categorical notion of enrichment, as described below. However, the connection, when it exists, depends on the existence of a suitable monoidal tensor on the relevant category of Σ -structures.

7.1. Enriched Category theory

Many interesting categorical structures arise when the hom-sets of one category are objects in some monoidal category. This the general area of enriched category theory, and the following definitions and diagrams (with minor notational differences) are taken directly from (Kelly 1982).

Definition 7.1. Enriched categories

Let $(V, I, \otimes, \alpha, l, r)$ be a monoidal category. A **category enriched over** V, or V-**category**, C consists of :

- a set Ob(C) of objects,
- for each pair $X, Y \in Ob(C)$, a **hom-object** $C(X, Y) \in Ob(V)$
- for each triple $X, Y, Z \in Ob(C)$, a composition law, i.e. a V-arrow

$$M = M_{X,Y,Z} : C(X,Y) \otimes C(Y,Z) \to C(X,Z)$$

— for each object X, an identity element in $V, j_X : I \to C(X, X)$.

These are required to satisfy the **associativity axiom**, and the **unit axioms**, given by the commutativity of the following diagrams :

and

(We have omitted subscripts on canonical morphisms, for readability). We also refer to (Kelly 1982) for the natural notion of a V-functor between V-enriched categories, as a functor that preserves the V-enrichment.

7.2. Enrichment over Σ -structures

Definition 7.2. Let S be some category of Σ -structures (e.g. PCM, PAM, or similar). Given $A, B, C \in Ob(\mathcal{C})$, a map $\Psi : A \times B \to C$ is called **2-additive** (following terminology of (Manes, Arbib 1986)) when, for all $a \in A$ and $b \in B$, the maps $\Psi_a : B \to C$ and $\Psi_b : A \to C$ defined by

$$\Psi_a(y) = \Psi(a, y) \quad , \quad \Psi_b(x) = \Psi(x, b)$$

are both arrows of C (i.e. summation-preserving functions). Now let $\otimes : S \times S \to S$ be a monoidal tensor on this category. We say that \otimes is a **tensor product** when it satisfies the following universal property :

There exists a 2-additive map $\Phi : A \times B \to A \otimes B$ such that for all 2-additive maps $\Psi : A \times B \to C$, there exists a unique morphism $\Psi' \in \mathcal{C}(A \otimes B, C)$ such that the following

diagram commutes



A tensor product can therefore be characterised as setting up a bijection between 2additive maps $\Psi : A \times B \to C$ and (sum-preserving) morphisms $\Psi' : A \otimes B \to C$. We emphasise that this is a very strong condition on the monoidal structure, and certainly is not satisfied in all cases (it is simple to check that neither the product nor the coproduct of PCMs given in Section 4.2 satisfies this property).

A tensor product \otimes on S satisfying the above universal property allows us to deduce that a category carrying an S-structure in the sense of Definition 5.1 is in fact a category enriched over (S, \otimes) , as in Definition 7.1.

Unwinding the above definitions of S-enrichment, a category C is S-enriched, if each homset C(X, Y) is an object of S (i.e. has a partial summation on indexed families satisfying the S axioms) satisfying the appropriate conditions. In particular, composition $C(X, Y) \otimes C(Y, Z) \xrightarrow{M} C(X, Z)$ is an S-morphism, (i.e. it preserves sums of summable families). Writing M(f, g) as $g \circ f$, as usual, this translates to the following:

- Each homset has a partial summation on indexed families that makes $\mathcal{C}(X, Y)$ an object of \mathcal{S} (in particular, there is a zero morphism $0_{XY} \in \mathcal{C}(X, Y)$).
- For summable families $\{f_i\}_{i\in I} \in \mathcal{C}(X,Y)$ and $\{g_j\}_{j\in J} \in \mathcal{C}(Y,Z)$, by the universal property of the tensor product, the family $\{(g_j \circ f_i)\}_{(j,i)\in J\times I}$ is summable and moreover

$$(\sum_{j \in J} g_j) \circ (\sum_{i \in I} f_i) = \sum_{(j,i) \in J \times I} (g_j \circ f_i) = \sum_{J,I} (g_j \circ f_i)$$
(1)

We also assume the unary sum axiom. This states that $\sum \{f\} = f$ for arbitrary arrows of \mathcal{C} . Hence, as a special case of (1) above, we have: for any arrows $f \in \mathcal{C}(X,Y)$ and $g \in \mathcal{C}(Y,Z)$, and summable families $\{f_i\}_{i \in I}$ and $\{g_j\}_{j \in J}$,

$$\sum_{j \in J} g_j) \circ f = \sum_{j \in J} (g_j \circ f) \tag{2}$$

$$g_{\circ}(\sum_{i \in I} f_i) = \sum_{i \in I} (g_{\circ} f_i)$$
(3)

The only assumptions we make on S are the existence of zero arrows and the unary sum axiom (and, of course, the existence of a suitable tensor product). When a category S does have a tensor product, the notion of 'categories with S-structure' due to (Manes, Arbib 1986) is then exactly the notion of 'enrichment over (S, \otimes) ', as found in (Kelly 1982).

Proposition 7.3. The following categories have tensor products :

1 Ab, the category of abelian groups and group homomorphisms.

- 2 **PAM**, the category of partial additive monoids.
- 3 Hilb and Ban, the categories of Hilbert of Banach spaces, and bounded linear maps (considered as subcategories of **PCM**).
- 4 **cHilb** and **cBan**, the categories of linear contraction maps on Hilbert or Banach spaces.

Proof.

- 1 This is a canonical example of enrichment, given in (Kelly 1982).
- 2 The existence of such a tensor product is is proved in (Bahamonde 1985), although an explicit description of the tensor product of PAMs is not given. This proof is based on a free PAM construction that relies on the limit axiom, and hence is not applicable to either **PCM** or Σ **Mon**.
- 3 The objects and hom-sets of **Hilb** and **Ban** have been shown to be PCMs. By forgetting about additional structure, we may consider them as subcategories of **PCM**. The usual tensor product ⊗ on Hilbert spaces then satisfies the above condition for a categorical tensor product. For Banach spaces, there are many different tensor products (we refer to (Ryan 2002) for a good exposition) — however the *projective tensor* (for example) described in this reference satisfies the required properties.
- 4 We have also seen that objects and arrows of **cHilb** and **cBan** are PCMs. We observe that the tensor product of two contraction maps is also a contraction map. Hence the usual tensor product \otimes of Hilbert spaces is a tensor product on **cHilb**, and the projective tensor is a tensor product on **cBan**, considered as subcategories of **PCM**.

We now demonstrate abstractly that the category **PCM** also has a tensor product. We will use (a corollary of) the special adjoint functor theorem to demonstrate that the internal hom functor [A, -] exhibited in Section 4.1 has a left adjoint (i.e. has a monoidal tensor on PCM) that makes **PCM** monoidal closed, in the sense above, and this monoidal tensor is a tensor product, as in Definition 7.2.

Proposition 7.4. In **PCM**, the internal hom [A, -] has a left adjoint $A \otimes -$, and this is a tensor product in the sense of Definition 7.2.

Proof.

- The existence of the left adjoint (Sketch) Observe that PCM is complete (by Proposition 4.2) and is locally small. Also note that I (the unity object) is a cogenerator, by the same argument as in the category of sets. Finally, [A, -] is continuous; so by the Corollary of the Special Adjoint Functor Theorem 2 ((MacLane 1998), Chap. V (8)), it has a left adjoint $A \otimes -$.
- \otimes is a tensor product As we have established monoidal closure,

 $Hom(A \otimes B, C) \cong Hom(A, [B, C])$

By definition of the internal hom, the term on the rhs (that is, Hom(A, [B, C])) is the set of maps that are 2-linear, in both A and B. Hence by the above bijection, $A \otimes B$ classifies maps that are 2-linear. By taking $C = A \otimes B$, it is immediate that the

canonical map $A \times B \to A \otimes B$ is 2-linear, and hence the required universal property holds.

Remark 7.5. Further work on the properties of such tensor products, including an explicit description of the tensor product of two PCMs, is currently being pursued with Tim Porter (Bangor).

Terminology Although we have established that the Manes-Arbib notion of, 'a category with a PCM-structure' is exactly the usual categorical notion of, 'a category enriched over $(\mathbf{PCM}, \otimes)^{2}$, we will use the Manes-Arbib terminology for the remainder of the paper.

8. Categories carrying Σ -structures, and matricial representations

In order to use Σ -structures on categories to provide a categorical trace based on iteration (the particle-style trace), we also need a notion of *matrix representation* of arrows. For a number of examples, matrices may be given in terms of quasi-projections and quasiinclusions (see (Haghverdi 2000; Manes, Arbib 1986)). In what follows, we write the monoidal tensor as \oplus :

Definition 8.1. (quasi- projections & inclusions, Σ -matrix categories, UDCs) We say that a category carrying a Σ -structure has quasi-projections and quasi-inclusions when, for any object $\bigoplus_{i=1}^{n} X_i$, there exist quasi-projection and quasi-inclusions arrows

$$\pi_k: \oplus_{i=1}^n X_i \to X_k \quad , \quad \iota_k: X_k \to \oplus_{i=1}^n X_i$$

satisfying $\sum_{i=1}^{n} \iota_i \pi_i = 1_{\bigoplus_{i=1}^{n} X_i}$ and $\pi_i \iota_j = \begin{cases} 1_{X_i} & i = j \\ 0 & \text{otherwise.} \end{cases}$ Similarly, in the presence of infinitary monoidal tensors, $X = \bigoplus_{i=1}^{\infty} X_i$, we make the natural definition of infinitary quasi-projections and quasi-inclusions.

A Σ -matrix category, or Σ MC is a symmetric monoidal category (\mathcal{C}, \oplus) that carries a PCM structure, and has quasi-projections and quasi-inclusions.

In the special case where the category carries a Σ -monoid structure, this gives a Unique Decomposition Category, or a UDC. We refer to (Haghverdi 2000) for the full theory of UDCs, together with computational interpretations. Grouplike Decomposition Cate*gories* or *GDCs* are defined analogously to *UDCs*, using strong Σ -groups, rather than Σ -monoids.

Proposition 8.2. Matrix representations of arrows

Let $X = \bigoplus_{i=1}^{n} X_i$ and $Y = \bigoplus_{j=1}^{m} Y_j$ be objects in a Σ MC. Then any arrow $f: X \to Y$ has a decomposition as $\{f_{ij}: X_j \to Y_i\}_{i=1..n,j=1..m}$, where f_{ij} is given by $f_{ij} = \pi_i f_{ij}$: $X_j \to Y_i$. This decomposition may be written in matrix form as

$$f = \begin{pmatrix} f_{11} & f_{12} & \dots & f_{1n} \\ f_{21} & f_{22} & \dots & f_{2m} \\ \dots & & & \dots \\ f_{m1} & f_{m2} & \dots & f_{mn} \end{pmatrix}$$

and composition of arrows in this form is given by the familiar formula for matrix multiplication $(gf)_{ki} = \sum_{j=1}^{m} g_{kj} f_{ji}$.

Proof. We refer to (Haghverdi 2000) for the proof of this result for Unique Decomposition Categories, along with questions of existence and uniqueness, and observe that this proof does not require the Partition-Associativity axiom. Hence it is also applicable to arbitrary categories carrying Σ -structures that also have quasi-projections and quasi-inclusions.

We also have the following result connecting matrix representations and summation :

Proposition 8.3. Let $\{F^{(a)}: X \to Y\}_{a \in A}$ be an indexed family of arrows in a ΣMC , where

$$X = \bigoplus_{i=1}^{n} X_i$$
 and $Y = \bigoplus_{j=1}^{m} Y_j$

giving matrix representations for each $F^{(a)}$ as

$${f_{ij}^{(a)}: X_j \to Y_i}_{i=1..n, j=1..m}$$

Then

$$\{F^{(a)}\}_{a \in A}$$
 is summable $\Rightarrow \{F^{(a)}_{ij}\}_{a \in A}$ is summable $\forall i, j$

However, the reverse implication does not hold.

Proof. Assume that $\{F^{(a)} : X \to Y\}_{a \in A}$ is summable, so $\sum_{a \in A} F^{(a)}$ exists. Then $\pi_i \left(\sum_{a \in A} F^{(a)}\right) \iota_j$ exists and by the distributivity of composition over summation, $\sum_{a \in A} \left(\pi_i F^{(a)} \iota_j\right)$ exists. Therefore, $\{f_{ij}^{(a)} = \pi_i F^{(a)} \iota_j\}_{a \in A}$ is summable. To show that the converse does not hold, we present 2 examples :

1 (an arbitrary ΣMC) In the category of contraction maps on Hilbert spaces, the matrices $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ are both contraction maps, and are componentwise-summable. However,

$$\left(\begin{array}{cc}1&0\\0&1\end{array}\right)+\left(\begin{array}{cc}0&1\\1&0\end{array}\right)=\left(\begin{array}{cc}1&1\\1&1\end{array}\right)$$

which is not a contraction map.

2 (a UDC) Let X be an object in **pInj**, and let $M : X \to X$ be an isomorphism. Then $\begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix}$ and $\begin{pmatrix} 0 & M \\ M & 0 \end{pmatrix}$ are both (global) bijections; however, global bijections are not summable in **pInj**.

8.1. Partially Additive Categories

A computationally important subclass of UDCs (and hence Σ MCs) are the *Partially* Additive Categories, or PACs, of (Manes, Arbib 1986). These are computationally important in that they are guaranteed to have a *particle-style trace* (Section 9), and this

may be defined in terms of the Elgot Dagger (Section 10.1). The Elgot dagger is the taken as the definition of a *While* loop in (Manes, Arbib 1986), and this gives a flowchart interpretation of the particle-style trace, as used in Section 10.

Definition 8.4. Let (\mathcal{C}, \oplus) be symmetric monoidal category carrying a PAM structure ((Definition 3.4) that has quasi-projections and quasi-injections. (\mathcal{C}, \oplus) is called a *Partially Additive Category* when it satisfies the following axioms:

- *countable coproducts:* The monoidal tensor \oplus is a coproduct, and C has countable coproducts.
- compatible sum axiom: Let $\{f_i : X \to Y\}_{i \in I}$ be a countable family where there exists $f : X \to \bigoplus_{i \in I} Y$ such that if



commutes, then $\sum_{i \in I} f_i$ exists.

— untying axiom: If $(f+g): X \to Y$ exists, then so does $\iota_1 f + \iota_2 g: X \to Y + Y$

For numerous examples of PACs, we refer to (Manes, Arbib 1986) and (Haghverdi 2000).

8.2. Matrix representations without quasi-projections/inclusions

Observe that a category may have matrix representations for arrows, even though it does not have quasi-projections and quasi-inclusions. In this case, the entries of the matrix are arrows from another category (a canonical example being (\mathbf{uHilb}, \oplus) — unitary maps certainly have matrix representations, but the matrix components are not themselves unitary maps). We formalise this situation as follows:

Definition 8.5. Matrix representations

Let (\mathcal{C}, \oplus) be an arbitrary category, and let $(\mathcal{W}, \oplus, \Sigma)$ be a Σ MC. We say that (\mathcal{C}, \oplus) has **matrix representations in** (\mathcal{W}, \oplus) when there exists a faithful strict monoidal functor $\Gamma : (\mathcal{C}, \oplus) \to (\mathcal{W}, \oplus)$. It is immediate that every arrow $f : \bigoplus_{i=1}^{n} X_i \to \bigoplus_{j=1}^{m} Y_j$ has a representation as a matrix $[f_{ij}]_{i=1..n,j=1..m}$ of arrows in \mathcal{W} , and for all $X, Y \in Ob(\mathcal{C})$, the matrix representation of $1_X \oplus 1_Y$ is $\begin{pmatrix} \Gamma(1_X) & 0 \\ 0 & \Gamma(1_Y) \end{pmatrix}$.

When the functor Γ is the inclusion functor for some monoidal subcategory (\mathcal{C}, \oplus) of a Σ -matrix category $(\mathcal{W}, \oplus, \Sigma)$ we abuse notation, and elide the inclusion functor. Hence, we may write, for example, $1_X \oplus 1_Y = \begin{pmatrix} 1_X & 0 \\ 0 & 1_Y \end{pmatrix}$, with the understanding that the matrix entries are taken from \mathcal{W} rather than from \mathcal{C} .

Proposition 8.6. The category $(\operatorname{Bij}_{fin}, \uplus)$ of bijections on finite sets has matrix representations within $(\operatorname{pInj}, \uplus)$.

Proof. This is immediate from the definitions of **Bij** and **pInj**. We present the example \mathbf{Bij}_{fin} , rather than **Bij**, due to an interesting connection with the categorical trace (Proposition 9.6).

9. The particle-style Trace

A *particle-style* or *iterative Trace* is a categorical trace defined in terms of PCM-structures on categories, and matrix representations of arrows. We first present the iterative trace for UDCs, as decribed in (Haghverdi 2000), and demonstrate that it is equally applicable in a more general setting.

Theorem 9.1. The particle-style trace on UDCs

Let (\mathcal{C}, \oplus) be a UDC, where, for all objects X, Y, U and arrows $F = \begin{pmatrix} a & b \\ c & d \end{pmatrix} : X \oplus U \to Y \oplus U$, the sum $a + \sum_{i=0}^{\infty} bd^i c$ exists. Then \mathcal{C} is traced, with the categorical trace given by

$$Tr^U_{X,Y}(F) = a + \sum_{i=0}^{\infty} bd^i c$$

We refer to this trace as the **iterative** or **particle-style trace** of C.

Proof. We refer to (Haghverdi 2000) — alternatively, Theorem 9.3 considers this result in a more general setting. \Box

Corollary 9.2. Let (\mathcal{C}, \oplus) be a partially additive category. Then (\mathcal{C}, \oplus) is a traced monoidal category, with trace given by the iterative trace formula.

Proof. We refer to (Haghverdi 2000) for a demonstration that the PAC axioms imply the existence of the above summation – this is also implicit from the construction of the iterative trace from the Elgot dagger (Manes, Arbib 1986), given in Section 10.1. \Box

In order to use the iterative trace in a more general setting, we demonstrate the minimal conditions for a categorical trace:

Theorem 9.3. the general iterative trace Let (\mathcal{C}, \oplus) be a category carrying a Σ structure, with matrix representations given by an inclusion into a Σ MC, where for all $F = \begin{pmatrix} a & b \\ c & d \end{pmatrix} : X \oplus U \to Y \oplus U \text{ the sum } a + \sum_{i=0}^{\infty} bd^i c \text{ exists. Then } \mathcal{C} \text{ is traced, with}$ the categorical trace given by

$$Tr^U_{X,Y}(F) = a + \sum_{i=0}^{\infty} bd^i c$$

We refer to this trace as the **particle-style trace** of C.

Proof. We postpone the proof of this result to Appendix A. The proof presented is based on a close analysis, and graphical interpretation, of the proof given in (Haghverdi 2000) for UDCs. \Box

9.1. Examples

The following *UDCs* have an iterative trace :

- -- (**Rel**, \uplus), the category of relations with disjoint union. This is also a PAC -- however, observe that the all families are summable, so we are immediately guaranteed the existence of the iterative trace summation.
- (**pFun**, \uplus), the category of partial functions with disjoint union. This is a PAC, and so is guaranteed to have an iterative trace.
- A closely related example is $(\mathbf{pFun}_D, \uplus)$, where D is an arbitrary fixed set. This category has sets as objects, and an arrow from X to Y is a partial function from $X \times D$ to $Y \times D$. The proof that this is a PAC (and hence traced) is almost identical to that for **pFun**.
- (pInj, ⊎), the category of partial injections, with disjoint union. This is a UDC, but not a PAC. However, the required summation always exists — we refer to (Hines 1997; Haghverdi 2000; Abramsky et. al. 2002) for proofs of this fact.
- -- $(\ell_2(\mathbf{pInj}), \oplus)$, the image of \mathbf{pInj} under Barr's ℓ_2 functor also has an iterative trace. This follows from the fact that $\ell_2 : \mathbf{pInj} \to \mathbf{Hilb}$ is a faithful monoidal functor of Σ -matrix categories.
- SRel, the category of stochastic relations. The objects of SRel are measurable spaces (X, \mathcal{F}_X) and maps $f: (X, \mathcal{F}_X) \to (Y, \mathcal{F}_Y)$ are stochastic kernels (i.e. functions $f: X \times \mathcal{F}_Y \to [0, 1]$ that are bounded measurable in the first variable and subprobability measures in the second). Composition is given by $g \circ f(x, C) = \int_Y g(y, C) f(x, dy)$ where $f(x, _)$ is the measure for integration. A family $\{f_i\}_{i \in I}$ is summable exactly when $\sum_{i \in I} f_i(x, Y) \leq 1$, $\forall x \in X$. We refer to (Haghverdi 2000) for more details, and a proof that this is a PAC (and hence traced).

Note that all the above examples are UDCs.

To deal with Σ MCs generally, we require a theory of *partial traces* (however, we present an example of a UDC that has a partial, but not total, trace in Proposition 9.8).

9.2. Partiality and the iterative trace formula

From its description in terms of a summation, there is the possibility that the iterative trace formula is not globally defined, but 'converges' on a certain subclass of arrows. Alternatively, the sum may be defined, but only within some 'larger' category. This would seem particularly applicable to the 'analytic examples' of Example 6.3. To accommodate this, we need a theory of *partial traces*, and the notion of a category being 'traced within another category'.

Definition 9.4. Partial categorical traces, one category traced within another Given a symmetric monoidal category (\mathcal{C}, \otimes) , together with a family of partial functions

$$Tr^U_{A,B}: \mathcal{C}(X \otimes U, Y \otimes U) \to \mathcal{C}(X,Y)$$

we say that $Tr_{A,B}^U$ is a **partial categorical trace** when it satisfies the following axioms (we use \simeq for Kleene equality throughout):

Conditional quantum iteration from categorical traces

1 **Naturality** in X and Y: for any $f \in dom(Tr^U_{A,B}), g: X' \longrightarrow X$ and $h: Y \longrightarrow Y'$,

$$Tr_{X',Y'}^U((h\otimes 1_U)f(g\otimes 1_U)) \simeq h Tr_{X,Y}^U(f) g$$

2 **Dinaturality** in U: For any $f: X \otimes U \longrightarrow Y \otimes U', g: U' \longrightarrow U$,

$$Tr_{X,Y}^U((1_Y \otimes g)f) \simeq Tr_{X,Y}^{U'}(f(1_X \otimes g)).$$

- 3 **Vanishing I:** Given $f : X \otimes I \to Y \otimes I$, then $Tr_{X,Y}^{I}(f)$ exists, and $Tr_{X,Y}^{I}(f) = \rho f \rho^{-1} : X \to Y$.
- 4 **Vanishing II:** For any $g: X \otimes U \otimes V \longrightarrow Y \otimes U \otimes V$, then the existence of both $Tr_{X \oplus U, Y \oplus U}^V(g)$ and $Tr_{X, Y}^V(Tr_{X \oplus U, Y \oplus U}^U(g))$ implies the existence of $Tr_{X, Y}^{U \otimes V}(g)$, in which case

$$Tr_{X,Y}^{U\otimes V}(g) = Tr_{X,Y}^U(Tr_{X\otimes U,Y\otimes U}^V(g))$$

5 **Superposing**: For any $f: X \otimes U \to Y \otimes U$ and $g: W \longrightarrow Z$,

$$Tr^U_{W\otimes X,Z\otimes Y}(g\otimes f)\simeq g\otimes Tr^U_{X,Y}(f).$$

6 Yanking: For all objects U, $Tr_{U,U}^U(s_{U,U})$ exists and $Tr_{U,U}^U(s_{U,U}) = 1_U$.

Given a monoidal subcategory (\mathcal{D}, \oplus) of (\mathcal{C}, \oplus) , we say that \mathcal{D} is **traced in** \mathcal{C} if $Tr_{X,Y}^U(f)$ exists in \mathcal{C} , for all $f: X \oplus U \to Y \oplus U$ in \mathcal{D} . We do *not* require that $Tr_{X,Y}^U(f)$ is a member of \mathcal{D} , or that \mathcal{C} carries a Σ -structure, or has matrix representations, &c.

Note that the above definition of partial trace is essentially the usual notion of traced monoidal category, with equality of partial functions defined in the usual (Kleene) sense (Freyd and Scedrov 1990): "one side is defined iff the other side is defined, and in that case they are equal". There are many other theories of partial trace and/or traced ideals in monoidal categories, developed for special purposes. For a theory of partial traces with applications to a typed version of Girard's Geometry of Interaction, see (Haghverdi, Scott 2005). For a study of partial traces and trace ideals in monoidal categories related to nuclearity in functional analysis, see (Abramsky et. al. 1999); however, we emphasize that for our purposes, we do not require that \mathcal{D} be a multiplicative ideal of \mathcal{C} . In fact, we are often interested in the case where \mathcal{D} is a monoidal subcategory of \mathcal{C} , not necessarily closed under composition with arrows of \mathcal{C} .

Theorem 9.5. The iterative trace formula defines a partial trace on every Σ MC.

Proof. We refer to Appendix B for a full statement of this result, and a proof. \Box

An interesting example of an iterative trace on a category that does not carry any Σ -structure is given in (Abramsky 2005) :

Proposition 9.6. Consider the category $(\operatorname{Bij}_{fin}, \uplus)$ of bijections on finite sets, as a monoidal subcategory of $(\operatorname{pInj}, \uplus)$. Then $(\operatorname{Bij}_{fin}, \uplus)$ has a (globally defined) iterative trace.

Proof. This is proved (albeit using different terminology) in (Abramsky 2005), where it is demonstrated that the iterative trace of a bijection between finite sets is itself a bijection between finite sets. \Box

9.3. Partially and globally traced UDCs

So far, all the examples of UDCs given are 'algebraic' examples that have a globally defined iterative trace, whereas all Σ MCs that are not UDCs are 'analytic', and have a partially defined iterative trace. However, this is not a reliable pattern – we now present a UDC that is very analytic in nature, and has a partially defined trace. Various versions of this category are studied in (Selinger 2004(ii)), in the context of higher-order operations on quantum-data classical-control programming languages:

Definition 9.7. Real cones

The category **Cone** of cones over \mathbb{R} has as objects *n*-fold Cartesian products of the nonnegative real numbers, denoted \mathbb{R}^+ . The arrows of **Cone** are linear maps specified by matrices with non-negative entries. There is a partial summation defined component-wise on arrows by: given a family $\{F_i: (\mathbb{R}^+)^a \to (\mathbb{R}^+)^b\}_{i \in I}$, then $\sum_{i \in I} F_i$ is defined when it is summable component-wise, as a sum of positive real numbers. The category **Cone**, also has a monoidal tensor \oplus , where

- On objects
$$(\mathbb{R}^+)^x \oplus (\mathbb{R}^+)^y = (\mathbb{R}^+)^{x+y}$$

- On arrows, $F \oplus G = \begin{pmatrix} F & \underline{0} \\ \underline{0} & G \end{pmatrix}$

It is then easy to demonstrate that this is a unique decomposition category, where all finite sums exist.

Proposition 9.8. The iterative trace formula on **Cone** defines a *partial* categorical trace. This example is based on constructions from (Selinger 2004(ii))

Proof. Given an arrow
$$F = \begin{pmatrix} A & B \\ C & D \end{pmatrix} : (\mathbb{R}^+)^{x+u} \to (\mathbb{R}^+)^{y+u}$$
, then the iterative race formula

trace formula

$$Tr_{x,y}^{u}(F) = A + \sum_{i=0}^{\infty} BD^{i}C$$

converges for some, but not all, arrows $F: (\mathbb{R}^+)^{x+u} \to (\mathbb{R}^+)^{y+u}$.

Characterising when this converges is non-trivial. However, when u = v = 1, the commutativity of real multiplication makes the characterisation simple. For a (2×2) matrix, $Tr^{(\mathbb{R}^+)}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = a + \sum b d^i c$ exists when either 1 b = 0 or c = 0, in which case

$$Tr^{(\mathbb{R}^+)^2} \left(\begin{array}{cc} a & b \\ c & d \end{array} \right) = a$$

2 d < 1, in which case

$$Tr^{(\mathbb{R}^+)^2} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = a + b \left(\frac{1}{1-d}\right)c$$

by a simple summation.

Note that in an arbitrary Σ MC, the existence of the trace of a matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ does not depend on the existence of $\sum_{i=0}^{\infty} d^i$, as the following example demonstrates :

Proposition 9.9. Let $F = \begin{pmatrix} A & B \\ C & D \end{pmatrix} : X \oplus U \to Y \oplus U$ be an arrow in the UDC **pInj** of partial injections. Then the iterative trace

$$Tr^{U}(F) = A + \sum_{i=0}^{\infty} BD^{i}C$$

exists for arbitrary F. However $\sum_{i=0}^{\infty} D^i$ exists exactly when $D = 0_U$.

Proof. We refer to (Hines 1997) for a proof that **pInj** has a global trace. However, recall the definition of summation in **pInj** from Example 6.1. We observe that the partial identity on $dom(D) \cap dom(D^2)$ is given by $(D^2)^{-1}D$, and this is required to be 0_U for $D + D^2$ to exist. However, this implies that $D = 0 = D^2$, and so $\sum_{i=0}^{\infty} D^i$ exists exactly when $D = 0_U$.

10. Flowchart Interpretations

10.1. Elgot Dagger and Iteration

The semantic treatment of While loops and conditional iteration in flowcharts, for classical, irreversible computation is given by the theory of the *Elgot Dagger*. Although we present the general definition, we give the computational interpretation for **pFun**, the PAC of partial functions, and refer to (Manes, Arbib 1986) for the general theory (applicable to all PACs).

Definition 10.1. Let (\mathcal{C}, \oplus) be a partially additive category, and let $f : X \to X \oplus Y$ be an arbitrary arrow in this category. Then, as \mathcal{C} has projections and inclusions, we may write f in matrix form as

$$f = \begin{pmatrix} f_1 & f_2 \end{pmatrix} \quad f_1 : X \to X \quad , \quad f_2 : X \to Y$$

The **Elgot dagger**, $f^{\dagger}: X \to Y$ is then defined by

$$f^{\dagger} = \sum_{n=0}^{\infty} f_2 f_1^n : X \to Y$$

We refer to (Manes, Arbib 1986) for a proof that this sum exists, in all PACs.

For an interpretation in the category **pFun**, note that the matrix decomposition forces a partition of the set X as $X = A \cup B$ for some disjoint subsets $A, B \subseteq X$. The application of f^{\dagger} to some $x \in X$ may be given by the flowchart in Figure 1.

As well as the flowchart formalism, the Elgot dagger is also taken as the *definition* of the semantics of a *While* loop:

$$f^{\dagger} =_{def} input(x); \{ (while \ x \in A) \ x \mapsto f(x); \} return(x) \}$$

Fig. 1. Flowchart intepretation of the Elgot dagger



(see (Manes, Arbib 1986) for details of this, and the general flowchart semantics for arbitrary PACs.)

The close connection between the Elgot dagger and the categorical trace is given by the following:

Proposition 10.2. Every partially additive category has a particle-style trace, defined in terms of the codiagonal and the canonical inclusions, by

$$Tr_{X,Y}^{U}(F) = [1_Y, f_2^{\dagger}](\iota_1 f_{11} + \iota_2 f_{21})$$

for all
$$F = \begin{pmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{pmatrix}$$
, where we take $f_2 = \begin{pmatrix} f_{12} & f_{22} \end{pmatrix} : U \to Y \oplus U$.

Proof. (Outline) By definition of the codiagonal and the Elgot dagger,

$$Tr_{X,Y}^{U}(F) = [1_Y, f_2^{\dagger}](\iota_1 f_{11} + \iota_2 f_{21}) = f_{11} + \left(\sum_{n=0}^{\infty} f_{12} f_{22}^n\right) f_{21} = f_{11} + \sum_{n=0}^{\infty} f_{12} f_{22}^n f_{21}$$

which is the required formula. For a proof that this does indeed define a categorical trace in a PAC (and for a more categorical construction), we refer to (Haghverdi 2000). \Box

10.2. Guarded While loops

It is immediate that the category **pInj** of partial injections, as a subcategory of **pFun** is not closed under the Elgot dagger; given a partial injection $f \in \mathbf{pFun}(X, X \uplus Y)$ then $f^{\dagger} \in \mathbf{pFun}(X, Y)$ need not be a partial injection. Computationally, this states that a program built up using reversible operations, together with a full "While loop" control structure may not have a reversible semantic interpretation. As a simple example, consider the almost trivial bijection:

$$f: \{1, 2, \ldots\} \to \{1, 2, \ldots\} \cup \{0\}$$
 given by $f(n) = n - 1$.

Then the Elgot dagger of this is the constant function $f^{\dagger} : \mathbb{N}^+ \to \{0\}$. The interpretation of the Elgot dagger as a *While* loop describes a subroutine on the integers:

$$input(x); \{(while \ x > 0) \ x \mapsto x - 1; \} \ return(x);$$

Although this is built up from a single globally reversible function, together with a simple conditional iteration, it has the semantic interpretation of the constant function const(x) = 0 for all $x \in \mathbb{N}^+$.

However, we have seen that the category (\mathbf{pInj}, \uplus) has an iterative trace, which has the intuition of 'eliminating a subspace through conditional iteration'. More generally, from Proposition 10.2, the categorical trace on (\mathbf{pFun}, \uplus) may (informally) be described as 'an Elgot dagger, guarded by partial functions' as follows.

Given a partial function

$$f = \begin{pmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{pmatrix} : X \uplus U \to Y \uplus U,$$

we define $A = dom(f_{11})$ and $B = dom(f_{22})$ and give a flowchart interpretation to the iterative trace as shown in Figure 2:

Fig. 2. Flowchart intepretation of the particle-style Trace



We may also give a 'guarded While loop' interpretation to the iterative trace , based

on this flowchart formalism:

$$Input(x);$$

$$If (x \in A) \qquad \{x \mapsto f_{11}(x) \\ Return(x)\} \qquad \{x \mapsto f_{21}(x) \\ (While (x \in B) \\ x \mapsto f_{12}(x) \\ Return(x) \qquad \{x \mapsto f_{22}(x)\} \end{cases}$$

Observe that the central *While* loop is guarded by conditionals & function applications that preserve the reversibility. As **pInj** is a traced monoidal subcategory of **pFun**, the categorical trace on **pFun** maps partial injections to partial injections. Therefore, 'guarded *While* loops' cannot be used to create *irreversible programs* from *reversible building blocks*.

11. Conditional feedback in the quantum world: a physical viewpoint

In the classical world, the particle-style trace may be given a physical interpretation — as noted in Sections 1 and 10, it corresponds to notions of conditional iteration that have been widely implemented, and are at the core of most computer architectures.

We have now introduced a framework that allows us to describe and reason about the iterative trace in categories of Banach and Hilbert spaces. This naturally raises the following questions:

- 1 Are 'conditionals' and 'conditional iteration' meaningful concepts in a purely quantum setting ?
- 2 What, if anything, is the connection with the iterative trace in categories of Hilbert spaces?

We emphasise that we are considering the purely quantum world (pure states and unitary operations), and hence are not considering iteration conditioned on the result of measurements, which would require a formalism based on density matrices such as (Selinger 2004(i)).

11.1. Basics of quantum information

We briefly reprise some fundamentals of quantum information and computation; a fuller introduction, and the alternative *density matrix formulation* may be found in either (Gruska 1999) or (Nielsen, Chuang 1991).

Definition 11.1. Qubits, computational basis, quantum registers

The atomic building-blocks of quantum information are *qubits*, norm-1 vectors in a 2dimensional complex Hilbert space Qu. These play an analogous rôle to bits in classical computation, and are assumed to have a fixed orthonormal basis set, the *computational basis*. In both quantum computation and quantum mechanics generally, it is common to use *Dirac notation* for both state vectors and linear maps. This is the very categorical idea that, instead of referring to a state vector $\psi \in \mathcal{H}$ we consider the linear map $|\psi\rangle : \mathbb{C} \to \mathcal{H}$, defined in the natural way as $|\psi\rangle(z) = z.\psi$. These linear maps are known as *Ket vectors*, and have duals, the *Bra vectors*, which are linear maps (functionals) $\langle \varphi | : \mathcal{H} \to \mathbb{C}$ defined by the condition that the composite $\langle \varphi | \circ | \psi \rangle$, as a linear endomap of \mathbb{C} , is the inner product of φ and ψ . A categorical framework for the Dirac notation in "strongly compact closed categories" is developed in (Abramsky, Coecke 2004).

Concatenation of qubits is given by the tensor product of Hilbert spaces, so n qubits are modelled by the space $\bigotimes_{i=1}^{n} Qu$. Spaces of this form are called *quantum registers* of n qubits, and are taken to have computational basis given by $\{|w\rangle\}_{w\in\{0,1\}^n}$, often denoted $\{|i\rangle\}_{i=0,\ldots,2^n-1}$. An n-qubit register has 2^n basis vectors, and it is this exponential property that is expected – via the resulting property of entanglement – to provide a computational advantage in using quantum-mechanical rather than classical computing devices (however, see (Jozsa, Linden 2003) for a more in-depth view).

Operations on quantum registers are taken to be either *unitary maps*, or *measurements*. Unitary maps, describing the evolution of isolated, or unobserved, quantum systems are used from Definition 6.3 onwards. Note that, as well as undisturbed evolution of a system over time, an arbitrary unitary map may be *applied* to a quantum register.

A measurement is determined by a self-adjoint operator, or Hermitian matrix. By the spectral decomposition theorem, every (finite) Hermitian matrix has a unique decomposition as the sum of projection operators — in this way a Hermitian matrix describes a set of projections, labelled by eigenvalues, and these are taken to be the experimental outcomes of a measurement — we refer to (Feynman et. al. 1965) for details.

We first present a negative result on the iterative trace on Hilbert spaces. This demonstrates that the iterative trace formula is not immediately a physical operation :

Proposition 11.2. The partial trace on Hilbert spaces

In the category $(\operatorname{Hilb}_{fd}, \oplus)$, there exist unitary maps where the iterative trace formula converges, but the result is not unitary.

Proof.

We prove this by example. Consider the 'square root of NOT' map, as commonly used in quantum computing :

$$\sqrt{NOT} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ -1 & 1 \end{pmatrix} : Qu \to Qu$$

Applying the iterative trace formula to the subspace spanned by $|1\rangle$ gives

$$Tr_{|0\rangle,|0\rangle}^{|1\rangle}(\sqrt{NOT}) = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}}\sum_{i=0}^{\infty} \left(\frac{1}{\sqrt{2}}\right)^{i} \frac{-1}{\sqrt{2}} = \frac{1-\sqrt{2}}{\sqrt{2}-1}$$

However, a unitary map on a one dimensional space is exactly scalar multiplication by a member of $S^1 = \{z : z\overline{z} = 1\}$, so the above map is not unitary (it is also, trivially, not Hermitian).

In the language of Definition 9.4, we say that **uHilb** is not a traced monoidal category; however, it may well be *traced within*, or *partially traced within* either (**Hilb**, \oplus) or (**cHilb**, \oplus). Given the intuition of the trace as 'eliminating a subspace by iteration', we can also see on purely physical grounds why (**uHilb**, \oplus) cannot be traced. Given an iterative trace, implemented as a physical unitary map, we could start with an arbitrary qubit $\psi = \alpha |0\rangle + \beta |1\rangle$, and 'trace out' the subspace given by the basis vector $|1\rangle$, leaving the norm-1 vector $|0\rangle$. This would violate the no-deleting theorem of (Pati, Braunstein 2001), which states that an unknown quantum state cannot be overwritten by a known quantum state, even in the presence of a copy (in fact, it would exhibit a stronger form of deletion known as *erasure*. We refer to (Pati, Braunstein 2001) for the distinction between deleting and erasure). From a logicians' viewpoint, the no-deleting theorem states that the contraction rule fails for quantum systems; similar considerations motivated linear logic (Girard 1987).

We now consider physical feedback in quantum-mechanical systems. A common example of qubits as physical systems is as *photon polarisation*. We use this in the following thought-experiments, together with some well-established illustrations of quantum phenomena, to both give examples of conditional quantum feedback, and to motivate constructions related to the categorical trace.

11.2. Single-photon interference

We now present a series of thought experiments in order to justify a construction to be introduced in Section 12, closely related to the iterative trace. The quantum-mechanical phenomenon we use for our interpretation is that of *single-particle interference*.

The phenomenon of interference, as in classical optics, is well-known and demonstrated by Young's double-slit experiment (Young 1807). However, a more detailed analysis is required when using a single-photon source in such an experiment. This was originally a thought-experiment[‡] (Feynman et. al. 1965), but practical demonstrations were soon given (for example, (Parker 1972)), and it is now recommended as an undergraduate-level lecture demonstration (L.D.S. 2006). This requires a quantum-mechanical description invoking the phenomenon of single-particle interference – the ability of a particle (photon) to not only take a superposition of physical locations, but to interfere with itself. As stated in (Pittman et. al. 1996),

"In his famous introduction (Feynman et. al. 1965) to the single particle superposition principle, Feynman stated that, '. . . it has in it the heart of quantum mechanics. In fact, it contains the only mystery.' ".

In what follows, we make heavy use of this principle, and also refer to (Pittman et. al. 1996) for a demonstration of why the many (entangled) particle case is qualitatively different to the single-photon case.

[‡] We refer to (Lamb 1995) for objections to single-photon thought experiments, as 'conflating a statistical description with physical reality'. However, such objects are harder to sustain for similar experiments performed with (for example) electrons (Smith 1955) or neutrons (Greenberger 1983).
11.3. Quantum phenomena and classical wave-mechanics

Although we take a single-photon description of the devices used in Section 11, we will mention neither measurement nor entanglement – features that are taken to distinguish quantum phenomena from classical wave-mechanics. The intention is to provide a notion of conditional iteration that is applicable in the quantum setting (in stark contrast to, for example, the classical *While* loop, since the latter can create irreversible programs). To demonstrate that the constructions presented are indeed valid in the quantum setting, we refer to (Cerf et. al. 2005) for a demonstration that single-photon experiments, using the toolkit presented, can model any quantum computational procedure based on the circuit model (Nielsen, Chuang 1991).

11.4. The polarisation analyser

Many experiments in introductory quantum mechanics make use of the optical properties of calcite $(CaCO_3)$ crystals. We refer to (Brom, Rioux 2002) for the following example :

Example 11.3. Calcite as a polarisation analyser

A calcite crystal may be used as an optical device with a single input channel and two output channels, as shown in Figure 11.3.

Fig. 3. An optical property of calcite



The input is unpolarised, and (using a classical description) is 'split into two distinct beams, with perpendicular polarisations'. If we consider the same experiment with a single-photon source[§], we must take a quantum description, and state that an incident photon with vertical polarisation produces an output on the upper channel, and an incident photon with horizontal polarisation produces an output on the lower channel.

Linearity then requires that an incident photon in a superposition of horizontal and vertical polarisations produces a single output $photon^{\P}$ in a superposition of locations

[§] Despite being a common feature of thought-experiments, single-photon sources are technically very difficult. We refer to (Kuhn et. al. 2002) for a physical realisation, (Kuhn et. al. 2003) for some questions associated with this, and observe that in many cases (including the lecture demonstrations of (L.D.S. 2006)) a low probability of multi-photon emission is sufficient.

This experiment should be sharply distinguished from parametric down-conversion (Kurtsiefer et. al. 2001), where a single high-energy input photon may produce 2 entangled output photons of lower-energy. The output channel, in parametric down-conversion, requires the tensor product of two single-photon states.

(i.e. the upper and lower channels). We now analye this type of experiment with reference to the standard toolkit of quantum optics devices.

11.5. Standard quantum optics devices

We now present various devices commonly used in linear and quantum optics experiments. This exposition is based on (Gerry, Knight 2005), with thanks to (Beige 2005). Note that the devices presented are properly modelled in Fock space – however, we restrict ourselves to the single-photon case, and give a simplified description. We refer to (Beige 2005; Gerry, Knight 2005) for a justification of this approach.

Example 11.4. The phase plate

A simple optical device is the **phase plate (PP)**. This has a single input and output channel and is drawn schematically as in Figure 4.

Fig. 4. The phase plate



Intuitively, this transmits all photons on the input channel, and adds a θ rotation to the phase. Given an incoming photon, described by an element of the Hilbert space H_{in} , and an outgoing photon described by a member of the space $H_{out} \cong H_{in}$, then the action of the phase plate is given by a unitary map $U_{PP} : H_{in} \to H_{out}$, specified by

$$U_{PP}(|\psi\rangle) = e^{i\theta} |\psi\rangle$$

Example 11.5. The half-wave plate

An equally simple optical device, also part of the standard toolkit for quantum optics, is the **half wave plate (HWP)**. This has a single input and output channel and is drawn schematically as in Figure 5.

Fig. 5. The half wave plate



Intuitively, this transmits all photons on the input channel, and adds a $\frac{\pi}{2}$ rotation to the polarisation. Let an incoming photon be an element of the Hilbert space H_{in} spanned by $\{|V_{in}\rangle, |H_{in}\rangle\}$, and let an outgoing photon be a member of the space H_{out} spanned

by $\{|V_{out}\rangle, |H_{out}\rangle\}$. Then the action of the half wave plate is given by a unitary map $U: H_{in} \to H_{out}$. This is specified by its action on the basis of H_{in} , as follows :

$$U_{HWP}(|H_{in}\rangle) = \frac{1}{\sqrt{2}} (|H_{out}\rangle + |V_{out}\rangle)$$
$$U_{HWP}(|V_{in}\rangle) = \frac{1}{\sqrt{2}} (-|H_{out}\rangle + |V_{out}\rangle)$$

Example 11.6. The polarising beamsplitter

A common device, closely related to Example 11.3 is the **polarising beamsplitter** (**PBS**). This has 2 input channels and two output channels, and is drawn schematically as in Figure 6.

Fig. 6. The polarising beamsplitter



Intuitively, this transmits photons with horizontal polarisation and reflects (through $\pi/2$) photons with vertical polarisation. We again restrict ourselves to the case where there is a single input photon^{||}.

Let us denote a horizontally (resp. vertically) polarized photon input in channel 1. by $|H_{in1}\rangle$ (resp. $|V_{in1}\rangle$, and similarly denote a horizontally (resp. vertically) polarized photon input in channel 2. by $|H_{in2}\rangle$ (resp. $|V_{in2}\rangle$).

Similarly, a horizontally (resp. vertically) polarized output photon in channel 1. is denote $|H_{out1}\rangle$ (resp. $|V_{out1}\rangle$, and similarly for a horizontally (resp. vertically) polarized photon output in channel 2., denoted $|H_{out2}\rangle$ (resp. $|V_{out2}\rangle$).

The polarising beamsplitter (at least in the special case where there is a single input photon) is then modelled by a unitary map U_{PBS} . This is defined as follows :

$$U_{PBS}(|H_{in1}\rangle) = |H_{out1}\rangle \qquad U_{PBS}(|V_{in1}\rangle) = |V_{out2}\rangle$$
$$U_{PBS}(|H_{in1}\rangle) = |H_{out2}\rangle \qquad U_{PBS}(|V_{in2}\rangle) = |V_{out1}\rangle$$

Precisely, we allow for a photon in Channel 1, or Channel 2, or a photon in a superposition of these locations. We do *not* allow for an input photon in each channel – not only would this require a more sophisticated mathematical treatment, but would also take us away from the underlying motivation of single-particle interference. The mathematical treatment given can be considered as 'neglecting the vacuum states, for simplicity of notation'.

Note that we do not explicitly give the source / target spaces for this example, as this would involve discussing the appropriate Fock spaces. We refer to (Gerry, Knight 2005) for a fuller treatment, and (Beige 2005) for the special case presented. Wherever we need an explicit description of the source / target space for a given experiment, we will give it directly, in terms of some orthonormal basis.

Example 11.7. A modified polarising beamsplitter

An alternative, equally common, polarising beamsplitter is given by taking the apparatus described in Figure 6 above, and adding 2 half-wave plates and a phase plate into channel 2, as shown in Figure 7. Although this is not the standard terminology, we refer to this as the **modified polarizing beamsplitter (MPBS)**.

Fig. 7. A modified polarising beamsplitter



By composing the appropriate unitary maps, we see that, given an arbitrary single photon input on channel 1, the output *regardless of the original polarisation* is horizontally polarised. Similarly, given a single photon input on channel 2, the output is vertically polarised.

At first sight, it appears that this violates the quantum no-deleting theorem (Pati, Braunstein 2001). However, consider the case where a photon with polarization $\alpha |H_{in1}\rangle + \beta |V_{in1}\rangle$ is input on channel 1. A simple analysis shows that the output photon is in the state $\alpha |H_{out1}\rangle + \beta |H_{out2}\rangle$ – that is, the qubit that was encoded on the photon polarisation (as a superposition of horizontal and vertical polarisation) is now encoded on the output channel (i.e. a superposition of channel 1 and channel 2).

Therefore, this device does not delete any information from the system. We have merely exchanged uncertainty about the polarization of a photon for uncertainty about its location. This is as described in (Jozsa 2002),

Considering no-cloning and no-deleting together we see that quantum information (of nonorthogonal states) has a quality of "permanence": creation of copies can only be achieved by importing the information from some other part of the world where it had already existed; destruction (deletion of a copy) can only be achieved by exporting the information out to some other part of the world where it must continue to exist.

11.6. An optical example of a quantum conditional

We now present a common application of the above toolkit, as intuition for the notion of a 'purely quantum conditional'.

Example 11.8. Interference Microscopy

A common application of the polarizing beamsplitter is in the field of *Interference Microscopy*. In an example such as (Carl et. al. 2005), a coherent input beam is divided into its horizontally and vertically polarized components, and the microscope sample is placed in one of the two output channels. A reversed polarising beamsplitter is then used to recombine the two channels, as shown in Figure 8 :





This enables identification of the optical properties of the test sample – for example it is the industry-standard technique for identification of asbestos fibres (Asbestosis Research Council 1978). We refer to (Strong 1958) for a classical overview of interference microscopy, and other applications.

For our purposes, we take this (using a single-photon description) as an example of a quantum-mechanical conditional, so interaction of a photon with the test sample is *conditioned* on the polarisation of the photon.

In general, unitary maps may be considered as describing a conditional operation — this intuition of 'unitary matrices as quantum conditionals' is used to give 'quantum conditionals' in the QML language of (Altenkirch, Grattage 2005)). Given a unitary map $U: Q \to Q$ on a two-dimensional space, with computational basis $\{|0\rangle, |1\rangle\}$, then U may be written in terms of its action on this basis as $U = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$. The application of U to a state vector ψ has a simple interpretation as a conditional:

(Cond
(
$$(\psi = |0\rangle)$$
 (Replace ψ by $\varphi_0 = a|0\rangle + c|1\rangle$))
($(\psi = |1\rangle)$ (Replace ψ by $\varphi_1 = b|0\rangle + d|1\rangle$))

where a superposition $\psi = \alpha |0\rangle + \beta |1\rangle$ results in ψ being replaced by $\alpha |\varphi_0\rangle + \beta |\varphi_1\rangle$.

Note that a unitary, *per se*, cannot be interpreted as a conditional map. In order to describe a unitary map in terms of a *conditional*, we need to take a matrix decomposition

— from Section 8, this is giving the space Q as the direct sum of two subspaces. Physically, this is via the specification of complete disjoint sets of distinguishable experimental outcomes (Feynman et. al. 1965).

11.7. Conditional quantum feedback

We now present a thought-experiment, closely related to the apparatus and examples presented in previous sections. However, we postpone a formal analysis until we have presented and justified the categorical tools needed.

Example 11.9. A P.I.M. with feedback

Based on the example of polarizing interference microscopy given above, we consider the conditional application of a unitary map to a photon. However, instead of recombining the two channels with a reversed polarizing beamsplitter (and hence producing a useful interference pattern), the result of the application is returned to the second input channel, as shown in Figure 9.

Fig. 9. Conditional feedback



There is a strong temporal aspect to this thought-experiment^{††}. Let us (as usual) take a single-photon description, and introduce a horizontally polarised photon on channel 1. We assume that the unitary map shown modifies the photon polarisation (otherwise the experiment is a triviality) by a process such as $|H\rangle \rightarrow \alpha |H\rangle + \gamma |V\rangle$ and $|V\rangle \rightarrow \gamma |H\rangle + \delta |V\rangle$. Assuming $\gamma \neq 0 \neq \beta$, we see that at any subsequent time, the photon is in a superposition of locations — both within the feedback loop, and on the output channel. In particular, the 'number of times the photon has traversed the feedback loop' is not a well-defined quantity, and the phenomenon of single-particle interference has a large part to play in any formal description.

Because of this temporal aspect, it is not immediate how to give a treatment in terms of input and output spaces. Instead, we describe this apparatus in terms of a unitary operator that is repeatedly applied to a single space.

^{††} We emphasis that this is a *thought-experiment*. Practically the apparatus shown will rapidly amplify any small errors in the alignment of (for example) the mirrors. However, we refer to (Casati1, Prosen 1995) for numerical simulations of a similar setup involving a perfectly reflecting spherical cavity.

11.8. Analysing Example 11.9

In order to analyse the above thought-experiment, we first use the assumption of discrete space and time, as in the 'toy models' of (Griffiths 2002) — we refer to this for justification and interpretations. We still require a single-photon thought experiment — however, we allow this photon to be in a coherent superposition of any of the locations shown in Figure 10. The set of possible locations is then $\{\ldots, in_2, in_1, current, out_1, out_2, \ldots\}$.

Fig. 10. Input / output streams in a conditional feedback apparatus



As well as the possible locations of the photon, a complete description of the configuration requires the photon polarisation, which is horizontal $|H\rangle$ or vertical $|V\rangle$. Hence, an instantaneous configuration of this system is a member of the (infinite-dimensional) Hilbert space $LOC \otimes POL$, where LOC has orthonormal basis $\{\ldots, |in_2\rangle, |in_1\rangle, |current\rangle, |out_1\rangle, |out_2\rangle, \ldots\}$, and POL has orthonormal basis $\{|H\rangle, |V\rangle\}$.

From the interpretation of the individual components, it is then straightforward to write down a description of the unitary evolution of the configuration space over time, in terms of the basis elements of $LOC \otimes POL$, as follows:

1 For 'input modes'

— When i > 1,

 $|in_i\rangle \otimes |p\rangle \mapsto |in_{i-1}\rangle \otimes |p\rangle$ for all $|p\rangle \in POL$

— When i = 1,

 $|in_1\rangle \otimes |V\rangle \mapsto |out_1\rangle \otimes |V\rangle$ and $|in_1\rangle \otimes |H\rangle \mapsto current\rangle \otimes |H\rangle$

2 For 'current modes'

— For horizontal polarisation :

$$|current\rangle \otimes |H\rangle \mapsto \alpha |out_1\rangle \otimes |H\rangle + \gamma |current\rangle \otimes |V\rangle$$

— For vertical polarisation :

 $|current\rangle \otimes |V\rangle \mapsto \beta |out_1\rangle \otimes |H\rangle + \delta |current\rangle \otimes |V\rangle$

3 For 'output modes'

— In every case,

 $|out_i\rangle \otimes |p\rangle \mapsto |out_{i+1}\otimes |p\rangle$

We may combine these descriptions of the action of this apparatus on basis vectors in order to form a unitary giving a global description of the action; however, there is no sense in which this 'takes an input space to an output space'. Instead we consider a restricted sub-experiment, where we have such a notion (as a limit, where the number of time-steps tends to infinity).

11.9. A restricted quantum feedback experiment

We now restrict the thought-experiment presented in Section 11.8 by imposing (physically reasonable) initial conditions, and eliminating those starting configurations that have no non-trivial interaction with the feedback loop.

The assumptions we make are

- 1 A photon in location **current** has vertical polarisation.
- 2 The input stream is horizontally polarised.
- 3 At the start of the experiment, the output stream is empty.

Assumption 1. may readily be justified in that no input stream can lead to a horizontally polarised photon in this location — any vertically polarised input will be reflected into the output stream. Assumption 2. is again because a vertically polarised input is simply reflected into the output stream without interacting with the feedback loop. Finally, assumption 3. is simply to make calculation simple — the case where the output stream is initially non-empty is a trivial extension of the case we consider. Note that, under this assumption, the output stream is always *horizontally polarised*.

A simple corollary of these initial conditions is that, in this experiment :

The location of a photon determines its polarisation.

Hence we may give a significantly simplified description of the evolution over time of this apparatus.

As a final simplifying step, we do not assume that the unitary evolution is from a some fixed space H to itself. Instead, we consider that at each timestep, we have unitary evolution F_i from space H_i to space H_{i+1} . This is as shown in Figure 11.

Hence we may give orthonormal bases for the space H_i , as follows

- the space H_0 has basis { $|current\rangle, |in_1\rangle, |in_2\rangle, |in_3\rangle, \ldots$ }
- the space H_1 has basis $\{|out_1\rangle, |current\rangle, |in_2\rangle, |in_3\rangle, |in_4\rangle, \ldots\}$
- the space H_2 has basis $\{|out_1\rangle, |out_2\rangle, |current\rangle, |in_3\rangle, |in_4\rangle, |in_5\rangle, \ldots\}$

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— . . .
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Fig. 11. Timesteps in a simplified conditional feedback apparatus

Using the description of the actions of the individual components, we may write down the linear maps $\{F_i: H_{i-1} \to H_i\}_{i>0}$ as follows :

$$--F_1 = \begin{pmatrix} \beta & \alpha & 0 & \dots \\ \delta & \gamma & 0 & \\ 0 & 0 & 1 & \\ \dots & & \dots \end{pmatrix}$$

$$--F_{2} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & \beta & \alpha & 0 & \\ 0 & \delta & \gamma & 0 & \\ 0 & 0 & 0 & 1 & \\ \dots & & & \dots \end{pmatrix}$$
$$--F_{3} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & 0 & \\ 0 & 0 & \beta & \alpha & 0 & \\ 0 & 0 & \delta & \gamma & 0 & \\ 0 & 0 & 0 & 0 & 1 & \\ \dots & & & \dots \end{pmatrix}$$

Proposition 11.10. The composite $F_{k-1}F_{k-2}\ldots F_1$ is given by

Proof. This follows by direct calculation. Of more interest is the similarity between column 1. and the summands of the Elgot dagger, and columns 2. onwards and the summands of the iterative trace. We consider the convergence of this process, the general categorical setting, and potential applications in terms of a computational theory of iteration in the following sections. \Box

12. Factoring the Trace and Twisted Daggers

We have seen in Proposition 11.2 that the iterative trace on Hilbert spaces may converge, but does not have an immediate physical interpretation. However, from Proposition 11.10, we recover the summands of both the particle-style trace and the Elgot dagger from a single physical experiment. We now investigate this in a more general setting. We will demonstrate that the iterative trace on a Σ MC *factored* as a canonical inclusion, followed by an iterative step, followed by a 'forgetful' step (a codiagonal, in the appropriate setting).

In the physical setting, this central iterative step is the repeated application of unitary maps. Hence the non-unitarity of the iterative trace on **Hilb** arises, not from its interpretation as conditional iteration, but from the 'forgetting of information' encoded by the application of the codiagonal.We also demonstrate in Section 14 that this central iterative part is also gives iterative trace, albeit in a larger category.

12.1. The 'twisted dagger' construction

We now introduce a construction on Σ MCs with infinite matrices. Intuitively, this construction is similar to the Elgot dagger, up to an additional symmetry map, or twist. Because of this, we refer to it as the *twisted dagger operation*.

Definition 12.1. The twisted dagger

Given a $\Sigma MC(C, \oplus, \Sigma)$, and an arrow $L: X \oplus U \to Y \oplus U$ with matrix representation $L = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, we define the **Twisted Dagger** of L to be the matrix

	$\begin{pmatrix} b \end{pmatrix}$	a	0	0	0	0	0	0	\
$\dagger^U(L) =$	bd	bc	a	0	0	0	0	0	
	bd^2	bdc	bc	a	0	0	0	0	
	bd^3	bd^2c	bdc	bc	a	0	0	0	
	bd^4	bd^3c	bd^2c	bdc	bc	a	0	0	
	bd^5	bd^4c	bd^3c	bd^2c	bdc	bc	a	0	
	bd^6	bd^5c	bd^4c	bd^3c	bd^2c	bdc	bc	a	
	()

(Note that we do *not* yet claim this is the matrix representation of an arrow in a Σ MC. At this stage, the twisted dagger is simply a formal matrix of arrows in a Σ MC. Questions about when it represents an arrow in some appropriate category form the substance of this section).

The twisted dagger matrix is based on Proposition 11.10, extended to both block matrices, and the limit as the number of timesteps increases. As before, we note the correspondence between the first column and the summands of the Elgot dagger, $(d b)^{\dagger} = \sum_{i=0}^{\infty} bd^i$, and the correspondence between the remaining columns and the summands of the iterative trace $Tr^U(L) = a + \sum_{i=0}^{\infty} bd^i c$. We now investigate the existence and properties of this matrix, with particular reference to unitary maps on Hilbert spaces.

Lemma 4. Given
$$L = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \operatorname{Hilb}_{\operatorname{fd}}(X \oplus U, Y \oplus U)$$
, and arbitrary $\varphi = \begin{pmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \\ \vdots \end{pmatrix} \in$

 $U \oplus X^{\oplus \omega}$, let us define the formal matrix

$$\zeta = \begin{pmatrix} \zeta_0 \\ \zeta_1 \\ \zeta_2 \\ \vdots \end{pmatrix}$$

to be given by the formal matrix composition $\zeta = \dagger^U(L)(\varphi)$. so

$$\zeta_n = \begin{cases} bd^n(\varphi_0) + \sum_{i=1}^n bd^{n-i}c(\varphi_i) + a(\varphi_{n+1}) & (n>0) \\ b(\varphi_0) + a(\varphi_1) & (n=0) \end{cases}$$

Then ζ_n exists, for all $n \in \mathbb{N}$.

Proof. Observe that ζ_n is given by a finite sum of continuous linear maps applied to a finite vector of elements.

Note that we do not claim that $\sum_{n=0}^{\infty} \|\zeta_n\|^2$ exists, or (equivalently) that ζ is an element of $Y^{\oplus \omega}$ — a sufficient condition for this is given by Theorem 12.2 below.

Theorem 12.2. Let $L = \begin{pmatrix} a & b \\ c & d \end{pmatrix} : X \oplus U \to Y \oplus U$ be a linear map between finitedimensional Hilbert spaces. Then :

- 1 A sufficient, but not necessary, condition for $\dagger^U(L)$ to be the matrix representation of an arrow in **Hilb** is that the component d is a strict contraction (i.e. ||d|| < 1).
- 2 When L is a unitary map, a sufficient condition for the component $\dagger^U(L)$ to be unitary is that the component d is a strict contraction.

Proof. As a preliminary to these proofs, we define

$$\{F_i: Y^{\oplus i} \oplus U \oplus X^{\oplus \omega} \to Y^{\oplus i+1} \oplus U \oplus X^{\oplus \omega}\}_{i=0}^{\infty}$$

by

$$F_i = (1_{Y^{\oplus i}}) \oplus Ls_{X,U} \oplus (1_{X^{\oplus \omega}})$$

and define

$$\{G_n: U \oplus X^{\oplus \omega} \to Y^{\oplus (n+1)} \oplus U \oplus X^{\oplus \omega}\}_{n=0}^{\infty}$$

by $G_n = F_n F_{n-1} F_{n-2} \dots F_0$.

We may write $\{F_i\}$ explicitly as :

$$F_{0} = \begin{pmatrix} b & a & 0 & \dots \\ d & c & 0 & \\ 0 & 0 & 1 & \\ \dots & & & \dots \end{pmatrix} \qquad F_{1} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & b & a & 0 & \\ 0 & d & c & 0 & \\ 0 & 0 & 0 & 1 & \\ \dots & & & \dots \end{pmatrix}$$
$$F_{2} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & b & a & 0 & \\ 0 & 0 & d & c & 0 & \\ 0 & 0 & 0 & 0 & 1 & \\ \dots & & & \dots \end{pmatrix} \qquad \qquad \dots$$

and, using the formula for matrix composition,

It is immediate that F_i is a well-defined linear map for all $i \ge 0$, and is unitary exactly when L is unitary. Similarly, for all $k \in \mathbb{N}$, the map G_k is the composite of a finite series of linear bounded maps, and hence is linear bounded, and unitary when L is unitary.

We now use these preliminaries to prove 1 - 2 above :

1 Consider arbitrary $\varphi \in U \oplus X^{\oplus \omega}$. We now study the sequence

$$\varphi = \varphi^{(0)} \xrightarrow{F_0} \varphi^{(1)} \xrightarrow{F_1} \varphi^{(2)} \xrightarrow{F_2} \varphi^{(3)} \xrightarrow{F_3} \cdots$$

so $\varphi^{(n)} = G_n(\varphi)$. We write $\varphi^{(n)}$ explicitly as

$$\varphi^{(n)} = \begin{pmatrix} \varphi_0^{(n)} \\ \varphi_1^{(n)} \\ \varphi_2^{(n)} \\ \varphi_3^{(n)} \\ \vdots \end{pmatrix} \quad \text{where} \quad \begin{cases} \varphi_n^{(n+i)} \in Y \\ \varphi_n^{(n)} \in U \\ \varphi_n^{(n)} \in U \\ \varphi_{n+i}^{(n)} \in X \end{cases} \quad \text{for all } n \in \mathbb{N} \ , \ i > 0$$

In particular, we make the identification $\varphi_i^{(0)} = \varphi_i$, for all $i \in \mathbb{N}$.

From the explicit description of $\{F_i\}_{i\in\mathbb{N}}$, we may use standard diagrammatic notation for matrix composition, and draw the calculation of the components of $\varphi^{(n)}$ as From either this diagram, or by direct calculation, we may inductively calculate these components by, for all p, q > 0:

$$\varphi_q^{(p)} = \begin{cases} \varphi_q^{(0)} & q > p \\ b(\varphi_{p-1}^{(p-1)}) + a(\varphi_p^{(0)}) & q = p - 1 \\ \\ d(\varphi_{p-1}^{(p-1)}) + c(\varphi_p^{(0)}) & p = q \\ \\ \varphi_q^{(q+1)} & p > q + 1 \end{cases}$$

Fig. 12. Calculating components of $\varphi^{(n)}$



It is immediate that, comparing these elements with the formal matrix $\zeta = \begin{pmatrix} \zeta_0 \\ \zeta_1 \\ \zeta_2 \\ \vdots \end{pmatrix}$ from Lemma 4, that for all $n \in \mathbb{N}$

from Lemma 4, that for all
$$n \in \mathbb{N}$$
,

$$\zeta_i = \varphi_i^{(j)} , \quad \forall \ i < N , \ j > i$$

By direct calculation, and the Cauchy-Bunyakovski-Schwarz inequality,

$$\|\varphi_k^{(k)}\| \le \|d^k\| . \|\varphi_0^{(0)}\| + \sum_{n=1}^k \|d^n\| . \|c\| . \|\varphi_{k-n}^{(0)}\|$$

However, by assumption $d: U \to U$ is a strict contraction map, so ||d|| < 1. Also, $\varphi \in X^{\oplus \omega}$ and so $\sum_{i=0}^{\infty} ||\varphi_i^{(0)}||^2 < \infty$. Therefore, we deduce that $\sum_{k=0}^{\infty} ||\varphi_k^{(k)}||^2 < \infty$, and hence the 'diagonal element'

$$\Delta_{\varphi} = \begin{pmatrix} \varphi_0^{(0)} \\ \varphi_1^{(1)} \\ \varphi_2^{(2)} \\ \vdots \end{pmatrix}$$

is a member of $U^{\oplus \omega}$. Finally, observe that

$$\zeta = \begin{pmatrix} b & 0 & 0 & \cdots \\ 0 & b & 0 & \cdots \\ 0 & 0 & b & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \varphi_0^{(0)} \\ \varphi_1^{(1)} \\ \varphi_2^{(2)} \\ \vdots \end{pmatrix} + \begin{pmatrix} a & 0 & 0 & \cdots \\ 0 & a & 0 & \cdots \\ 0 & 0 & a & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \varphi_0^{(0)} \\ \varphi_0^{(0)} \\ \varphi_2^{(0)} \\ \vdots \end{pmatrix}$$

and hence $\zeta \in Y^{\oplus \omega}$, as required.

To show that the condition ||d|| < 1 is not necessary, consider the simplest possible counterexample – the identity matrix $\begin{pmatrix} 1_X & 0\\ 0 & 1_U \end{pmatrix}$: $X \oplus U \to X \oplus U$. It is immediate that

$$\dagger^{U}(L) = \begin{pmatrix} 0 & 1_{X} & 0 & 0 & 0 & \dots \\ 0 & 0 & 1_{X} & 0 & 0 & \dots \\ 0 & 0 & 0 & 1_{X} & 0 & \dots \\ 0 & 0 & 0 & 0 & 1_{X} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

and this is a partial isometry, a *shift map* in the sense of (Page 1971).

2 In this part of the proof, we use the characterisation of unitary maps as

- 'partial isometries, with full initial and final subspaces'.

The proof using the characterisation as

- 'Invertible, with inverse given by the matrix conjugate transpose',

is significantly more complex; however, we refer to the supplementary materials (Hines, Scott 2007) for this proof in the 2×2 case.

We know from 1/ above that $\dagger^U(L)$ exists, for all unitary $L = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ satisfying

- $\|d\| < 1.$ We now need to show that
- (a) $\dagger^U(L)$ is a partial isometry,
- (b) The initial and final subspaces of $\dagger^U(L)$ are the whole of $U \oplus X^{\oplus \omega}$ and $Y^{\oplus \omega}$ respectively.

These results may be seen as follows :

(a) We first define $Term_N: Y^{\oplus (N+1)} \oplus U \oplus X^{\oplus \omega} \to Y^{\oplus \omega}$ for all $N \in \mathbb{N}$, by

$$Term_{N}\left(\begin{array}{c}y_{0}\\\vdots\\y_{N-1}\\u\\x_{1}\\\vdots\end{array}\right)=\left(\begin{array}{c}y_{0}\\\vdots\\y_{N}\\0_{Y}\\0_{Y}\\\vdots\end{array}\right)$$

Clearly, $Term_N$ is a linear map, and is a partial isometry, with initial subspace

 $Y^{\oplus(N+1)} \leq Y^{\oplus(N+1)} \oplus U \oplus X^{\oplus\omega}$. Hence, as $G_N : U \oplus X^{\oplus\omega} \to Y^{\oplus(N+1)} \oplus U \oplus X^{\oplus\omega}$ is unitary, the composite $Term_N G_N : U \oplus X^{\oplus\omega} \to Y^{\oplus\omega}$ is a partial isometry. Now consider arbitrary fixed $\varphi \in U \oplus X^{\oplus\omega}$. From part 1/ above, for all $\epsilon > 0$, there exists $M \in \mathbb{N}$ such that

$$\|Term_M(G_M(\varphi)) - \dagger^U(L)(\varphi)\| < \epsilon$$

So, by completeness, $\lim_{N\to\infty} Term_N(G_N(\varphi)) = \dagger^U(L)(\varphi)$, and so in the space $\operatorname{Hilb}(U \oplus X^{\oplus \omega}, Y^{\oplus \omega})$, the series of partial isometries $\{Term_NG_N\}_{N=1}^{\infty}$ converges to $\dagger^U(L)$. However, by (Andruchow, Corach 2004), the set of partial isometries between spaces H_1, H_2 forms a smooth submanifold of the space $\operatorname{Hilb}(H_1, H_2)$ (we also refer to (Andruchow, Corach 2005) for a close connection between partial isometries and Hilbert-Schmidt maps). Therefore, we deduce that the limit $\dagger^U(L)$ is a partial isometry.

(b) We prove that the initial subspace is full by contradiction.

First recall that $L = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$: $X \oplus U \to Y \oplus U$ is a unitary map satisfying ||d|| < 1. Now assume there exists some $u \in U$ such that b(u) = 0. Then $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 0 \\ u \end{pmatrix} = \begin{pmatrix} 0 \\ d(u) \end{pmatrix}$. However, $\left\| \begin{pmatrix} 0 \\ u \end{pmatrix} \right\| = \|u\|$, and by the assumption that d is a strong contraction, $\left\| \begin{pmatrix} 0 \\ d(u) \end{pmatrix} \right\| = \|d(u)\| < \|u\|$. This is a contradiction of the unitarity of L, so we deduce that $b(u) \neq 0$, for all $u \in U$.

Now let $\chi \in U \oplus X^{\oplus \omega}$ be in the complement of the initial subspace of $\dagger^U(L)$, so $\dagger^U(L)(\chi) = 0$. As $\lim_{n \to \infty} Term_n(G_n(\varphi)) = \dagger^U(L)(\varphi)$, we deduce that $\{\chi^{(n)} = Term_nG_n(\chi)\}_{n=1}^{\infty}$ is a series of elements of $Y^{\oplus \omega}$ that converges to 0. Writing these explicitly as

$$\chi^{(n)} = \begin{pmatrix} \chi_0^{(n)} \\ \chi_1^{(n)} \\ \chi_2^{(n)} \\ \vdots \end{pmatrix}$$

We observe from part 1. that $\chi_{n+k}^{(n)} = \chi_{n+2}^{(n)}$ for all $k \ge 2$. Hence $\chi = 0$ implies that $\chi_{n+2}^{(n)} = 0$, for all $n \in \mathbb{N}$. However, by close inspection of diagram 12, this is only possible when b(u) = 0, for some $u \in U$, contradicting the preliminary result above.

We now demonstrate that the final subspace is full

Consider arbitrary $\zeta \in Y^{\oplus \omega}$, written as

$$\zeta = \begin{pmatrix} \zeta_0 \\ \zeta_1 \\ \zeta_2 \\ \vdots \end{pmatrix}$$

As $\zeta \in Y^{\oplus \omega}$, for all $\epsilon > 0$, there exists some $N \in \mathbb{N}$ such that $\sum_{i=N}^{\infty} \|\zeta_i\| < \epsilon$. Using the adjoint of the partial isometry $Term_M$ above, it is immediate that

$$Term_{M}^{*}(\zeta) = \begin{pmatrix} \zeta_{0} \\ \vdots \\ \zeta_{M} \\ 0_{U} \\ 0_{X} \vdots \end{pmatrix}$$

and, for all M > N, $\|\zeta\| = \|Term_M^*(\zeta)\| < \epsilon$. We now define $\lambda^{(M)} \in U \oplus X^{\oplus \omega}$ by $\lambda^{(M)} = G_M^{-1}(Term_M^*(\zeta))$, where the unitary map G_M^{-1} is given by $F_M^{-1}F_{M-1}^{-1}\dots F_0^{-1}$, for F_i as defined in part 1. Since G_M^{-1} is unitary, $\|\lambda^{(M)}\| = \|Term_M^*(\zeta)\|$. By taking sufficiently large $M > N \in \mathbb{N}$, it follows that $\dagger^U(L)(\lambda^{(M)} \to \zeta$ as $M \to \infty$, and as ζ was chosen arbitrarily, the terminal subspace of $\dagger^U(L)$ is exactly $Y^{\oplus \omega}$. This then completes our proof of unitarity.

Discussion^{‡‡}Unitarity, Convergence, and Termination

The usual interpretation of unitarity is that a unitary map on Hilbert space is *physically* reasonable – i.e. it corresponds to a valid evolution of an undisturbed quantum system. However (based on the thought-experiment in Section 11.9) the twisted dagger is the *limit* of an iterated physical process as the number of time-steps tends to infinity. The twisted dagger, applied to a finite-dimensional unitary map L, has a physical interpretation – but this arises from the interpretation of the intermediate steps (described by the unitary maps $G_n(L)$), rather than unitarity of the limit (which has the distinctly unphysical interpretation of the 'result' after an infinite number of iterated steps).

How, then, should we interpret unitarity in the limit? It can only be a strong form of convergence, or termination of an iterated process. At any finite time K, we have a physical interpretation (i.e. $G_K(L)$ is unitary, for unitary L). When the limit exists, we deduce that after a suitable number T of timesteps, further iterations have a negligible effect on the state of the system — a direct comparison may be drawn with Cauchy sequences. However, this is simply the statement that the twisted dagger is an isometry & unitarity is a stronger result than this. Via the characterisation of unitaries as special cases of partial isometries, it also implies that every element of the image space arises via such an iterated process.

^{‡‡} Many thanks to Sam Braunstein for the following comments on physical interpretations

Because of this interpretation, we consider the twisted dagger of any (finitedimensional) unitary map to be physically motivated, even when the limit is not unitary. Conversely, if a linear map L is not unitary, we do not consider the twisted dagger to have a physical interpretation (at least, as an undisturbed quantum system), even when $\dagger^{U}(L)$ is itself unitary.

Note also that the traced out subspace U does not appear in the image of the twisted dagger, although it is part of the image for all finite intermediary steps. Hence, for the twisted dagger to be a unitary map, the projection onto this subspace must, at some point, become and remain empty. In the finitary, or physically reasonable case, this raises the possibility of using a measurement on this subspace as a test that a completed computation has indeed terminated.

12.2. The twisted dagger, and the trace

In a Σ MC, there is clearly a close connection between the *twisted dagger*, the iterative trace, and the Elgot dagger. Precisely, columns 1,2,3, ... of the twisted dagger matrix give the summands of the iterative trace, and column 0 gives the summands of the Elgot dagger. We now study the connection between the twisted dagger and the iterative trace in the category **Hilb**_{fd}.

Theorem 12.3. Let $L = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \operatorname{Hilb}_{\operatorname{fd}}(X \oplus U, Y \oplus U)$ be a linear map, where $\dagger^{U}(L)$ exists, and let $\iota_{k} : X \to U \oplus (\oplus^{\omega} X)$ be the canonical inclusion into the k^{th} component, $\psi \to (0, \ldots, 0, \psi, 0, 0, \ldots)$ (where k > 1). Then the trace $Tr_{X,Y}^{U}(L) : X \to Y$ exists, and is given by the following composite



for arbitrary $k \geq 1$. Note this factorization lives in **Hilb**, not **Hilb**_{fd}.

Proof.

This is immediate from the description of the twisted dagger matrix. For k = 1, observe that

$$\begin{pmatrix} b & a & 0 & 0 & 0 & \dots \\ bd & bc & a & 0 & 0 & \dots \\ bd^2 & bdc & bc & a & 0 & \dots \\ bd^3 & bd^2c & bdc & bc & a & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} 0 \\ \psi \\ 0 \\ 0 \\ \vdots \end{pmatrix} = \begin{pmatrix} a(\psi) \\ bc(\psi) \\ bdc(\psi) \\ bd^2c(\psi) \\ \vdots \end{pmatrix}$$

Composition with the codiagonal gives $\nabla \dagger^U(L) \iota_2(\psi) = a + \sum_{i=0}^{\infty} bd^i c = Tr^U_{X,Y}(L)(\psi)$ for arbitrary $\psi \in X$, as required. The case where k > 1 follows similarly.

Corollary 12.4. Let the **shift map** $Shift : \oplus^{\omega}Y \to \oplus^{\omega}Y$ be the partial isometry defined by

$$Shift(y_0, y_1, y_2, \ldots) = (0, y_0, y_1, y_2, \ldots)$$

Then $\dagger^U(L) \iota_k = Shift^k \ \dagger^U(L) \iota_1$, for k > 1.

Proof. This is also immediate from the structure of the twisted dagger matrix. \Box

Remark 12.5. The twisted dagger of a unitary matrix is the limit of an entirely unitary, and hence reversible, process (and is, under relatively light conditions, itself unitary). The canonical inclusion is an isometry (i.e. a partial isometry with full initial space) and is also an information-preserving operation. Hence, we may identify the irreversibility of the iterative trace on Hilb_{fd} as arising from the codiagonal, which (speaking informally) 'forgets information about the computation'. From a categorical point of view, observe that we have specified the iterative trace on Hilb_{fd} in terms of canonical inclusions, composition, and countable codiagonals, without explicit reference to notions of summation.

13. Convolved lists in Hilbert space

We have seen above how the twisted dagger of a unitary matrix $L = \begin{pmatrix} a & b \\ c & d \end{pmatrix} : X \oplus U \to U$

 $Y \oplus U$ may be used to produce the categorical trace $Tr^U(L) : X \to Y$ via an inclusion and a (strictly information-forgetting) codiagonal. We may interpret the inclusion as either 'preparation in a known state', or 'the addition of a suitable ancilla'. The physically unreasonable part of the construction of the categorical trace is therefore the codiagonal, due to the no-deleting theorem of (Pati, Braunstein 2001).

We now consider how close we may come to the iterative trace without using the codiagonal — i.e. in a purely physically reasonable manner. Thus, instead of using the twisted dagger to produce a linear map from X to Y, we consider the linear map from $X^{\oplus \omega}$ to $Y^{\oplus \omega}$, given by an inclusion, followed by the twisted dagger operation. Precisely, given a unitary map $L: X \oplus U \to Y \oplus U$ where $\dagger^U(L): U \oplus X^{\oplus \omega} \to Y^{\oplus \omega}$ exists, we consider the composite

$$\oplus^{\omega} X \xrightarrow{\iota_2} U \oplus (\oplus^{\omega} X) \xrightarrow{\dagger^U(L)} \oplus^{\omega} Y$$

Proposition 13.1. Let $L = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathbf{Hilb}_{\mathbf{fd}}(X \oplus U, Y \oplus U)$ be a linear map where $\dagger^{U}(L) \in \mathbf{Hilb}(X^{\oplus \omega}, Y^{\oplus \omega})$ exists. Then the above composite has matrix representation of the form

$$\dot{\tau}^{\mathcal{T}}(L) \circ \iota_{2} = \begin{pmatrix} r_{0} & 0 & 0 & 0 & 0 & \dots \\ r_{1} & r_{0} & 0 & 0 & 0 & \dots \\ r_{2} & r_{1} & r_{0} & 0 & 0 & \dots \\ r_{3} & r_{2} & r_{1} & r_{0} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} : \oplus^{\omega} X \to \oplus^{\omega} Y$$

Proof. This follows by explicit calculation, giving $r_0 = a$, and $r_i = bd^{i-1}c$, for i > 0.

We now observe that matrices of this form specify a subcategory of Hilb, as follows :

Definition 13.2. We define the subcategory \mathcal{T} **Hilb** of **Hilb** as follows:

- Objects of \mathcal{T} **Hilb** are infinite direct sums of the form $X^{\oplus^{\omega}}$, for finite-dimensional Hilbert spaces X.
- The arrows $\mathcal{T}\mathbf{Hilb}(X^{\oplus\omega}, Y^{\oplus\omega})$ are bounded linear maps of the form

$$R = \begin{pmatrix} r_0 & 0 & 0 & 0 & 0 & \dots \\ r_1 & r_0 & 0 & 0 & 0 & \dots \\ r_2 & r_1 & r_0 & 0 & 0 & \dots \\ r_3 & r_2 & r_1 & r_0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} : \oplus^{\omega} X \to \oplus^{\omega} Y$$

— Composition of arrows is the usual composition of linear maps.

Lemma 13.3. *T***Hilb**, as defined above, is a subcategory of (**Hilb**, \oplus).

Proof. The identity matrices at each object are trivially of the required form; we then need to demonstrate that matrices of this form are closed under composition. Consider $R: \oplus^{\omega} X \to \oplus^{\omega} Y$ and $S: \oplus^{\omega} Y \to \oplus^{\omega} Z$ in \mathcal{T} **Hilb**, given by

$$R = \begin{pmatrix} r_0 & 0 & 0 & 0 & 0 & \dots \\ r_1 & r_0 & 0 & 0 & \dots \\ r_2 & r_1 & r_0 & 0 & 0 & \dots \\ r_3 & r_2 & r_1 & r_0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \text{ and } S = \begin{pmatrix} s_0 & 0 & 0 & 0 & 0 & \dots \\ s_1 & s_0 & 0 & 0 & 0 & \dots \\ s_2 & s_1 & s_0 & 0 & 0 & \dots \\ s_3 & s_2 & s_1 & s_0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Then a direct calculation gives that

$$SR = \begin{pmatrix} t_0 & 0 & 0 & 0 & 0 & \cdots \\ t_1 & t_0 & 0 & 0 & 0 & \cdots \\ t_2 & t_1 & t_0 & 0 & 0 & \cdots \\ t_3 & t_2 & t_1 & t_0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

where $t_k = \sum_{k=j+i} s_j r_i$. Associativity is inherited from **Hilb**, and so our result follows.

Corollary 13.4. The category \mathcal{T} **Hilb** is a representation in **Hilb** of (summable) lists of linear maps, together with a convolution product.

Proof. It is immediate that arrows $R : \bigoplus^{\omega} X \to \bigoplus^{\omega} Y$ and $S : \bigoplus^{\omega} Y \to \bigoplus^{\omega} Z$ in \mathcal{T} **Hilb** are uniquely specified by (summable) lists of linear maps $\{R_i : X \to Y\}_{i \in \mathbb{N}}$ and $\{S_j : Y \to Z\}_{j \in \mathbb{N}}$. Lemma 13.3 demonstrates that the composite SR is uniquely specified

by the list

$$\left\{ t_k = \sum_{k=j+i} S_j R_i : X \to Y \right\}_{k \in \mathbb{N}}$$

At this point, we wish to give a full categorical theory of convolved lists over Hilbert space, with special emphasis on those arising from the twisted dagger of unitary maps. However, in order to give a systematic treatment of this theory, we do it for the general case of categories carrying PCM structures.

14. Convolution Categories

We give a general categorical construction based on convolutions of lists, applicable to categories carrying PCM structures. The setting for this operation is the category of all categories carrying a PCM-structure :

Definition 14.1. The category PCM-Cat is defined as follows :

- Objects The objects of PCM-Cat are categories carrying PCM-structures, as in Definition 5.1.
- Arrows An arrow $\Gamma \in \mathbf{PCM-Cat}(\mathcal{C}, \mathcal{D})$ is a functor from \mathcal{C} to \mathcal{D} that 'respects the summation'. That is, for all summable indexed families $\{f_i \in \mathcal{C}(X, Y)\}_{i \in I}$, the family $\{\Gamma(f_i) \in \mathcal{D}(\Gamma(X), \Gamma(Y))\}_{i \in I}$ is also summable, and $\Gamma(\sum_{i \in I} f_i) = \sum_{i \in I} (\Gamma(f_i))$.

Definition 14.2. The convolution category construction

Let C be a category carrying a PCM structure. The **convolution category** over C, denoted **Con**(C), is defined as follows:

- The objects of $\mathbf{Con}(\mathcal{C})$ are exactly the objects of \mathcal{C} .
- An arrow $F \in \mathbf{Con}(\mathcal{C})(X,Y)$ is an infinite summable list (F_0, F_1, F_2, \ldots) over $\mathcal{C}(X,Y)$. Equivalently, an arrow $F : X \to Y$ in $\mathbf{Con}(\mathcal{C})$ is simply a function $F : \mathbb{N} \to \mathcal{C}(X,Y)$ where $\{F(i) : X \to Y\}_{i \in \mathbb{N}}$ is a summable family.
- Composition of arrows is given by the *convolution of lists*, so

$$(GF)(k) = \sum_{i+j=k} G(j)F(i)$$

Theorem 14.3. Let C be a category carrying a PCM structure (i.e. a member of **PCM-Cat**). Then

- 1 $\mathbf{Con}(\mathcal{C})$ is well-defined as a category.
- 2 C is a *retract* of $\mathbf{Con}(C)$, so there exists a pair of functors $\sigma_{\mathcal{C}} : \mathbf{Con}(C) \to C$ and $\eta_{\mathcal{C}} : C \to \mathbf{Con}(C)$ satisfying $\sigma_{\mathcal{C}}\eta_{\mathcal{C}} = Id_{\mathcal{C}}$.
- 3 $\mathbf{Con}(\mathcal{C})$ carries a PCM structure.

Proof.

1 Given $F \in \mathbf{Con}(\mathcal{C})(X, Y)$ and $G \in \mathbf{Con}(\mathcal{C})(Y, Z)$, we must show that $(GF)(k) = \sum_{i+j=k} G(j)F(i)$ is well-defined, i.e. we need to show that (GF)(k) exists for all

 $k \in \mathbb{N}$, and the family $\{(GF)(k)\}_{k \in \mathbb{N}}$ is summable. Observe that (by definition), $\sum_{i=0}^{\infty} F(i) \in \mathcal{C}(X, Y)$ exists, as does $\sum_{j=0}^{\infty} G(j) \in \mathcal{C}(Y, Z)$. Thus their composite $(\sum_{j=0}^{\infty} G(j))(\sum_{i=0}^{\infty} F(i)) = \sum_{i,j} G(j)F(i)$ exists. In particular, the doubly indexed family $\{G(j)F(i)\}_{i,j}$ is summable. Consider the sets $H_k = \{(i,j) \mid i+j=k\}$. These sets form a partition of \mathbb{N}^2 , by the usual Cantor enumeration. For each $k \in \mathbb{N}$, the family $\{G(j)F(i)\}_{(i,j)\in H_k}$ is a (finite) subfamily of the summable family $\{G(j)F(i)\}_{i,j}$ and is thus summable. So by weak partition associativity, $\sum_{i,j} G(j)F(i) = \sum_{k \in \mathbb{N}} \sum_{(i,j)\in H_k} G(j)F(i)$ exists, as required. The associativity of composition follows from the associativity of composition in \mathcal{C} , together with the associativity of the partial summation given by the Σ -structure: $(HGF)(l) = \sum_{l=k+j+i} H(k)G(j)F(i)$. Finally, the existence of identities follows from the existence of zeros in PCMs. The identity at an object X is simply $Id_X(i) = \int 1_X i = 0$

- $\begin{cases} 1_X & i = 0\\ 0_{XX} & i \neq 0 \end{cases}$
- 2 We give the functors $\sigma_{\mathcal{C}} : \mathbf{Con}(\mathcal{C}) \to \mathcal{C}$ and $\eta_{\mathcal{C}} : \mathcal{C} \to \mathbf{Con}(\mathcal{C})$ explicitly. They are both the identity on objects; on arrows,

$$\sigma_{\mathcal{C}}(F) = \sum_{i=0}^{\infty} F(i) : X \to Y \ \forall \ F \in \operatorname{\mathbf{Con}}(\mathcal{C})(X,Y)$$

similarly,

$$\eta_{\mathcal{C}}(L)(i) = \begin{cases} L & i = 0\\ 0_{X,Y} & i \neq 0 \end{cases} \quad \forall \ L \in \mathcal{C}(X,Y)$$

It is almost immediate that these are functors, and satisfy $\sigma_{\mathcal{C}}\eta_{\mathcal{C}} = Id_{\mathcal{C}}$. Hence \mathcal{C} is a *retract* of **Con**(\mathcal{C}).

3 The notion of summation is inherited in a pointwise manner. A countable indexed family $\{F_{\alpha}\}_{\alpha \in A}$ is summable, denoted $\sum_{\alpha \in A} F_{\alpha}$ exactly when, for each $i \in \mathbb{N}$, the sum $\sum_{\alpha \in A} F_{\alpha}(i)$ exists, as does $\sum_{\alpha \in A} F_{\alpha}(i)$. In this case, we define

$$\left(\sum_{\alpha \in A} F_{\alpha}\right)(i) = \sum_{\alpha \in A} F_{\alpha}(i)$$

It is almost immediate that $\mathbf{Con}(\mathcal{C})$ carries the same Σ -structure as \mathcal{C} i.e. when \mathcal{C} carries (for example) a PAM structure, so does $\mathbf{Con}(\mathcal{C})$.

Corollary 14.4. Con is a functor from PCM-Cat to itself.

Proof. Let C and D objects in **PCM-Cat**. From Theorem 14.3, Con(C) and Con(D) are objects in **PCM-Cat**. It remains to give the definition of **Con** on arrows of **PCM-Cat** (i.e functors between categories carrying PCM structures), and check functoriality of **Con** : **PCM-Cat** \rightarrow **PCM-Cat**.

Given $\Gamma \in \mathbf{PCM-Cat}(\mathcal{C}, \mathcal{D})$ (i.e. a summation-preserving functor from \mathcal{C} to \mathcal{D}), we define

$$\operatorname{Con}(\Gamma) : \operatorname{Con}(\mathcal{C})(X,Y) \to \operatorname{Con}(\mathcal{D})(\Gamma(X),\Gamma(Y))$$

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as follows:

Given $F \in \mathbf{Con}(\mathcal{C})(X, Y)$, specified by

$$F: \mathbb{N} \to \mathcal{C}(X, Y)$$

we define

$$Con(\Gamma)(F) : \mathbb{N} \to \mathcal{D}(\Gamma(X), \Gamma(Y))$$

by $\operatorname{Con}(\Gamma)(F)(n) = \Gamma(F(n))$. To show that this is functorial, consider $\Delta \in \operatorname{PCM-Cat}(\mathcal{D}, \mathcal{E})$ (i.e. a summation-preserving functor from \mathcal{D} to \mathcal{E}). From the definition,

$$\mathbf{Con}(\Delta)\mathbf{Con}(\Gamma)(F)(n) = \Delta\Gamma(F(n)) = \mathbf{Con}(\Delta\Gamma)(F)(n)$$

and hence **Con** is functorial.

The **Con** functor preserves a number of interesting structures within **PCM-Cat**, as follows :

Theorem 14.5. Let C be a category carrying a Σ -structure, with a (symmetric) monoidal tensor \oplus that is **compatible with summation** in the sense that, for all families $\{f_i\}_{i \in I} \subseteq C(X, Y)$ and $\{g_j\}_{j \in J} \subseteq C(A, B)$,

$$\sum_{(i,j)\in I\times J}f_i\oplus g_j\ \simeq\ \left(\sum_{i\in I}f_i\right)\oplus \left(\sum_{j\in J}g_j\right)$$

(note the use of Kleene equality). Then

- 1 $\mathbf{Con}(\mathcal{C})$ is a (symmetric) monoidal category.
- 2 When \mathcal{C} has quasi-projections and quasi-inclusions, so does $\mathbf{Con}(\mathcal{C})$.
- 3 When C has a (possibly partial) categorical trace, so does $\mathbf{Con}(C)$, and this trace satisfies, for all $F \in \mathbf{Con}(C)(X \oplus U, Y \oplus U)$,

$$Tr_{X,Y}^U(F)$$
 exists, exactly when $Tr_{X,Y}^U\left(\sum_{i=0}^{\infty} F(i)\right)$ exists in \mathcal{C}

4 The functors $\sigma_{\mathcal{C}}$ and $\eta_{\mathcal{C}}$ of Theorem 14.3 preserve the categorical trace.

Proof.

- 1 The monoidal tensor on $\mathbf{Con}(\mathcal{C})$ is defined in terms of the monoidal tensor of \mathcal{C} :
 - The object $A \oplus B$ in $\mathbf{Con}(\mathcal{C})$ exactly the object $A \oplus B$ in \mathcal{C} .
 - The tensor on arrows is defined by a convolution,

$$(F \oplus G)(k) = \sum_{k=j+i} F(j) \oplus G(i)$$

The assumption that the monoidal tensor is compatible with the summation, and similar considerations to the proof of Theorem 14.3 demonstrate that this is well-defined. To show that this is indeed a monoidal tensor, consider

$$K \in \mathbf{Con}(\mathcal{C})(Y, V) \quad G \in \mathbf{Con}(\mathcal{C})(B, Y) H \in \mathbf{Con}(\mathcal{C})(X, U) \quad F \in \mathbf{Con}(\mathcal{C})(A, X)$$

Then $(H \oplus K)(F \oplus G)(n) = \sum_{x+y=n} (H \oplus K)(x)(F \oplus G)(y)$, and by definition

$$(H \oplus K)(x) = \sum_{a+b=x} H(a) \oplus K(b) \quad , \quad (F \oplus G)(y) = \sum_{p+q=y} F(p) \oplus G(q)$$

Therefore,

$$(H \oplus K)(F \oplus G)(n) = \sum_{x+y=n} \left(\sum_{a+b=x} H(a) \oplus K(b) \right) \left(\sum_{p+q=y} F(p) \oplus G(q) \right)$$

Using the distributivity of summation over composition, and rearranging indices

$$(H \oplus K)(F \oplus G)(n) = \sum_{a+b+p+q=n} (H(a)F(p) \oplus K(b)G(q))$$

Conversely, $(HF \oplus KG)(n) = \sum_{n=\alpha+\beta} HF(\alpha) \oplus KG(\beta)$ and by the definition of composition in **Con**(C),

$$(HF \oplus KG)(n) = \sum_{n=\alpha+\beta} \left(\left(\sum_{\alpha=\gamma+\delta} H(\gamma)F(\delta) \right) \oplus \left(\sum_{\beta=\lambda+\mu} K(\lambda)G(\mu) \right) \right)$$

Again using the distributivity of composition over summation and rearranging indices,

$$(HF \oplus KG)(n) = \sum_{\gamma + \delta + \lambda + \mu = n} (H(\gamma)F(\delta) \oplus K(\lambda)G(\mu))$$

so we deduce that $(H \oplus K)(F \oplus G)(n) = (HF \oplus KG)(n)$, as required. The proof that $1_X \oplus 1_Y = 1_{X \oplus Y}$ is also immediate. For the symmetry and associativity conditions, we denote the symmetry and associativity isomorphisms of \mathcal{C} by $s_{X,Y}$ and $\alpha_{X,Y,Z}$ respectively, and define

$$S_{XY} = \eta_{\mathcal{C}}(s_{X,Y}) \in \mathbf{Con}(\mathcal{C})(X \oplus Y, Y \oplus X)$$
$$T_{XYZ} = \eta_{\mathcal{C}}(\alpha_{X,Y,Z}) \in \mathbf{Con}(\mathcal{C})(X \oplus (Y \oplus Z), (X \oplus Y) \oplus Z)$$

As $\eta_{\mathcal{C}}$ is a functor, S_{-} and T_{-} also satisfy the MacLane Pentagon and Commutativity Hexagon conditions (MacLane 1998). Hence, by the uniqueess of canonical isomorphisms, $\mathbf{Con}(\mathcal{C})$ is a symmetric monoidal category.

- 2 Given $U = X \oplus Y$, the quasi-projections in $\mathbf{Con}(\mathcal{C})$ are given by $\eta_{\mathcal{C}}(\pi_X)$ and $\eta_{\mathcal{C}}(\pi_Y)$ respectively. Similarly for the quasi-inclusions, and it is readily verified that these satisfy the conditions given in Definition 8.1.
- 3 Let $F: X \oplus U \to Y \oplus U$ be an arrow in $\mathbf{Con}(\mathcal{C})$. Then, as $\mathbf{Con}(\mathcal{C})$ has quasi-projections and quasi-inclusions, we may write

$$F = \left(\begin{array}{cc} P & Q \\ R & S \end{array}\right) \colon X \oplus U \to Y \oplus U$$

However, as the quasi-projections and quasi-inclusions at an object $A \in Ob(\mathbf{Con}(\mathcal{C}))$ are given in terms of the inclusion functor $\eta_{\mathcal{C}}$ by

$$\eta_{\mathcal{C}}(\pi_A) = (\pi_A, 0, 0, \ldots) , \quad \eta_{\mathcal{C}}(\iota_A) = (\iota_A, 0, 0, \ldots)$$

respectively, we may find the elements P, Q, R, S as follows:

$$- P(i) = (\eta_{\mathcal{C}}(\pi_Y)F\eta_{\mathcal{C}}(\iota_X))(i) = \pi_Y F(i)\iota_X \in \mathcal{C}(X,X) - Q(i) = (\eta_{\mathcal{C}}(\pi_Y)F\eta_{\mathcal{C}}(\iota_U))(i) = \pi_Y F(i)\iota_U \in \mathcal{C}(U,Y) - R(i) = (\eta_{\mathcal{C}}(\pi_U)F\eta_{\mathcal{C}}(\iota_X))(i) = \pi_U F(i)\iota_X \in \mathcal{C}(X,U) - S(i) = (\eta_{\mathcal{C}}(\pi_U)F\eta_{\mathcal{C}}(\iota_U))(i) = \pi_U F_(i)\iota_U \in \mathcal{C}(U,U)$$

Hence we may deduce that

$$\sigma(F) = \left(\begin{array}{cc} \sigma(P) & \sigma(Q) \\ \sigma(R) & \sigma(S) \end{array}\right)$$

and as \mathcal{C} is traced,

$$Tr^U_{X,Y}(\sigma(F)) = \sigma(P) + \sum_{i=0}^{\infty} \sigma(Q)\sigma(S)^i \sigma(R)$$

and further,

$$\sigma(Tr^U_{X,Y}(F)) = Tr^U_{X,Y}(\sigma(F)).$$

Therefore,

$$P + \sum_{i=0}^{\infty} QS^i R$$
 exists in $\mathbf{Con}(\mathcal{C})$

4 A corollary of 3. above is that $\sigma_{\mathcal{C}}$ preserves the categorical trace. The proof that the functor $\eta_{\mathcal{C}} : \mathcal{C} \to \mathbf{Con}(\mathcal{C})$ also preserves the trace of ΣMCs follows immediately from the fact that it is an embedding of \mathcal{C} into $\mathbf{Con}(\mathcal{C})$, and from the definition of summation in $\mathbf{Con}(\mathcal{C})$.

14.1. A monad based on Convolution

We now demonstrate that the **Con** functor, together with two natural transformations that we give below, forms a monad. We refer to (Moggi 1991) for the classic work on monads and computation, and to (Jones, Wadler 1993) for a common interpretation of monads as implementations of input / output and other side-effects within functional programming languages.

Lemma 14.6. The indexed family of functors

$$\eta_{\mathcal{C}}: \mathcal{C} \to \mathbf{Con}(\mathcal{C}) \ \forall \ \mathcal{C} \in Ob(\mathbf{PCM-Cat})$$

given in Theorem 14.3, part 2., are the components of a natural transformation from the identity functor on **PCM-Cat** to the convolution functor on **PCM-Cat**.

Proof. To demonstrate that the indexed family $\eta_{\mathcal{C}}$, for $\mathcal{C} \in Ob(\mathbf{PCM-Cat})$ gives the components of a natural transformation, consider objects of **PCM-Cat**, \mathcal{C}, \mathcal{D} together with a summation-preserving functor (i.e. an arrow of **PCM-Cat**) $\Gamma : \mathcal{C} \to \mathcal{D}$. By

functoriality, it is almost immediate that the following diagram commutes



and hence the family $\eta_{\mathcal{C}}$ gives the components of a natural transformation. We denote this natural transformation by $\eta: I_{\mathbf{PCM-Cat}} \twoheadrightarrow \mathbf{Con}$.

In a similar way, there is a natural transformation from the endofunctor $Con(Con(_))$ to the endofunctor $Con(_)$ with components given in Theorem 14.3.

Lemma 14.7. Let us define an indexed family of functors $\mu_{\mathcal{C}}$, for all \mathcal{C} in $Ob(\mathbf{PCM-Cat})$, by $\mu_{\mathcal{C}} = \sigma_{\mathbf{Con}(\mathcal{C})}$, where for arbitrary $X \in Ob(\mathbf{PCM-Cat})$, the summation-preserving functor (i.e. arrow in **PCM-Cat**) $\sigma_{\mathcal{X}} : \mathbf{Con}(\mathcal{X}) \to \mathcal{X}$ is as defined in Theorem 14.3. Then the family

$$\mu_{\mathcal{C}} : \mathbf{Con}(\mathbf{Con}(\mathcal{C})) \to \mathbf{Con}(\mathcal{C}) \quad \forall \ C \in Ob(\mathbf{PCM-Cat})$$

gives the components of a natural transformation from Con(Con()) to Con().

Proof. Consider arbitrary objects of **PCM-Cat** \mathcal{C}, \mathcal{D} , together with an arrow $\Gamma \in \mathbf{PCM-Cat}(\mathcal{C}, \mathcal{D})$ (i.e. a summation-preserving functor). By functoriality, it is immediate that the following diagram commutes :



Hence the family $\mu_{\mathcal{C}}$ gives the components of a natural transformation. We denote this natural transformation by $\mu : \mathbf{Con}(\mathbf{Con}(_)) \to \mathbf{Con}(_)$.

As may be expected, we now use Lemmas 14.6 and 14.7 above to give a monad based on the **Con** functor. However, we first give a preliminary result on the structure of **Con**^K(\mathcal{C}), for an category \mathcal{C} carrying a PCM-structure.

Lemma 14.8. Let \mathcal{C} be an object of **PCM-Cat**. Then

- 1 The objects of $\mathbf{Con}^{K}(\mathcal{C})$ are exactly the objects of \mathcal{C} .
- 2 An arrow $F \in \mathbf{Con}^{K}(\mathcal{C})(X,Y)$ is specified by an arrow

 $\tilde{F}: \mathbb{N}^K \to \mathcal{C}(X, Y)$ such that $\{\tilde{F}(i_1, i_2, \dots, i_K)\}_{(i_1, i_2, \dots, i_K) \in \mathbb{N}^K}$ is summable.

Proof.

1 This is immediate, since for an category \mathcal{M} carrying a PCM-structure, both $\mathbf{Con}(\mathcal{M})$ and \mathcal{M} have the same objects.

2 Recall that an arrow $G \in \mathbf{Con}(\mathcal{C})(X,Y)$ is specified by a function $G : \mathbb{N} \to \mathcal{C}(X,Y)$. Hence an arrow $F \in \mathbf{Con}^{K}(\mathcal{C})(X,Y)$ is specified by a function $F : \mathbb{N} \to \mathbf{Con}^{K-1}(\mathcal{C})(X,Y)$. Extending this process by induction we have that

$$F: \mathbb{N} \to [\mathbb{N} \to [\dots [\mathbb{N} \to (\mathcal{C}(X, Y)] \dots]]$$

By currying, we observe that $F \in \mathbf{Con}^{K}(\mathcal{C})(X, Y)$ is exactly equivalent to an arrow $\tilde{F} : \mathbb{N}^{K} \to \mathcal{C}(X, Y)$. Now recall that for an arbitrary arrow $G \in \mathbf{Con}(\mathcal{C})(X, Y)$ specified by a function $G : \mathbb{N} \to \mathcal{C}(X, Y)$, the family $\{G(n) \in \mathcal{C}(X, Y)\}_{n \in \mathbb{N}}$ is required to be summable. Hence, for the arrow $F \in \mathbf{Con}^{K}(\mathcal{C})(X, Y)$, this is the requirement that $\{F(n_1) \in \mathbf{Con}^{K-1}(\mathcal{C})(X, Y)\}_{n_1 \in \mathbb{N}}$ is a summable family in $\mathbf{Con}^{K-1}(\mathcal{C})$. However, by definition of summation in a convolution category (from Theorem 14.3), we deduce that $\{F(n_1)(n_2) \in \mathbf{Con}^{K-2}(\mathcal{C})(X, Y)\}_{n_1, n_2 \in \mathbb{N}}$ must also be a summable family. Iterating this process, it follows that $\{F(n_1)(n_2) \ldots (n_K) \in (\mathcal{C})(X, Y)\}_{n_1, n_2, \ldots, n_K \in \mathbb{N}}$ is a summable family, and our result holds by currying.

Remark From Lemma 14.8, we observe a close connection between multiple applications of the **Con** functor, isomorphisms $\mathbb{N}^K \cong \mathbb{N}$, and partitions of \mathbb{N} into multiple countably infinite subsets^{§§}. This raises the intriguing possibility of using the self-embedding techniques of (Hines 1997; Hines 1999) to study the convolution construction. Unfortunately, this is beyond the scope of this paper.

Theorem 14.9. The triplet $(\mathbf{Con}, \eta, \mu)$ is a monad.

Proof. Consider an arbitrary category C carrying a PCM-structure. Then by Lemma 14.8, the following diagram commutes :



Similarly, using the same currying technique as Lemma 14.8, the following diagram

^{§§} Note that such partitions require and rely on the weak partition-associativity axiom — in particular the Higgs (I) and Higgs (II) Σ -group axioms are *not* strong enough to allow for such partitions

 $\operatorname{commutes}$:



Finally, by Lemma 14.6 and Lemma 14.7 above, the various η_X and μ_Y in the above diagrams are the components of natural transformations $\eta : I_{\mathbf{PCM-Cat}} \twoheadrightarrow \mathbf{Con}$ and $\mu : \mathbf{Con}(\mathbf{Con}(\underline{)}) \to \mathbf{Con}(\underline{)}$. Therefore, we deduce that $(\mathbf{Con}, \eta, \mu)$ is a monad.

Hence, the convolution construction (which, broadly speaking, keeps track of the passage of time within a computation), together with the above natural transformations is a monad (i.e. the type of structure generally used to represent side-effects within functional programming (Jones, Wadler 1993)).

We now consider the connection between the partial iterative trace in the convolution category $Con(Hilb_{fd})$, and the twisted dagger construction of Section 12.

15. Embedding $Con(\mathcal{C})$ into \mathcal{C}

Given the intuitive description of **Con** as 'forming convolved lists', it is perhaps unsurprising that there exists an embedding of C into **Con**(C), as shown in Theorem 14.3, part 2. What is less intuitive is the existence (under relatively straightforward assumptions) of an embedding of **Con**(C) into C.

Definition 15.1. The rearrangement axiom

Let \mathcal{C}, \oplus be a category carrying a PCM structure that has countably infinite monoidal tensors and quasi-projections and quasi-injections (as in Definition 8.1).

Given an arbitrary summable family $\{f_i : X \to Y\}_{i \in I}$ and arbitrary families $\{\iota_i : Y \to \oplus^{\omega} Y\}_{i \in I}$ and $\{\pi_i : \oplus^{\omega} X \to X\}_{i \in I}$ of quasi-injections and quasi-projections *indexed* by the same index set I, we say that (\mathcal{C}, \oplus) satisfies the **rearrangement axiom** when $\{\iota_i f_i \pi_i : \oplus^{\omega} X_i \to \oplus^{\omega} Y_i\}_{i \in I}$ is also a summable family.

A simple consequences of the rearrangement axiom is that given a summable family $\{f_i : X \to Y\}_{i \in \mathbb{N}}$, then the infinite monoidal tensor $\bigoplus_{i=0}^{\infty} f_i : \bigoplus X^{\omega} \to \bigoplus Y^{\omega}$ exists, as does the map $\pi_0 \sum_{i=0}^{\infty} (\iota_0 f_i \pi_i) : \bigoplus^{\omega} X \to Y$.

It is straightforward to check that all categories carrying PCM structures (that also have infinite quasi-projections and quasi-injections) from Examples 6.1 and 6.3 satisfy this axiom.

Theorem 15.2. Let \mathcal{C} be a category carrying a PCM structure that also has countably infinite monoidal tensors and matrix representations, and satisfies the rearrangement axiom. Then there exists a faithful functor $\Gamma_{\mathcal{C}} : \mathbf{Con}(\mathcal{C}) \to \mathcal{C}$.

Proof. We define $\Gamma_{\mathcal{C}}$ as follows :

- (on objects) $\Gamma_{\mathcal{C}}(X) = \bigoplus^{\omega} X$, for all $X \in Ob(\mathbf{Con}(\mathcal{C})) = Ob(\mathcal{C})$.
- on arrows Given $f \in \mathbf{Con}(\mathcal{C})(X, Y)$, as a function $f : \mathbb{N} \to \mathcal{C}(X, Y)$, we define $F = \Gamma_{\mathcal{C}}(f) \in \mathcal{C}(\bigoplus^{\omega} X, \bigoplus^{\omega} Y)$ by the matrix

$$F = (F_{ij})_{i,j \in \mathbb{N}}$$
 where $F_{ij} = \begin{cases} f(j-i) & j \ge i \\ 0 & \text{otherwise.} \end{cases}$

By the rearrangement axiom, this is the matrix representation of an arrow of C, since the family $\{f(i)\}_{i \in \mathbb{N}}$ is summable. Functoriality follows from the usual formula for matrix composition : given $r \in \mathbf{Con}(\mathcal{C})(X, Y)$ and $s \in \mathbf{Con}(\mathcal{C})(Y, Z)$, then

$$\Gamma_{\mathcal{C}}(r) = \begin{pmatrix} r(0) & 0 & 0 & \dots \\ r(1) & r(0) & 0 & \dots \\ r(2) & r(1) & r(0) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \text{ and } \Gamma_{\mathcal{C}}(s) = \begin{pmatrix} s(0) & 0 & 0 & \dots \\ s(1) & s(0) & 0 & \dots \\ s(2) & s(1) & s(0) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Direct calculation gives $\Gamma_{\mathcal{C}}(s)\Gamma_{\mathcal{C}}(r) = \begin{pmatrix} t_0 & 0 & 0 & \dots \\ t_1 & t_0 & 0 & \dots \\ t_2 & t_1 & t_0 & \dots \end{pmatrix}$ where $t_k = \sum_{k=j+i} s_j r_i$.

Direct calculation gives $\Gamma_{\mathcal{C}}(s)\Gamma_{\mathcal{C}}(r) = \begin{pmatrix} t_2 & t_1 & t_0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$ where $t_k = \sum_{k=j+i} s_j r_i$.

Hence $\Gamma_{\mathcal{C}}(s)\Gamma_{\mathcal{C}}(r) = \Gamma_{\mathcal{C}}(sr)$. The proof that $\Gamma_{\mathcal{C}}(1_X) = 1_{\bigoplus_{\omega X}}$ is then straightforward. \Box

Corollary 15.3. The subcategory \mathcal{T} Hilb of Definition 13.2 is the image of Con(Hilb_{fd}) under the functor Γ_{Hilb} .

16. Applications to quantum computation

Using the twisted dagger of a unitary matrix, we now use the interpretation as a categorical trace (Section 12.3), and the flowchart interpretation of the iterative trace (Section 10) to give a notion of conditional iteration in quantum computation. As a preliminary, we describe how such iteration works in the classical setting. Given a classical iterative algorithm expressed in these terms, we demonstrate how to produce a quantum subroutine that behaves like this classical algorithm on the computational basis, and acts linearly on superpositions of basis states.

Such subroutines are important in Grover's search algorithm (Grover 1996), and the canonical example of a quantum subroutine that behaves in this way is the computation of superpositions of modular exponentials required for Shor's algorithm (Shor 1999). Although our scheme for quantum-mechanical iteration may indeed be used to calculate such a superposition, this particular calculation is amenable to a great deal of optimisation before any iterative steps are required (R. van Meter, K. Itoh 2005). Instead of going through this particular example, we present a general scheme for producing a quantum-mechanical reversible algorithm.

There is a slight complication in that the notion of iteration we have for quantummechanical systems (i.e. the twisted dagger on unitary maps) requires an ancillary register that 'keeps track of the number of iterative cycles' in the computation. In the course of the computation, this register becomes entangled with the result of the computation, and hence causes decoherence (Myers 1997; Linden, Popescue 1998; Hagar, Korolev 2004). To produce a usable quantum resource we must disentangle the result of the computation from the ancillary space — this is achieved using techniques similar, but not identical, to those found in (Bennett 1973).

16.1. Classical reversible iteration, via the trace

For a (classical reversible) notion of iteration provided by the particle-style trace, we require :

— A set of k variables, $\{v_1, v_2, \ldots, v_k\}$, where each v_i is a member of \mathbb{Z}_{n_i} .

— A reversible operation F that updates these variables.

— A set of halting conditions.

Mathematically, the complete set of variables is specified by a vector $\underline{x} = (v_1, \ldots, v_n) \in X = \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_1} \times \ldots \times \mathbb{Z}_{n_k}$, and F is a bijection on this set. As X is finite, the bijection $F: X \to X$ is trivially a computable function – for simplicity, we assume F is defined by primitive arithmetic operations (but *not* primitive recursion) on the set of k variables.

The halting conditions may be specified either by conditions on the variables x_1, \ldots, x_k , or (equivalently) a subset $H \subseteq X$ that we call the **halting subset**. For example, setting the halting condition " $(v_1 = v_2) OR (v_2 = 5 AND v_3 = 17)$ " is equivalent to specifying the halting subset

$$\{(n,n): n \le \min(n_1,n_2)\} \times \mathbb{Z}_{n_3} \times \ldots \times \mathbb{Z}_{n_k} \bigcup \mathbb{Z}_{n_1} \times \{5\} \times \{17\} \times \ldots \times \mathbb{Z}_{n_k}$$

We will denote the complement of H by C, so $X \cong H \uplus C$, and write $F : H \uplus C \to H \uplus C$. The iterative trace (in the category **pInj**) may be used to eliminate the behaviour of F on the subspace C, giving a partial injection $Tr^{C}(F) : H \to H$, and we have seen in Proposition 9.6 that as X is a finite set, $Tr^{C}(F)$ is in fact a bijection.

The flowchart and algebraic semantics interpretations given in Section 10 (together with the simplification provided by the fact that F is a bijection) may by used to give an interpretation of $Tr^{C}(F)$ as the following subroutine :

Input
$$\underline{x} \in H$$
;
 $Do \{\underline{x} \mapsto F(\underline{x});\}$ (While $\underline{x} \in C$)
 $Return \ x \in H$;

Note that the typing of the categorical trace forces H to act both as a starting and a halting subset^{¶¶}. We denote the bijection computed by this subroutine by $M: H \to H$.

Our stated aim is then to produce a quantum-mechanical version of the subroutine, that computes M on the computational basis, and is superposition-preserving.

^{¶¶} This constraint can be relaxed to give distinct starting / halting subsets $S, H \subseteq X$, simply by conjugating F by a bijection σ that interchanges S and H. We do not present this extension explicitly, but note that in this generalisation the starting and halting subsets must be of the same size.

16.2. Classical reversible iteration, via the twisted dagger

Classically, the modifications required in order to use the twisted dagger, rather than the iterative trace, as a notion of iteration are straightforward. We simply need an extra variable that keeps track of the number of iterative cycles in a computation — this allows us to work in the convolution category **Con**(**pInj**). Given **variables**, $\{v_1, v_2, \ldots, v_k\}$, a **reversible operation** F updating these variables, and a set of **halting conditions**, as before, a canonical inclusion followed by twisted dagger (as in Section 12.2) has the following interpretation

$$Input \ (n, \underline{x}) \in \mathbb{N} \times H;$$

$$Do \qquad \{ \underline{x} \ \mapsto \ F(\underline{x}); \\ n \mapsto n+1; \} \ (While \ \underline{x} \in C)$$

$$Return \ (n, x) \in \mathbb{N} \times H;$$

We thus see that the convolution construction has the simple interpretation of 'keeping track of the number of iterative cycles required in a computation', so instead of simply computing the function $M : H \to H$ given above, the twisted dagger computes the function $M' : \mathbb{N} \times H \to \mathbb{N} \times H$, given by M'(n,h) = (n+k, M(h)) where k is the number of steps required for the algorithm in Section 16.1 to terminate on the input h.

Finally, note that as the configuration set X is finite, not only do we have guaranteed termination (Proposition 9.6), but there exists an upper bound K to the number of possible iterative cycles required before termination. Although an upper bound may be given by basic combinatorics, this will be, in most cases, a vast overestimate — the arithmetic structure of the update function F may often be used to provide a substantially tighter, if not exact, upper bound^{||||}

17. Quantum-mechanical iteration

We now consider how the twisted dagger may be used to provide a notion of conditional iteration in quantum-mechanical systems. Precisely, given a classical, reversible, algorithm based on iteration (presented in terms of the constructions of Section 16.2 above), we demonstrate how to produce a quantum-mechanical subroutine that not only reproduces the behaviour of this classical algorithm on the computational basis, but is superposition-preserving. We emphasise that this is just one application of our general notion of quantum iteration; further applications (including iterating operations with no classical counterpart) will be considered in subsequent papers.

Also, although the twisted dagger provides a notion of iteration, recall from the discussion following Theorem 12.2 that the twisted dagger is properly thought of as the limit of

III The existence of an upper bound is crucial, not only for termination, but also to allow us to disentangle the 'clock space' from the result of the computation – although we only require an upper bound, not the least upper bound or the exact number of steps to termination. This is in contrast to the approach of (Bernstein, Vazirani 1997), where iteration (based on quantum Turing machines) is restricted to the case where computation must terminate in a fixed number of steps, regardless of the input.

a series of physical operations, rather than a physical operation in its own right. Because of this, we first express the computation in terms of the twisted dagger, and then justify using the finite iterates, rather than the twisted dagger itself.

17.1. The twisted dagger, as quantum-mechanical iteration

In the classical reversible algorithm give above, we have

- A vector $\underline{x} = (v_1, \ldots, v_n) \in X = \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_1} \times \ldots \times \mathbb{Z}_{n_k}$ of variables.
- An update bijection $F: X \to X$.
- A starting / halting subset $H \subseteq X$, and its complement $C \subseteq X$.

We require complex spaces with bases indexed by the sets X, H and C respectively, giving

- $-l_2(X)$, with basis $\{|x\rangle : x \in X\}$
- $-l_2(H)$, with basis $\{|h\rangle : h \in H \subseteq X\}$
- $-l_2(C)$, with basis $\{|c\rangle : c \in C \subseteq X\}$

(Note that $l_2(X) \cong l_2(H) \oplus l_2(C)$). We also 'lift' the bijection F to a linear map, $U_f : l_2(X) \to l_2(X)$ defined by $U_f|x\rangle = |F(x)\rangle$ and as U_f is simply a permutation of basis vectors, it is trivially unitary. As (by assumption) F is defined by primitive arithmetic operations (*excluding* recursion), this unitary map be efficiently constructed — although the construction of quantum-mechanical versions of arithmetic operations is an interesting non-trivial field in its own right. We refer to (Nielsen, Chuang 1991; Vedral et. al. 1996; van Meter et. al. 2006) for a good overview.

For the twisted dagger, we require an additional ancillary 'clock space' T, with orthonormal basis $\{|0\rangle, |1\rangle, |2\rangle, \ldots\}$. This allows us to construct the required infinite coproduct using the distributivity isomorphism, giving $\bigoplus^{\omega} l_2(H) \cong T \otimes l_2(H)$.

The twisted dagger (composed with a canonical inclusion, as in Section 12.2) then provides a map $\Psi = \dagger^{l_2(C)}(U_f)\iota : T \otimes l_2(H) \to T \otimes l_2(H)$ that acts on the computational basis as follows :

$$\Psi(|t\rangle|h\rangle) = |t+k_h\rangle|M(h)\rangle$$

where k_h is the number of steps required for the algorithm of Section 16.1 to terminate on the input *h*. Finally, recall from Section 16.2 that we may set an upper bound *K* so that $h_k < K$, for all inputs.

17.2. Disentangling the clock space

In Section 17.1 above, we have produced an algorithm that implements the following function

$$\Psi_F(|t\rangle|h\rangle) = |t+k_h\rangle|M(h)\rangle$$

where M is the (classical) function implemented by the algorithm of Section 16.1, and k_h is the number of steps required for this algorithm to halt on the input h. However, for a superposition of basis states of $l_2(H)$ this algorithm will, in general entangle of the clock space with the result of the computation (see (Myers 1997; Linden, Popescue 1998;

Hagar, Korolev 2004) for why this is undesirable for quantum algorithms). Hence, we require a procedure to disentangle the clock space from the result of the computation. This is done as follows :

1 For an computational basis vector $|h\rangle \in l_2(H)$, we tensor this with the zero of the clock space, giving $|0\rangle|h\rangle \in C \otimes l_2(H)$. We then apply the algorithm implementing Ψ_F above, to give

$$\Psi_F(0\rangle|h\rangle) = |h_k\rangle|M(h)\rangle$$

2 Using an almost identical procedure to that of Section 17.1 on the function F^{-1} instead of F, we may produce an algorithm that implements the function $\Psi_{F^{-1}}(|t\rangle|h\rangle) = |t+k_h\rangle|M^{-1}(h)\rangle$ on computational basis vectors. We apply this to the output of step 1., to get

$$\Psi_{F^{-1}}\Psi_F(0\rangle|h\rangle) = |2h_k\rangle|h\rangle$$

(This 'uncomputation' step is a familiar part of the approach to reversible computation given in (Bennett 1973)).

3 We now apply elementary arithmetic operations to the clock space. Precisely, for an arbitrary even number 2n < 2K (where K is an upper bound to the number of iterative cycles required in the computation) we require a unitary map P satisfying $P(|2n\rangle) = |K-n\rangle$. We refer to (Vedral et. al. 1996) for implementations of arithmetic operations on quantum registers, and Section 16.2 for discussion of this upper bound. Applying P to the clock space only gives

$$(P \otimes 1)\Psi_{F^{-1}}\Psi_F(|0\rangle|h\rangle) = |K - k_h\rangle|h\rangle$$

4 Finally, we re-apply the algorithm implementing Ψ_F to the output of step 3. above, giving

$$\Psi_F(P \otimes 1)\Psi_{F^{-1}}\Psi_F(|0\rangle h\rangle) = |K\rangle |M(h)\rangle$$

Note that the content of the clock space is no longer a function of h, but is instead a constant.

Now consider performing the above steps, not with a computational basis vector, but with an arbitrary superposition of computational basis vectors $\sum_{i \in I} \alpha_i |h_i\rangle$. By linearity, the above procedure acts as :

$$|0\rangle \otimes \sum_{i \in I} \alpha_i |h_i\rangle \quad \mapsto \quad |K\rangle \sum_{i \in I} \alpha_i |M(h_i)\rangle$$

and we observe that the clock space is no longer entangled with the result of the computation. Hence we may measure (or simply ignore) the contents of the clock space, and are left with the required superposition $\sum_{i \in I} \alpha_i |M(h_i)\rangle$.

17.3. Approximations to the twisted dagger, in finite time \mathcal{E} finite-dimensional space

We now consider how the above computations (In particular those of Section 17.1 and 17.2) may be performed in finite time, using finite resources.

Recall the interpretation of the twisted dagger as the limit of an infinite series of applications of unitary maps given in Theorem 12.2. We write the unitary map U_f above in matrix form as

$$U_f = \begin{pmatrix} p & q \\ r & s \end{pmatrix} : l_2(H) \oplus l_2(C) \to l_2(H) \oplus l_2(C)$$

It is shown in Theorem 12.2 how the twisted dagger of a unitary map arises as the limit of a series of applications of unitary matrices, F_0, F_1, F_2, \ldots , where these matrices have distinct infinite-dimensional spaces as their sources / targets. This is physically unreasonable in that we cannot apply an infinite number of unitary operations in a finite time. Also, to conform with the traditional approach to quantum computation, we wish to work within a finite-dimensional space.

What makes this a physically reasonable quantum-computational procedure is the existence of an upper bound K to the number of steps before termination (from Section 16.2). Hence, for an input $|0\rangle|x\rangle$ (we assume that $|x\rangle$ is a computational basis vector, for simplicity – the general case follows by linearity), there exists some $h_x < K$ such that

$$F_{h_k}F_{h_k-1}\dots F_0(|0\rangle|x\rangle) = |h_k\rangle|M(x)\rangle$$

where M is the function computed by the iterative procedure of Section 16.2, and this is *unchanged* (up to trivial permutations of the basis states of the form

$$\left(\bigoplus^{i} H\right) \oplus C \oplus \left(\bigoplus^{j} H\right) \cong \left(\bigoplus^{a} H\right) \oplus C \oplus \left(\bigoplus^{b} H\right) \quad \text{where} \quad i+j=K=a+b$$

i.e. simply shifting the postion of the non-halting subspace) by applications of F_N for all N > K.

The key point now is that, since the solution is reached within some finite time $\leq K$, we do not require a countable infinite clock space — a 'limited' version T_K with computational basis $\{|0\rangle|1\rangle, \ldots, |K\rangle\}$ is sufficient for the procedure described in Section 17.1. We also only require a finite series of unitary maps that are the finitary analogues of F_0, \ldots, F_K . Finally for the 'disentangling' procedure (including unitary arithmetic) of Section 17.2, we require a larger space of dimension 2K — and this is simply given by tensoring T_K with one additional qubit.

18. Conclusions and Discussion

18.1. Summary

The main results of this paper may be summarised as follows:

- The particle-style trace (a categorical trace based on conditional iteration) trace is applicable in a wider setting than the UDCs of (Haghverdi 2000); this setting includes categories where the summation on hom-sets does not satisfy the positivity property
 including categories of Hilbert spaces and linear maps.
- Although linear maps representing isolated physical operations (unitary maps) have an iterative trace within the category of Hilbert spaces, this is not a physical operation

— not only does it not correspond to usual notions of conditional iteration, but the result is neither unitary (describing isolated time-evolution) nor Hermitian (specifying measurement outcomes).

- We may factor the iterative trace on (finite-dimensional) Hilbert spaces into three parts: a canonical inclusion, a (possibly non-terminating) series of unitary operations (the 'twisted dagger'), and a codiagonal. We identify the irreversibility (or non-physicality) of the iterative trace with the 'forgetful' codiagonal, rather than the interpretation as conditional iteration. The (unitary) twisted dagger thus arises as the infinite product of local unitary operations.
- There exists an embedding into **Hilb** of a traced monoidal category based on convolved lists (over **Hilb**_{rd}). Under this embedding the trace becomes the canonical inclusion followed by the twisted dagger. These are the two physically reasonable parts of the factorization above. This arises from a general construction on categories carrying a Σ-structure that we call the Convolution Category Construction.
- Using the close connection between the iterative trace and algebraic program semantics for conditional iteration, we are able to give algorithms based on conditional iteration. In the example given, we demonstrate that an arbitrary reversible algorithm based on conditional iteration has a quantum-mechanical analogue that is i/ superposition-preserving, and ii/ behaves like the classical algorithm on the computational basis.

18.2. Future directions

There are many possible future directions for this work. Quantum-physically, the natural step is to consider a full Fock-space treatment of the thought experiments of Section 11, and use these to motivate a more physically sophisticated treatment of conditional iteration. Also, although necessary conditions for unitarity of the twisted dagger are given, these are not also sufficient conditions — whether sufficient conditions can be given explicitly remains open.

Categorically, there remain many questions to be answered — the Convolution construction may well provide a Kleisli or Eilenberg-Moore category. However, the natural numbers seem to play too large a role in this construction, and (subject to minor restrictions) may be replaced with an arbitrary abelian monoid (particularly interesting examples begin the finite cyclic monoids \mathbb{Z}_p). A full theory would take this generality into account. Computationally, we have also only given a restricted case — the next natural step is to consider iterating unitary matrices that are not definable in terms of a classical bijection on some orthonormal basis. In this case, convergence could not be established as simply as the combinatorics of Section 16, and the analytic results of Section 12 would become more important.

Finally, the subtleties of the tensor product of Σ -structures and the associated theory of enrichment appears to be of considerable interest. We are currently examining such notions in joint work with Tim Porter.

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Appendix A: Minimal conditions for the particle-style trace

For completeness we analyse the proof, presented in (Haghverdi 2000), that the iterative trace formula is indeed a categorical trace, in the sense of (Joyal et. al. 1996). We demonstrate that this proof does *not* require all the axioms for a unique decomposition category - in particular, it holds for categories carrying a Σ structure with matrix representations (and hence UDCs, PACs, & c.).

Theorem 19.1. Let $(\mathcal{C}, \oplus, \Sigma)$ be a Σ matrix category, such that for all $F = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$: $X \oplus U \to Y \oplus U$, the sum

$$a + \sum_{i=0}^{\infty} b d^i c : X \to Y$$
 exists

Then $(\mathcal{C}, \oplus, \Sigma)$ is a traced monoidal category, with $Tr^U_{X,Y}(F) : X \to Y$ given by the above summation.

Proof. Note that, as $(\mathcal{C}, \oplus, \Sigma)$ has matrix representations, the monoidal tensor $F \oplus G$ is given by the matrix $\begin{pmatrix} F & 0 \\ 0 & G \end{pmatrix}$. We now consider the axioms for a categorical trace: — Naturality in X: $Tr_{X,Y}^U(F)G = Tr_{X',Y}^U(F(G \oplus 1_U))$

We write F in matrix form as $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$. Then, as (\mathcal{C}, \oplus) has matrix representations $G \oplus 1_U = \begin{pmatrix} G & 0 \\ 0 & 1_U \end{pmatrix}$. Then by definition,

$$Tr^U_{X',Y}(F(G\oplus 1_U)) \ = \ Tr^U_{X',Y}\left(\begin{array}{cc} ag & b \\ cg & d \end{array}\right) \ = \ ag + \sum_{i=0}^\infty bd^i cg$$

By assumption, the trace formula converges, so $Tr_{X,U}^U(F) = a + \sum_{i=0}^{\infty} bd^i c$ exists, and by the distributivity of composition over summation, $Tr_{X,U}^U(F)G = (a + b)$ $\sum_{i=0}^{\infty} bd^i c) G = Tr^U_{X',Y}(F(G \oplus 1)).$ Naturality in $Y: hHTr^U_{X,Y}(F) = Tr^U_{X,Y'}((H \oplus 1_U)F)$

This follows by the dual calculation, using left-distributivity, rather than rightdistributivity. Again, the only assumptions needed are the Σ -structure on hom-sets, distributivity, and matrix representations.

— Dinaturality in $U: Tr_{X,Y}^U((1_Y \oplus G)F) = Tr^{U'}(F(1_X \oplus G))$ $\begin{pmatrix} 1 & 0 \end{pmatrix}$

Using matrix representations, write
$$F = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$
, $1_Y \oplus G = \begin{pmatrix} 1_Y & 0 \\ 0 & G \end{pmatrix}$, and

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similarly
$$1_X \oplus G = \begin{pmatrix} 1_X & 0\\ 0 & G \end{pmatrix}$$
. Then
 $Tr^U_{X,Y}((1_Y \oplus G)F) = Tr^U_{X,Y}\begin{pmatrix} a & b\\ Gc & Gd \end{pmatrix} = a + \sum_{i=0}^{\infty} b(Gd)^i Gc$

and

$$Tr_{X,Y}^{U'}(f(1_X \oplus G)) = Tr_{X,Y}^{U'} \begin{pmatrix} a & Gb \\ c & Gd \end{pmatrix} = a + \sum_{i=0}^{\infty} (bG)(dG)^i c$$

and by the distributivity of composition over summation, these are the same. — Vanishing I $Tr_{X,Y}^{I}(\rho_{Y}^{-1}F\rho_{X}) = F$

By definition of the units arrows, and the existence of zero morphisms,

$$Tr_{X,Y}^{I}(\rho_{Y}^{-1}F\rho_{X}) = Tr_{X,Y}^{I}\begin{pmatrix} F & 0_{I,Y} \\ 0_{X,I} & 1_{I} \end{pmatrix} = F + \sum_{i=0}^{\infty} 0_{IY}1_{I}^{i}0_{XI} = F$$

- Vanishing II $Tr_{X,Y}^{U\oplus V}(F) = Tr_{X,Y}^U(Tr_{X\oplus U,Y\oplus U}^V(F))$ We write $F: X \oplus U \oplus V \to Y \oplus U \oplus V$ in matrix form as

$$F = \left(\begin{array}{rrr} a & b & c \\ d & e & f \\ g & h & k \end{array}\right)$$

 \mathbf{so}

$$Tr_{X\oplus U,Y\oplus U}^{V}(F) = \begin{pmatrix} a & b \\ d & e \end{pmatrix} + \sum_{i=0}^{\infty} \begin{pmatrix} c \\ f \end{pmatrix} k^{i} \begin{pmatrix} g & h \end{pmatrix}$$
$$= \begin{pmatrix} a + \sum_{i=0}^{\infty} ck^{i}g & b + \sum_{i=0}^{\infty} k^{i}h \\ p + \sum_{i=0}^{\infty} fk^{i}g & e + \sum_{i=0}^{\infty} fk^{i}h \end{pmatrix}$$

Therefore, by direct calculation,

$$Tr_{X,Y}^{U}(Tr_{X\oplus U,Y\oplus U}^{V}(F)) = a + \sum_{i=0}^{\infty} ck^{i}g + (b + \sum_{i=0}^{\infty} ck^{i}h)(\sum_{j=0}^{\infty} (e + \sum_{i=0}^{\infty} fk^{i}h)^{j})(d + \sum_{i=0}^{\infty} fk^{i}g) + \sum_{i=0}^{\infty} ck^{i}g + (b + \sum_{i=0}^{\infty} ck^{i}h)(\sum_{j=0}^{\infty} (e + \sum_{i=0}^{\infty} fk^{i}h)^{j})(d + \sum_{i=0}^{\infty} fk^{i}g) + \sum_{i=0}^{\infty} ck^{i}g + (b + \sum_{i=0}^{\infty} ck^{i}h)(\sum_{j=0}^{\infty} (e + \sum_{i=0}^{\infty} fk^{i}h)^{j})(d + \sum_{i=0}^{\infty} fk^{i}g) + \sum_{i=0}^{\infty} ck^{i}g + (b + \sum_{i=0}^{\infty} ck^{i}h)(\sum_{j=0}^{\infty} (e + \sum_{i=0}^{\infty} fk^{i}h)^{j})(d + \sum_{i=0}^{\infty} fk^{i}g) + \sum_{i=0}^{\infty} ck^{i}g + (b + \sum_{i=0}^{\infty} ck^{i}g) + \sum_{i=0}^{\infty} ck^{i}g + (b + \sum_{$$

However,

$$Tr_{X,Y}^{U\oplus V}(F) = a + \sum_{i=0}^{\infty} \left(\begin{array}{cc} b & c \end{array} \right) \left(\begin{array}{cc} e & f \\ h & k \end{array} \right)^{i} \left(\begin{array}{cc} d \\ g \end{array} \right)$$

and straightforward calculations (given explicitly in (Haghverdi 2000)) will demonstrate that these infinite sums are equal. It may also be checked that these calculations only require matrix manipulations and the distributivity of composition over (infinite) sums.

However, equality may also be established using a graphical notation. Let us draw ${\cal F}$ as in Figure 13 :

We may calculate $Tr^{V}(F)$ by introducing a feedback loop, as in Figure 14

We calculate $Tr^{V}(F)$ by summing over all paths from X to Y, X to U, etc., to get a digraph representation for the matrix of $Tr^{V}(F): X \oplus U \to Y \oplus U$, as in Figure 15

Fig. 13. The matrix of F as a digraph



Fig. 14. The matrix of F, with a feedback loop



Finally, to calculate $Tr^{U}(Tr^{V}(F))$, we may take the digraph in Figure 15, and introduce a feedback loop, to get the digraph shown in Figure 16. We then sum over all paths from X to Y, to give $Tr^{V}(Tr^{U}(F)) = p + \sum_{j=0}^{\infty} qs^{j}r$. We now use the same formalism to calculate $Tr^{U\oplus V}(F)$. Let us draw $F: X \oplus (U \oplus V) \to Y \oplus (U \oplus V)$ (together with the appropriate feedback loop) as in Figure 17. We may then sum over all paths from X to Y, in order to calculate $Tr^{U\oplus V}(F)$. However, as a simplification, we may first replace all matrix-labelled arrows in Figure 17 to y the appropriate digraphs, giving the digraph shown in Figure 18.

We then sum over all paths from X to Y, giving an explicit formula for $Tr^{U\oplus V}(F)$, and it follows, either by graphical manipulations or explicitly writing out the appropriate sums, that $Tr^{U}(Tr^{V}(F)) = Tr^{U\oplus V}(F)$.

- Superposing $G \oplus Tr_{X,Y}^U(F) = Tr_{W \oplus X,Z \oplus Y}^U(G \oplus F)$ Writing $F = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, and using the characterisation of the monoidal tensor in Fig. 15. The digraph of $Tr^V(F)$

$$\begin{array}{c} X \\ \downarrow \\ p \\ Y \end{array} \begin{array}{c} V \\ \downarrow \\ V \end{array} \begin{array}{c} U \\ \downarrow \\ V \\ V \end{array} \end{array} \text{ where } \begin{cases} p = a + \sum_{i=0}^{\infty} ck^{i}g \quad q = b + \sum_{i=0}^{\infty} hk^{i}c \\ r = d + \sum_{i=0}^{\infty} gk^{i}f \quad s = c + \sum_{i=0}^{\infty} hk^{i}f \end{cases}$$

Fig. 16. Calculating $Tr^U(Tr^V(F))$



where p, q, r, s are as in Figure 15.

terms of matrices, gives
$$G \oplus F = \begin{pmatrix} G & 0 & 0 \\ 0 & a & b \\ 0 & c & d \end{pmatrix}$$
 and so
$$Tr^{U}_{W \oplus X, Z \oplus Y}(F) = \begin{pmatrix} G & 0 \\ 0 & a \end{pmatrix} + \sum_{i=0}^{\infty} \begin{pmatrix} 0 \\ b \end{pmatrix} d^{i} \begin{pmatrix} 0 & c \end{pmatrix}$$

By the formulæ for matrix composition, and the matrix characterisation of the monoidal tensor,

$$Tr_{W\oplus X,Z\oplus Y}^{U}(F) = \begin{pmatrix} G & 0\\ 0 & a + \sum_{i=0}^{\infty} bd^{i}c \end{pmatrix} = \begin{pmatrix} G & 0\\ 0 & Tr_{X,Y}^{U}(F) \end{pmatrix} = G \oplus Tr_{X,Y}^{U}(F)$$

— Yanking: $Tr_{U,U}^U(s_{U,U}) = 1_U$

As C has matrix representations, $Id_{U\oplus U} = \begin{pmatrix} 1_U & 0 \\ 0 & 1_U \end{pmatrix}$, and so $\begin{pmatrix} 0 & 1_U \\ 1_U & 0 \end{pmatrix}$ satisfies the axioms for the commutativity isomorphism. It is then trivial that the trace of this is 1_U .

Observe that the only requirements for this proof to hold are the following:

- $-(\mathcal{C},\oplus)$ has matrix representations, with monoidal tensor is given by $f\oplus g = \begin{pmatrix} f & 0 \\ 0 & g \end{pmatrix}$.
- There exists a partial (associative commutative) summation, where composition distributes over summation.
- If a family of arrows is summable, then so are all its subfamilies this is required for

Fig. 17. Calculating $Tr^{U \oplus V}(F)$



Fig. 18. The matrix of F, with a double feedback loop



the proof of Vanishing II, and is implied by the 'summable subfamilies' property of both Σ -monoids and Σ structures (By contrast, the weak Higgs I axiom of Definition 3.6. only allows for the summability of finite subfamilies).

— The trace formula converges.

Hence the iterative trace formalism is equally applicable to PACs, UDCs, Σ -matrix categories, strong GDCs, &c.

Appendix B : The existence of partial traces in arbitrary ΣMCs

We now demonstrate that every Σ MC has a partial trace, provided by the iterative trace formula. Note that this is not a triviality satisfied by some condition such as 'the class of trace-class arrows is empty', since the axioms for a partial trace require the existence of certain tracable arrows (the Vanishing I, and Yanking axioms). **Theorem 19.2.** Let $(\mathcal{C}, \oplus, \Sigma)$ be a Σ -Matrix category. Then the iterative trace formula defines a partial trace on $(\mathcal{C}, \oplus, \Sigma)$.

Proof. We demonstrate that the iterative trace formula satisfies the axioms given in Definition 9.4.

1 (Naturality) (We give a proof for naturality in X. The proof for naturality in Y follows similarly.

Given
$$f = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$
 and $g: X' \to X$, then $g \oplus 1_U = \begin{pmatrix} g & 0 \\ 0 & 1_U \end{pmatrix}$, and :

(⇒) existence Let us assume that $Tr^{U}(f)g$ exists. The iterative trace formula gives $Tr^{U}(f(g \oplus 1_{U})) = ag + \sum_{i=0}^{\infty} bd^{i}cg$. However, this is just $Tr^{U}(f)g$, which exists by assumption.

(\Leftarrow) existence Let us assume that $Tr^U(f(g \oplus 1_U))$ exists. The iterative trace formula gives $Tr^U(f(g \oplus 1_U)) = ag + \sum_{i=0}^{\infty} bd^i cg$. However, we have already seen that this is just $Tr^U(f)g$.

(Equality) It is immediate that these two expressions are equal.

2 (Dinaturality) Given
$$f = \begin{pmatrix} a & b \\ c & d \end{pmatrix} : X \oplus U \to Y \oplus U$$
 and $g : U' \to U$, then :

(⇒) existence Let us assume that $Tr^{U}((1_{Y} \oplus g)f) = Tr^{U}\begin{pmatrix} a & b \\ gc & gd \end{pmatrix} = a + \sum_{i=0}^{\infty} b(gd)^{i}gc$ exists. The particle-style trace formula gives

$$Tr^{U'}(f(1_X \oplus g)) = Tr^{U'} \begin{pmatrix} a & gb \\ c & gd \end{pmatrix} = a + \sum_{i=0}^{\infty} (bg)(dg)^i c$$

However, rebracketing gives

$$Tr^{U'}(f(1_X \oplus g)) = a + \sum_{i=0}^{\infty} b(gd)^i gd$$

and this is just $Tr^{U}(1_Y \oplus g)f)$, which exists by assumption.

The \Leftarrow proof of existence, and equality, then follow trivially.

3 (Vanishing I) Given $f: X \to Y$, then by definition

$$\rho^{-1}f\rho = \left(\begin{array}{cc} f & 0_{IY} \\ 0_{XI} & 1_I \end{array}\right)$$

From the iterative trace formula,

$$Tr^{I}(\rho^{-1}f\rho) = f + \sum_{j=0}^{\infty} 0_{IY} 1_{I}^{j} 0_{XI} = f + 0_{XY} = f$$

as required. (Note that similar reasoning gives that, for arbitrary $f: X \to Y$ and $g: U \to U, Tr^U(f \oplus g)$ exists, and is equal to f).

4 (Vanishing II)

Consider an arrow $f: X \oplus U \oplus V \to Y \oplus U \oplus V$ written in matrix form as

$$f = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & k \end{pmatrix} : X \oplus U \oplus V \to Y \oplus U \oplus V$$

From Appendix A, if both $Tr^{U}(Tr^{V}(f)) : X \to Y$ and $Tr^{U \oplus V}(f) : X \to Y$ exist, then they are equal. Without assuming existence, let us compare these formulæ:

$$Tr^{U\oplus V}(f) = a + \sum_{l=0}^{\infty} \begin{pmatrix} b & c \end{pmatrix} \begin{pmatrix} e & f \\ g & h \end{pmatrix}^{l} \begin{pmatrix} d \\ g \end{pmatrix}$$

This may also be written explicitly as

$$Tr^{U\oplus V}(f) = a + \begin{pmatrix} b & c \end{pmatrix} \begin{pmatrix} p & q \\ r & s \end{pmatrix} \begin{pmatrix} d \\ g \end{pmatrix}$$

where the components p, q, r, s are indexed sums given explicitly in (Haghverdi 2000) (Lemma 4.0.1).

Conversely

$$Tr^{V}(f) = \begin{pmatrix} a & b \\ d & e \end{pmatrix} + \sum_{i=0}^{\infty} \begin{pmatrix} c \\ f \end{pmatrix} k^{i} \begin{pmatrix} g & h \end{pmatrix}$$
$$= \begin{pmatrix} a & b \\ d & e \end{pmatrix} + \sum_{i=0}^{\infty} \begin{pmatrix} ck^{i}g & ck^{i}h \\ fk^{i}g & fk^{i}h \end{pmatrix} = \begin{pmatrix} a + \sum_{i=0}^{\infty} ck^{i}g & b + \sum_{i=0}^{\infty} ck^{i}h \\ d + \sum_{i=0}^{\infty} fk^{i}g & e + \sum_{i=0}^{\infty} fk^{i}h \end{pmatrix}$$

and

$$Tr^U(Tr^V(f)) = t + \sum_{j=0}^{\infty} uv^j w$$

where

$$\begin{split} t &= a + \sum_{i=0}^{\infty} ck^i g \qquad u = b + \sum_{i=0}^{\infty} ck^i h \\ v &= d + \sum_{i=0}^{\infty} fk^i g \qquad w = e + \sum_{i=0}^{\infty} fk^i h \end{split}$$

The question now is : What is the relationship between the doubly-indexed sum (indexed by $i, j \in \mathbb{N} \times \mathbb{N}$, and given explicitly by summing over all paths in Figure 16) in the calculation of $Tr^{U}(Tr^{V}(f))$, and the singly-indexed sum (indexed by $l \in \mathbb{N}$, and given explicitly by summing over all paths in Figure 17) in the calculation of $Tr^{U \oplus V}(f)$?

Writing out the summands explicitly in both cases demonstrates that the singlyindexed sum (indexed by $l \in \mathbb{N}$) arises from taking a partition of the doubly-indexed sum $\mathbb{N} \times \mathbb{N} = \biguplus_{l=0}^{\infty} N_l$ (where $N_l \cong \mathbb{N}$, for all $l = 0...\infty$), and summing over each $n \in N_l$, leaving a singly-indexed sum.

Hence, by the weak partition-associativity axiom, the existence of the single-indexed sum $Tr^{U \oplus V}(f)$ is implied by the existence of the doubly-indexed sum $Tr^{U}(Tr^{V}(f))$.

However, the converse implication does not hold, as we only assume the *weak* partition-associativity axiom.

5 (Superposing)

Given $g: W \to Z$ and $f = \begin{pmatrix} a & b \\ c & d \end{pmatrix} : X \oplus U \to Y \oplus U$, then :

(\Rightarrow existence) Let us assume that $Tr^U_{W\oplus X,Z\oplus Y}(g\oplus f)$ exists. From the iterative trace formula,

$$Tr^{U}(g \oplus f) = \begin{pmatrix} g & 0 \\ 0 & a \end{pmatrix} + \sum_{i=0}^{\infty} \begin{pmatrix} 0 \\ b \end{pmatrix} d^{i} \begin{pmatrix} 0 & c \end{pmatrix} = \begin{pmatrix} g & 0 \\ 0 & a + \sum_{i=0}^{\infty} b d^{i} c \end{pmatrix}$$

However, each matrix component is also an arrow in C, so $Tr^U(f) = a + \sum_{i=0}^{\infty} bd^i c$ exists.

(\Leftarrow existence) Let us assume that $Tr_{X,Y}^U(f)$ exists. Then from the iterative trace formula,

$$Tr^{U}(g \oplus f) = \left(\begin{array}{cc} g & 0\\ 0 & a + \sum_{i=0}^{\infty} bd^{i}c \end{array}\right)$$

and so $Tr^U_{W\oplus X,Z\oplus Y}(g\oplus f) = g\oplus Tr^U_{X,Y}(f)$, which exists, since $Tr^U_{X,Y}(f)$ exists.

(Equality) It is immediate that these two expressions are equal.

6 **Yanking)** By definition, $s_{U,U} = \begin{pmatrix} 0 & 1_U \\ 1_U & 0 \end{pmatrix}$. From the iterative trace formula,

$$Tr^{U}(s_{U,U}) = 0_{U} + \sum_{i=0}^{\infty} 1_{U} \cdot 0_{U}^{i} \cdot 1_{U}$$

However, $1_U . 0_U^i . 1_U = 0_U$ for all $i \neq 0$, so the only non-zero summand is 1_U , and hence this sum exists, giving $Tr_{U,U}^U(s_{U,U}) = 1_U$ as required.