The operator tensor formulation of quantum theory

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In this paper, we provide what might be regarded as a manifestly covariant presentation of discrete quantum theory. A typical quantum experiment has a bunch of apparatuses placed so that quantum systems can pass between them. We regard each use of an apparatus, along with some given outcome on the apparatus (a certain detector click or a certain meter reading for example), as an operation. An operation (e.g. $B_{b_{2}a_{3}}^{b_{1}a_{2}}$) can have zero or more quantum systems inputted into it and zero or more quantum systems outputted from it. The operation $B_{b_{2}a_{3}}^{b_{1}a_{2}}$ has one system of type $a$ inputted, and one system of type $b$ and one system of type $a$ outputted. We can wire together operations to form circuits, for example, $A^{a_{1}}B_{b_{2}a_{3}}^{b_{1}a_{2}}C_{b_{2}a_{3}}$. Each repeated integer label here denotes a wire connecting an output to an input of the same type. As each operation in a circuit has an outcome associated with it, a circuit represents a set of outcomes that can happen in a run of the experiment. In the operator tensor formulation of quantum theory, each operation corresponds to an operator tensor. For example, the operation $B_{b_{2}a_{3}}^{b_{1}a_{2}}$ corresponds to the operator tensor $\hat{B}_{b_{2}a_{3}}^{b_{1}a_{2}}$. Further, the probability for a general circuit is given by replacing operations with corresponding operator tensors as in

$$\text{Prob}(A^{a_{1}}B_{b_{2}a_{3}}^{b_{1}a_{2}}C_{b_{2}a_{3}}) = \hat{A}_{a_{1}}^{a_{1}}\hat{B}_{b_{2}a_{3}}^{b_{1}a_{2}}\hat{C}_{b_{2}a_{3}}.$$  (1)

Repeated integer labels indicate that we multiply in the associated subspace and then take the partial trace over that subspace. Operator tensors must be physical (namely, they must have positive input transpose and satisfy a certain normalization condition).

Keywords: operator tensors; quantum circuits; quantum reformulation

1. Introduction

One of Turing’s great insights was the idea that a computational process can be broken up into a series of steps to be implemented by a machine. The mathematical machinery that comes out of this insight constitutes a large part of the field of computer science. Physics, on the other hand, has been largely dominated by the mathematics of differential equations as evidenced by Newtonian dynamics, Maxwell’s equations, General Relativity and the Schrödinger equation. Recently, however, this has begun to change. The

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Techniques of computer science have seen a significant number of profound applications in quantum theory in the guise of the new field of quantum information. This has been accompanied by the importation of certain philosophical and methodological prejudices from computer science. In particular, we can think of a quantum process as a computational process in which there is a user interface. In fact, the idea of a user interface is very much in accord with the operational view of quantum theory where, on the users side of things, we make choices of measurements and make a note of measurement outcomes. This operational view of quantum theory is quite old. The techniques of computer science provide a natural mathematical language for operationalism. Operationalism is, here, a methodology. The success of such a methodology need not hinder an attempt to understand the world in ontological terms (where we ask what the underlying reality is). Rather, there is every reason to hope that the operational approach will ultimately bring us closer to such an ontological understanding. It is likely that, one hundred years from now, physics will owe as much to the work of Turing as computer science does already.

In this paper, we will present a new operational formulation of quantum theory—the operator tensor formulation—which provides an especially natural operational view of quantum theory. To appreciate this new formulation, we first need to consider how the old operational formulation of quantum theory works for circuits.

(a) Circuits and operations

A circuit is formed by wiring together operations such that there are no open wires left. For example,

\[
\begin{array}{c}
A \xrightarrow{a} B \xrightarrow{b} C \xrightarrow{c} E \xrightarrow{d} F
\end{array}
\]

The operations are represented by boxes. Systems pass along the wires. The type of system (electron, atom, photon, etc.) is denoted by \(a, b, c, \ldots\). At each operation is a certain specified classical outcome (not shown in the figure) which is read off, for example, flashing lights, a meter or something of this sort. Hence, the circuit represents something that may happen—it could so happen that we get the given outcome at each operation in the circuit. We can give the symbolic notation for this circuit as

\[
A^{a_1b_2}B^{a_3d_4}C^{a_5}_{b_2a_3}D^{b_6}_{a_1a_3d_4}F^{c_7}_{b_6c_7}.
\]
In this notation, the wires are indicated by integers. For example, in the above expression $a_5$ appears as a superscript on $C_{b_2a_3}^{a_5}$ and a subscript on $E_{a_5d_4}^{c_7}$, indicating a wire for a system of type $a$ from an output of $C$ to an input of $E$. The integers are merely labels and have no physical significance beyond this. Since all the wiring information is carried by these integers, the order of the operations in the symbolic representation makes no difference. We could, for example, equally represent the same circuit by

$$B_{a_3d_4}^{a_5}F_{b_6c_7}^{a_5}C_{b_2a_3}^{a_1b_2}D_{a_1}^{b_6}E_{a_5d_4}^{c_7}. \tag{1.3}$$

Relatedly, in the diagrammatic representation, the position (both vertical and horizontal) of the boxes on the page has no significance as long as the wiring remains the same and the boxes maintain their orientation.

(b) Calculation in old formulation of quantum theory

How do we calculate the probability that all the specified outcomes at each of the boxes are seen? The standard formulation of quantum theory, as usually applied to circuits of this sort, involves thinking in terms of a state evolving in time. Since we need to think of a state evolving in time, first we must foliate the circuit [1].

![Diagram](image)

The foliation lines pick out the circuit analogue of space–time hypersurfaces. In general, there are more than one such foliation for any given circuit. Now with respect to the chosen foliation we can write down an expression for the probability.

$$\text{Prob}(A_{a_1b_2} B_{a_3d_4} C_{b_2a_3}^{a_5} D_{a_1}^{b_6} E_{a_5d_4}^{c_7} F_{b_6c_7}^{a_5}) = \text{Trace}(\hat{P}_F[I_b \otimes \$E] \circ [\$D \otimes \$C \otimes I_d](\hat{\rho}_A \otimes \hat{\rho}_B)). \tag{1.5}$$

We get this expression by evolving the state prepared at time $t_1$ to time $t_2$, then to time $t_3$. For the final step, we take the trace with the operator associated with the final result $F$. Here $\hat{\rho}_A$ is a positive operator (having trace less than or equal to one) associated with the preparation $A$. Associated with the operation $D$ is the trace non-increasing completely positive map $\$D$. We will call an operation having both inputs and outputs, such as this, a transformation. We denote by $I_d$ the identity map on systems of type $d$. Finally, $\hat{P}_F$ is a positive operator (which is less than or equal to the identity) associated with $F$. We will call operations, such
as $F$, having only input wires results. An important subtlety in this calculation is that we do not assume that the state is normalized after each time step. The reason for this is that the normalization of the state is equal to the probability that the outcomes associated with the operations up to this time have happened and we do not want to lose this information.

There are three problems associated with doing calculations in the old formulation of quantum theory as evidenced by the calculation in (1.5):

— we need to choose an arbitrary foliation even though this is not part of the physics;
— we have to pad the calculation with identity maps (such as $I_d$) whenever two or more foliation lines intersect a given wire; and
— our treatment is disunified in that we use different types of mathematical objects for preparations (positive operator having trace less than or equal to one), transformations (trace non-increasing completely positive map) and results (positive operator less than or equal to the identity).

We will resolve these problems in the operator tensor formulation.

(c) Calculation in operator tensor formulation

In the operator tensor formulation, there is an operator corresponding to each operation. For example, the operator, $\hat{C}_{b_2a_3}^{a_5}$, corresponds to the operation, $C_{b_2a_3}^{a_5}$. The operator $\hat{C}_{b_2a_3}^{a_5}$ is an element of the space of Hermitian operators acting on the Hilbert space $\mathcal{H}_{b_2} \otimes \mathcal{H}_{a_3} \otimes \mathcal{H}_{a_5}$. These operators have subscripts and superscripts associated with the inputs and outputs of the corresponding operation. These subscripts and superscripts give the operators a tensor character, so we will sometimes refer to them as operator tensors.

In the operator tensor formulation, the probability is given by the formula

\[
\text{Prob}(A_{a_1b_2} B_{a_3d_4} C_{b_2a_3}^{a_5} D_{a_1} E_{a_5}^{c_7} F_{b_6c_7}) = \hat{A}_{a_1b_2} \hat{B}_{a_3d_4} \hat{C}_{b_2a_3}^{a_5} \hat{D}_{a_1} \hat{E}_{a_5}^{c_7} \hat{F}_{b_6c_7}.
\]

(1.6)

With standard tensor expressions, we sum over repeated labels. However, the label in the operator tensor corresponds to a Hilbert space rather than an integer and so we cannot simply sum over repeated labels here. Rather, when we have a repeated label in an operator tensor expression we multiply in the appropriate subspace and then take the partial trace in that subspace. We will explain in detail how this procedure works later on. Such repeated labels correspond to a wire such as $a_5$. Operators, such as $\hat{C}_{b_2a_3}^{a_5}$ for example, must be physical. We define an operator to be physical if it satisfies two properties.

— **It has positive input transpose.** If we take the partial transpose over the part of the space associated with the input, then we get a positive operator. For example, $\hat{C}_{b_2a_3}^{a_5 T} \geq 0$.

— **It has output trace less than the identity.** If we take the partial trace over the output, we get an operator that is less than or equal to the identity. For example, $\hat{C}_{b_2a_3}^{a_5} \hat{I}_{a_5} \leq I_{b_2a_3}$.

These properties are imposed to guarantee that any probabilities we calculate are between 0 and 1.
Penrose showed how we can represent tensorial calculations diagrammatically. This will be especially useful here. We can give a diagrammatic version of (1.6) as follows:

\[
\text{Prob}
\begin{pmatrix}
A & B & D & C & E & F \\
abla & & b & c & \nabla & \\
& a & d & a & & \\
\end{pmatrix}
= \\
\begin{pmatrix}
\hat{A} & \hat{B} & \hat{D} & \hat{C} & \hat{E} & \hat{F} \\
& & & & & \\
& & & & & \\
\end{pmatrix}
\]

(1.7)

The double border boxes on the right represent operators and the wires represent taking the partial trace over the corresponding Hilbert space (we will explain how to do this in detail later). Hence, the figure on the right is an operator tensor calculation.

We note that, in the operator tensor formulation, for both (1.6) and (1.7) the calculation (on the right-hand side) looks like the circuit description (inside the argument on the left-hand side) except that we have \(A \to \hat{A}, B \to \hat{B}, \ldots\) and (in the diagrammatic version) we have double border boxes. Further, with regard to the three points at the end of §1b, we note that we do not need to impose a foliation, we do not need to pad the calculation with identities and we give a unified treatment of preparations, transformations and results (the operators corresponding to them must be physical).

\((d)\) Previous work

The operator tensor formulation was first presented in [2] where it was used to aid a reconstruction of quantum theory from natural postulates. This paper is dedicated to presenting the operator tensor formulation (without the need to service a reconstruction effort) and consequently should be pedagogically clearer. The closest thing in the literature to the operator tensor formulation of quantum theory is the quantum combs approach of Chiribella et al. [3]. The relationship between the quantum combs approach and the present approach is discussed in detail in §8.5 of [2] and, more briefly, below.

One of the main ideas in this paper is that we do not have to restrict ourselves to evolving a state forward in time in formulations of physical theories. This idea has a long heritage. In the context of quantum theory, Aharonov et al. [4] have pursued such ideas for many years. Most recently, Aharonov et al. [5] have given the ‘multi-time’ formulation of quantum theory in which it is possible to have something analogous to a pure state pertaining to many times. Relatedly, motivated by considerations from quantum gravity, Oeckl [6] has presented a
general boundary formulation of quantum theory. In this it is possible to associate a quantum state with a general boundary of a space–time region. This is also restricted to the pure state case.

Also motivated by quantum gravity, the present author set up the causaloid formalism [7] (see also [8–10]). This is a general framework for physical theories that does not demand that we have definite causal structure. It was shown in [7] how to formulate quantum theory in the causaloid framework. This gave a formulation for the general (not just pure state) case in which we can associate mathematical objects that are analogous to quantum states with general space–time regions (actually this was a discrete situation, so the space–time regions correspond to fragments of a circuit). Such mathematical objects can be combined by taking the causaloid product to get the object for the union of the two space–time regions.

Subsequently, Chiribella et al. [3] gave the quantum combs formulation of quantum theory [3], which has much in common with the formulation presented in this paper (see also the related work of Gutoski & Watrous [11]). In particular, in the quantum combs approach, an operator is associated with an operation. This operator is equal to the input transpose of the operator introduced in §1c and is therefore positive. In the quantum combs formalism, it is possible to associate an operator with a fragment of a circuit and these operators can be combined using the link product. In the present framework, we can combine operators in an analogous way to the way we combine tensors, by having repeated indices (which correspond to taking the partial trace over the corresponding space). We call this the circuit trace. The circuit trace and, effectively, the link product are special cases of the causaloid product. The main differences between the quantum combs formalism and the operator tensor formalism of this paper are the following: (i) we work with operators that are positive under input transpose; (ii) the operators here are given a tensorial structure which is exploited to simplify quite considerably the formulas; (iii) we are able to abandon the use of the tensor product symbol, $\otimes$, and do not have to pad equations with the identity; and (iv) the connection with duotensors (to be discussed later) makes it clear how we can go from a circuit to the corresponding operator tensor calculation for the probability simply by implementing $A_{a_1}^{b_2} \to \hat{A}_{a_1}^{b_2}$.

Another reformulation of quantum theory which is clearly related to the present one is that of Leifer & Spekkens [12] (see also the earlier work of Leifer [13]). In this approach, a conditional state, $\rho_B|A$, playing an analogous role to $P(B|A)$ in classical probability theory, is defined. Quantum formulas can be written as instances of quantum belief propagation, $\rho_B = \text{Trace}_A(\rho_B|A\rho_A)$, which is analogous to classical belief propagation, $P(B) = \sum_R P(B|A)P(A)$. The conditional state, $\rho_B|A$, is positive after taking the transpose over the space associated with $A$ (which is basically the same as the property of having positive input transpose considered in this paper). Unlike the operator tensor formulation and the quantum combs formulation the approach of Leifer and Spekkens is not manifestly time asymmetric. It would be interesting to understand better the relationship to the present approach, especially with respect to this issue of time asymmetry.

Prior to the above-mentioned work, Markopoulou [14] gave the quantum causal histories formulation. These causal graphs were with matrix algebras at each vertex and completely positive maps on the edges. Motivated by Markopoulou's
work, Blute et al. [15] took the dual point of view, putting completely positive maps on the vertices and a similar point of view is adopted in this paper. Markopoulou’s work was very influential in getting people to think about putting quantum operations on a causal graph.

In this work, a pictorial approach to understanding structure and doing calculations has been adopted. This was motivated by the category theoretic approach of Abramsky & Coecke [16]. Pictures provide a powerful way of understanding the structure of calculations and their connection with the underlying physics. In particular, the main conceptual motivation behind this approach is that it puts process and composition at the forefront. The pictorialism revolution [17] initiated by Abramsky and Coecke is being more and more widely adopted. In particular, see [18] and the author’s own papers [19]. The use of pictures to represent calculations in this way goes back, of course, to Penrose’s diagrammatic calculus for tensors [20,21]. The diagrams in this paper were drawn using version 1.1 of the DUOTENZOR package [22].

Diagrammatic techniques have been used to represent ‘tensor network states’ [23] (see also [24]), and recently Wood et al. [25] have developed a tensor network graphical calculus for open quantum systems.

Sorkin and various co-workers have pursued the causal set approach to quantum gravity in which causal graphs are dynamically produced according to some growth dynamics [26]. Recently, Johnston [27] has shown how to put a discretized quantum field theory on a fixed causal set.

At the heart of the operator tensor formulation of quantum theory are duotensors. Duotensors are like tensors but with a bit more structure. They were introduced by the author in [19] to provide a way of formulating general probabilistic theories. Such general probabilistic theories (sometimes described as the convex probabilities framework) have a long history going back originally to Mackey and have been worked on by many others since then [28–35]. More recent works on this framework have been published [1,8,19,36–41].

2. The circuit model

(a) Apparatuses and operations

In quantum theory a typical experiment consists of a bunch of apparatuses, \( A, B, C, \ldots \), placed such that apertures are matched up, allowing systems (electrons, photons, atoms, etc.) to pass between them. Typically, we are interested in a use of an apparatus during some time interval that systems are passing through (typically, this is determined by gating the use of the apparatus with respect to an external clock). An apparatus may have settings (adjusted by knobs for example) and outcomes (read-off meters, flashing lights or the clicking of detectors for example). We denote the outcome by \( x_A \).

It is useful to associate what we will call an operation with a use of an apparatus. An operation has the following features:

- identification of some apertures as inputs and some apertures as outputs;
- a given choice of setting, \( s(A) \); and
- a given set of outcomes, \( o(A) \).
If the outcome that is seen is in the associated outcome set, i.e. \( x_A \in o(A) \), then we say that the operation happened (by associating an outcome set with an operation rather than just a single outcome allows course-graining over outcomes).

The different types of system that may be inputted or outputted are represented by \( a, b, c, \ldots \). Sometimes we will use a single letter to denote a composite system (e.g. \( d = ab \)). Throughout this paper, we will use both the diagrammatic and the symbolic notation. We denote an operation by, for example,

\[
\text{diagramatic notation} \quad A_{a_1 b_2 a_3}^{c_4 a_5} \quad \text{symbolic notation} \quad (2.1)
\]

In the diagrammatic notation, the inputs are shown coming in from the bottom and the outputs are shown coming out from the top. In the symbolic notation, the inputs are shown as subscripts and the outputs are shown as superscripts. In the symbolic notation, we have integer subscripts on the type labels. The purpose of these integers is to show where the wires go, as will be discussed below. Sometimes we will suppress the subscripts and superscripts and simply refer to the operation as, for example, \( A \).

For a given apparatus use with given identification of inputs and outputs and a given choice of settings, we may still have different outcome sets and, therefore, different operations. One interesting case is a set of such operations with disjoint outcome sets whose union is the set of all outcomes for this apparatus. We will call this a complete set of operations. For this situation, we will sometimes use the notation \( A[i] \) to represent the different operations in the complete set having associated (disjoint) outcome sets \( o[i] \) (whose union is the set of all outcomes).

\((b)\) Wires and fragments

We can wire together operations to build fragments. For example,

\[
\text{we give the diagrammatic representation on the left and the symbolic representation on the right. Note that, in the symbolic representation, repeated indices correspond to wires. The outcome set associated with this fragment is } o(A) \times o(B) \times o(C). \text{ If, in some run of the experiment, the outcomes seen at the}
\]

\[
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\]
operations belong to the outcome sets at each operation comprising the fragment, then we can say that the fragment happened for this run. There are certain wiring rules when building fragments.

One wire. At most one wire can be attached to any given input or output.

Type matching. We can only join outputs to inputs of the same type.

No closed loops. If we trace forward long wires from output to input going from one box to the next, then we cannot get back to the box where we started.

Fragments are the most general types of experimental arrangement we consider. Special cases include the following.

Circuits. A circuit is a fragment having no open inputs or outputs.

Preparations. A preparation is a fragment having open outputs but no open inputs.

Results. A result is a fragment having open inputs but no open outputs.

We will sometimes represent fragments by a single letter, $D$, for example. We can write the example in (2.2) above as

$$E_{b_4 a_5 a_9 b_11} \{ b_4, a_5 \rightarrow b_7, d_{10} a_9 \rightarrow d_{10} \}. \quad (2.3)$$

Here we have also specified the causal structure on the right. The causal structure tells us which outputs can be fed (directly or indirectly) into which inputs. For example, we can go from output $a_5$ through some intermediate operations and into input $d_{10}$. Often we will simply refer to a fragment as $E$, for example, without giving the inputs and outputs or causal structure information.

(c) Probabilities

The most general object we can consider is a fragment. In general, a fragment will have open inputs and outputs. Hence, we cannot expect the probability for the fragment to happen (i.e. that the outcomes on the apparatuses are in the outcome sets associated with the corresponding operations) to be independent of what is sent into the inputs (nor can we expect it to be independent of how we post-select on the outputs). Hence we should be careful before attempting to assign a probability to a fragment—we may be unable to sensibly do so. However, these considerations do not apply to circuits (this is the special case of a fragment when we have no open inputs or outputs). Hence we make the following assumption.

**Assumption 2.1.** We can assign a probability to any given circuit (the probability that the circuit ‘happens’), and this probability depends only on the specification of the given circuit (the knob settings and outcome sets at the operations, and the wiring).

In making this assumption, we are assuming that we have appropriately characterized our apparatus uses as operations. For example, if we had inadvertently omitted to include an input on the operation corresponding to some aperture on the apparatus, then an adversary could send some system into this aperture and alter the probabilities.
An important consequence of this assumption is that probabilities factorize for a circuit composed of two disjoint circuits. Thus, consider a circuit $AB$ composed of circuits $A$ and $B$. We have

$$\text{Prob}(AB) = \text{Prob}(A)\text{Prob}(B)$$  

(2.4)

since

$$\text{Prob}(AB) = \text{Prob}(x_A \in o(A) , x_B \in o(B) | \text{sw}(A), \text{sw}(B))$$

$$= \text{Prob}(x_A \in o(A) | x_B \in o(B), \text{sw}(A), \text{sw}(B))\text{Prob}(x_B \in o(B) | \text{sw}(A), \text{sw}(B))$$

$$= \text{Prob}(x_A \in o(A) | \text{sw}(A))\text{Prob}(x_B \in o(B) | \text{sw}(B))$$.

This property is essential for the framework we wish to set up. A similar property was taken as a basic assumption by Chiribella et al. [18].

3. Duotensors

In this section, we will set up the duotensor framework that provides the bridge between operations and operators. To do this, we need to define a notion of equivalence concerning operations.

(a) Equivalence

To define a notion of equivalence, first we define the $p(\cdot)$ function as follows:

$$p(\alpha A + \beta B + \cdots) := \alpha \text{Prob}(A) + \beta \text{Prob}(B) + \cdots$$

for circuits $A, B, \ldots$ and real numbers $\alpha, \beta, \ldots$ (these can be negative). Note that the $p(\cdot)$ function is defined for linear sums of circuits. We cannot define it for general fragments since assumption 2.1 only allows us to assign probabilities to circuits.

Before giving a general definition of equivalence, first consider the following example. We will say

$$\alpha A^{a_1} + \beta B^{a_1} \equiv \gamma C^{a_1} + \delta D^{a_1}$$

(3.1)

if

$$p([\alpha A^{a_1} + \beta B^{a_1}]E_{a_1}) = p([\gamma C^{a_1} + \delta D^{a_1}]E_{a_1}) \quad \text{for all } E_{a_1}.$$  

(3.2)

In general, we wish to consider expressions such as the following:

expression $= \alpha + \beta A + \gamma B + \cdots$,  

(3.3)

where $A, B, \ldots$ are fragments. Our definition of equivalence is the following. We write

expression$_1 \equiv $ expression$_2$  

(3.4)

if

$$p($expression$_1$E) \equiv p($expression$_2$E)$$

(3.5)

for any fragment $E$ that makes the contents of the argument on both sides of this equation a linear sum of circuits.
Clearly, (3.1) is an example of this if (3.2) is satisfied. Another example is the following:

\[ A \equiv \text{Prob}(A) \quad \text{for any circuit} \ A. \]  

(3.6)

To prove this, note that

\[ p(\mathbf{A} \mathbf{E}) = p(\mathbf{A})p(\mathbf{E}) = p(\text{Prob}(\mathbf{A})\mathbf{E}), \]  

(3.7)

where \( \mathbf{E} \) is an arbitrary circuit. This example illustrates that equivalence is a weaker notion than equality. A circuit is equivalent to a real number (its probability) even though these are two very different things (one exists in the laboratory and the other is a purely mathematical object).

In general, there are two types of equivalence.

— Each expression is a real number plus a linear combination of circuits:

\[ \alpha + \beta \mathbf{A} + \gamma \mathbf{B} + \cdots \equiv \delta + \epsilon \mathbf{C} + \zeta \mathbf{D} + \cdots, \]

where \( \mathbf{A}, \mathbf{B}, \ldots, \mathbf{C}, \mathbf{D}, \ldots \) are all circuits.

— Each expression is a linear combination of fragments

\[ \alpha \mathbf{A} + \beta \mathbf{B} + \cdots \equiv \gamma \mathbf{C} + \delta \mathbf{D} + \cdots, \]

where \( \mathbf{A}, \mathbf{B}, \ldots, \mathbf{C}, \mathbf{D}, \ldots \) are all fragments having the same causal structure.

An example of the first type is given by (3.6) and an example of the second type is given by (3.1) (when (3.2) is satisfied).

(b) Fiducial preparations

For any preparation, it is possible to find a sum over a fiducial set of preparations to which the preparation is equivalent. A fiducial set is essentially a basis. We will notate the elements in a fiducial set of preparations for a system of type \( \mathbf{a} \) in the following way:

\[ a_1 \mathbf{X}^{a_1} \iff \mathbf{a} \]

(3.8)

where \( a_1 = 1 \) to \( K_\mathbf{a} \) (this index labels the elements of the fiducial set). On the right we give the diagrammatic notation, and on the left we give the equivalent symbolic notation. We use sans serif font, \( \mathbf{a} \), to denote the type. We use normal math font, \( a \), to denote the index running from 1 to \( K_\mathbf{a} \). The reason for the odd placement of this index (as a pre-subscript) in the symbolic notation will become clear later. In the diagrammatic notation, we have a black dot on the fiducial elements. We set things up such that we must match black dots with white dots when we do calculations.
Since we have a fiducial set of preparations, any preparation $A^{a_1}$ can be written as

$$A^{a_1} = a_1 A_a^{a} X^{a_1} \iff \begin{array}{c} A \\ a \\ \end{array} = \begin{array}{c} a \\ \end{array}$$

(3.9)

In the symbolic notation on the left, we use Einstein summation convention over the repeated index $a_1$. In the diagrammatic notation on the right, we represent the summation over the index by the matching of a black and white dot. Since we always match black and white dots it is convenient to define

$$\begin{array}{c} A \\ a \\ \end{array} = \begin{array}{c} a \\ \end{array}$$

(3.10)

Note that the vertical wires (running from outputs to inputs on operations) are physical—they correspond to systems passing between operations. On the other hand, the horizontal links are mathematical—they correspond to summing over indices. In the diagrams, we write $a$ rather than $a_1$ because, even when we have many links (so we are summing over many indices), we can see where each link is by looking at the diagram without giving it an integer label.

The object $a_1 A$ is a list of numbers (it is an example of a duotensor) associated with the preparation. It is the state expressed with respect to the given fiducial set of preparations. Diagrammatically the state, $a_1 A$, is represented by

$$\begin{array}{c} A \\ a \\ \end{array}$$

(3.11)

In the case of quantum theory we will, later, see how we can also represent states by operators.

(c) Fiducial results

Recall that a result is a fragment having open inputs but no open outputs. Just as with preparations, we can set up a fiducial set of results which we can sum over (with some coefficients) to get an expression equivalent to any result. We denote the fiducial results by

$$X^{a_1} \iff \begin{array}{c} a \\ \end{array}$$

(3.12)

where $a_1 = 1$ to $K$. Note that, once again, we put a black dot on the fiducial element. Then, for an arbitrary result for a system of type $a$, we can write

$$B_a \equiv B_a^{a_1} X^{a_1} \iff \begin{array}{c} B \\ a \\ \end{array} = \begin{array}{c} a \\ \end{array}$$

(3.13)
As before, we define

\[
\begin{align*}
\triangleleft^a_{\downarrow a} \equiv \triangleleft^a_{\downarrow a} \boxed{B} & \quad (3.14)
\end{align*}
\]

\( (d) \) Simple circuits

We can form a circuit by following a preparation by a result for the same type of system. We will first illustrate all of this using the diagrammatic notation (similar equations can always be written down in symbolic notation).

\[
\begin{align*}
\boxed{B} & \equiv \triangleleft^a_{\downarrow a} \equiv \triangleleft^a_{\downarrow a} \boxed{B} & (3.15)
\end{align*}
\]

Using the linearity of the \( p(\cdot) \) function, we have

\[
\begin{align*}
\triangleleft^a_{\downarrow a} & \equiv \triangleleft^a_{\downarrow a} \triangleleft^a_{\downarrow a} \equiv \triangleleft^a_{\downarrow a} \triangleleft^a_{\downarrow a} \boxed{B} & (3.16)
\end{align*}
\]

where we define the hopping metric

\[
\begin{align*}
\bullet^a & \equiv p \left( \triangleleft^a_{\downarrow a} \right) \quad \Leftrightarrow \quad \triangleleft^a_{\downarrow a} & = \bullet^a & (3.17)
\end{align*}
\]

The equivalence on the right follows from the definition on the left by (3.6). The hopping metric is a very important object in this work. Its entries are the probabilities obtained when a fiducial preparation is followed by a fiducial result (and hence its entries are all positive).

\( (e) \) Black and white dots

We must match black and white dots. We can use the hopping metric to change a white dot into a black dot. Hence we have

\[
\begin{align*}
\boxed{A} \bullet & = \boxed{A} \bullet \bullet \quad \bullet \boxed{B} & = \bullet \bullet \boxed{B}
\end{align*}
\]

Hence

\[
\begin{align*}
\boxed{A} \bullet^a \bullet \boxed{B} & = \boxed{A} \bullet^a \boxed{B} = \boxed{A} \bullet^a \boxed{B} & = \boxed{A} \bullet^a \boxed{B}
\end{align*}
\]

We have
Hence, given the definitions we have set up, we can insert and delete pairs of black and white dots as we like. Consistency requires

- $\circ\rightarrow\circ$ to be the inverse of $\bullet\bullet$,
- $\circ\rightarrow\bullet$ to be equal to the identity, and
- $\bullet\rightarrow\bullet$ to be equal to the identity.

The entries of the inverse, $\circ\rightarrow\circ$, can be negative (in quantum theory they will be negative). We can use the inverse to change a black dot into a white dot. One example of this is for the fiducial elements themselves:

$$
\begin{align*}
\begin{array}{c}
\Diamond \\
a
\end{array}
&= 
\begin{array}{c}
\circ \\
a
\end{array}

\begin{array}{c}
a
\end{array}
&= 
\begin{array}{c}
\bullet \\
a
\end{array}

\end{align*}
$$

These correspond to a sum over fiducial elements weighted by the appropriate elements in $\circ\rightarrow\circ$.

\(f\) Symbolic notation for a simple circuit

In symbolic form, the calculation in (3.15) can be written as

$$
A^a_1 B_a_1 \equiv a_i^a \overline{a}_i^a A a_i A \equiv a_i^a A a_i^a B, \quad (3.19)
$$

where we define

$$
a_i^a \overline{a}_i^a := p(a_i^a X_{a_i}^a, \overline{a}_i^a). \quad (3.20)
$$

This is the hopping metric, $\bullet\bullet$, in symbolic notation. We define

$$
A^a_1 := a_i^a \overline{a}_i^a A \quad B := a_i^a \overline{a}_i^a B, \quad (3.21)
$$

so that the hopping metric can be used to ‘hop’ an index over. It hops a subscript to the left (so it becomes a pre-subscript) and it hops a pre-superscript to the right (so it becomes a superscript). The inverse of the hopping metric is $a_i^a \overline{a}_i^a$ (this is the symbolic representation of $\circ\rightarrow\circ$).

\(g\) Full decomposability

Now we introduce our second assumption for the duotensor framework.

**Assumption 3.1 (full decomposability).** Any operation is equivalent to a linear combination of operations each of which consists of a result for each input and a preparation for each output.

Each preparation and result in this decomposition can be expanded in terms of fiducial preparations and results, respectively. Hence, we do not lose any generality by choosing these results and preparations to belong to fiducial sets. Hence we can give a more useful equivalent formulation of the assumption.
Assumption 3.2 (full decomposability). Any operation $A_{a_1b_2\cdots c_3}^{d_4e_5\cdots f_6}$ can be written, in diagrammatic notation, as

$$A_{a_1b_2\cdots c_3}^{d_4e_5\cdots f_6} \equiv \begin{array}{c}
\begin{array}{c}
A \\
ad \cdots b \cdots c
\end{array}
\end{array} \equiv 
\begin{array}{c}
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(h) Duotensors

Inserting black and white dots (with black next to the fiducial elements)

\[
\begin{array}{c}
\begin{array}{c}
\text{A} \text{ } \Rightarrow \text{A}
\end{array}
\end{array}
\]

(3.26)

Therefore,

\[
\begin{array}{c}
\begin{array}{c}
\text{A} \\
\text{with all white dots}
\end{array}
\end{array}
\]

(3.27)

(with all white dots) provides the weights in the sum over fiducial elements. This is an example of a duotensor. Duotensors are like tensors except that each index is associated with two bases (a fiducial basis for preparations and a fiducial basis for results). Duotensors transform like tensors but with respect to two bases (see \[1,2\] for a full discussion of how duotensors transform). We can write duotensors symbolically; for example,

\[
\begin{array}{c}
\begin{array}{c}
\text{A} \\
\text{is written as}
\end{array}
\end{array}
\]

(3.28)

The following map is useful in converting between the diagramatic and symbolic notations:

\[
\text{A}
\]

(3.29)

Importantly, duotensors are accompanied by a hopping metric for each system type which is used to convert between different forms of the duotensor. In diagrammatic notation, we can use \(\text{○}\text{─○}\) and \(\text{●}\text{─●}\) to change the colours of the dots.

\[
\begin{array}{c}
\begin{array}{c}
\text{A} \\
\text{is written as}
\end{array}
\end{array}
\]

(3.30)

It follows from full decomposability that the duotensor with all black dots corresponds to the fiducial probabilities. For example,

\[
\begin{array}{c}
\begin{array}{c}
\text{Prob}
\end{array}
\end{array}
\]

(3.31)
The operator tensor formulation

follows by inserting (3.26) in the diagram on the right-hand side, substituting in the hopping metric (3.17) and cancelling over matched black and white dots. Hence, we can obtain the duotensor with all black dots by process tomography using fiducial preparations and results. We can then use the hopping metrics to convert to any other form. In particular, the form with all white dots is the coefficients in the expansion of an operation in terms of fiducial elements. This will be particularly important when we go over to operators where the duotensor with all white dots will be the weights in the decomposition of an operator tensor in terms of fiducial preparation operators and result operators (see §5b). Another form of note is the standard form in which we have white dots on the left and black dots on the right. In this case, when we put the duotensors next to each other a black dot will always meet a white dot. The duotensor associated with a preparation will have all black dots when in standard form and so constitutes a list of fiducial probabilities.

(i) General circuits

Now we have set up the machinery sufficient to convert a general circuit into an equivalent duotensor calculation which, therefore, gives the probability for this circuit to happen. To see this consider

In the first step, we have replaced each operation with its fully decomposed form using (3.22). At this stage we have a linear sum of products of fiducial circuits. In the second step, we apply the \( p(\cdot) \) function and use the definition of the hopping metric in (3.17). We also make use of the property that the \( p(\cdot) \) function factorizes over disjoint circuits (since probabilities factorize over disjoint circuits as in (2.4)).
The bottom line is

\[
\text{Prob} \begin{pmatrix}
A & B & C & D \\
 a & b & c & d \\
 a & a & c & a
\end{pmatrix} = \begin{pmatrix}
A & B & C & D \\
 a & a & b & d \\
 a & a & c & a
\end{pmatrix}
\]

(3.32)

This clearly follows for any circuit. In other words, the probability for a circuit is given by a duotensor diagram that looks the same (except that the font has changed and it has been rotated through $90^\circ$).

4. The machinery of operator tensors

(a) Operator tensors

We will now set up another mathematical structure, namely that of operator tensors. In the next section, we will see how to use these to reformulate quantum theory. We define complex Hilbert spaces $\mathcal{H}_{a_1}, \mathcal{H}_{b_2}, \ldots$ having dimensions $N_a, N_b, \ldots$. We define complex Hilbert spaces $\mathcal{H}^{a_1}, \mathcal{H}^{b_2}, \ldots$ having dimensions $N_a, N_b, \ldots$. We define

$$\mathcal{H}_{a_1 b_2 \ldots c_3}^{d_4 e_5 \ldots f_6} := \mathcal{H}_{a_1} \otimes \mathcal{H}_{b_2} \otimes \cdots \otimes \mathcal{H}_{c_3} \otimes \mathcal{H}^{d_4} \otimes \mathcal{H}^{e_5} \otimes \cdots \otimes \mathcal{H}^{f_6}. \quad (4.1)$$

We define

$$\mathcal{V}_{a_1 b_2 \ldots c_3}^{d_4 e_5 \ldots f_6}$$

as the space of Hermitian operators acting on $\mathcal{H}_{a_1 b_2 \ldots c_3}^{d_4 e_5 \ldots f_6}$. We write

$$A_{a_1 b_2 \ldots c_3}^{d_4 e_5 \ldots f_6} \leftrightarrow \begin{array}{c}
d \ e \ f \\
\cdots \\
\end{array}$$

(4.2)

for elements of $\mathcal{V}_{a_1 b_2 \ldots c_3}^{d_4 e_5 \ldots f_6}$. We call operators having only superscripts preparation operators and we call operators having only subscripts result operators.
The operator tensor formulation

(b) Fiducial operators

We introduce a fiducial (spanning) set of preparation operators for \( V^a \)

\[ a \hat{X}^a_1 \iff a \bullet \triangleleft^a \]  

(4.3)

where \( a_1 = 1 \) to \( K_a \). We have that \( K_a = N_a^2 \) as this is the number of linearly independent operators spanning the space of Hermitian operators on an \( N_a \) dimensional complex Hilbert space. Similarly, we introduce a fiducial (spanning) set of result operators for the space \( V_{a_1} \)

\[ \hat{X}_{a_1}^a \iff \triangleleft^a \]  

(4.4)

where \( a_1 = 1 \) to \( K_a \).

(c) Full decomposability of operator tensors

Since the Hilbert spaces we are using are complex we have

\[ V^d_{a_1b_2\ldots c_3} = V_{a_1} \otimes V_{b_2} \otimes \cdots \otimes V_{c_3} \otimes V^d \otimes V^e \otimes \cdots \otimes V^f \]  

(4.5)

for the space of Hermitian operators. Hence, we can write any operator as a linear sum over fiducial operators for the inputs and outputs:

\[ \hat{A}^d_{a_1b_2\ldots c_3} = d_1 c_3 \ldots f_6 A_{a_1 b_2 \ldots c_3} \hat{X}_{a_1}^a \hat{X}_{b_2}^b \cdots \hat{X}_{c_3}^c \hat{X}_{d_4}^d \hat{X}_{c_5}^e \cdots f_6 \hat{X}_{f_6}^f \]  

(4.6)

in symbolic notation or

\[ \begin{array}{ccc} d & e & f \\ \cdots & \cdots & \cdots \\ a & b & c \\ \end{array} = \begin{array}{ccc} a & b & c \\ \cdots & \cdots & \cdots \\ d & e & f \\ \end{array} \]  

(4.7)

in diagrammatic notation. This is clearly analogous to the assumption of full decomposability for operations. Notice, however, that (i) it is just a fact about the space of Hermitian operators on a (complex) Hilbert space and (ii) we have equality here rather than equivalence.

(d) Combining operator tensors

Usually, when dealing with operators, much use is made of the tensor product symbol \( \otimes \) and there is, correspondingly, a need to pad expressions with the
identity. We will follow a different route here. The tensor product of \( \hat{A}^{a_1} \) and \( \hat{B}^{b_2} \) is written as \( \hat{A}^{a_1} \hat{B}^{b_2} \) (in \( V^{a_1 b_2} = V^{a_1} \otimes V^{b_2} \)) rather than \( \hat{A}^{a_1} \otimes \hat{B}^{b_2} \). More generally, we write the tensor product of \( \hat{C}^{c_3 b_5} \) and \( \hat{D}^{b_8 c_9} \) as

\[
\hat{C}^{c_3 b_5} \hat{D}^{b_8 c_9}
\]

(4.8)

The order is not important, so we could, instead, write

\[
\hat{D}^{b_8 c_9} \hat{C}^{c_3 b_5}
\]

(4.9)

since all the relevant information that is normally conveyed by the order in which the tensor product is taken is, here, contained in the integer subscripts on the type labels.

If have a repeated integer, this corresponds to taking the product in the Hilbert space corresponding to the repeated index and then taking the partial trace in that space. To do this in the general case, we will use full decomposability. However, it is worth illustrating this first for the simple case

\[
\hat{A}^{a_1} \hat{B}^{a_1} \iff \hat{B}
\]

(4.10)

In conventional notation, this is equal to \( \text{Trace}(\hat{A}^{a_1} \hat{B}^{a_1}) \).

Now consider the example

\[
\hat{A}^{b_3 c_4} \hat{B}^{d_6 c_7} = A^{b_1 c_4} X^{a_1} X^{b_2} X^{c_3} X^{c_4} B^{d_6 c_7} X^{b_5} X^{b_6} X^{b_7}
\]

(4.11)

Here the \( b_3 \) label is repeated so it is implicit that we are taking the trace of the product of \( b_3 X^{b_3} \) and \( X^{b_3} \). We can also write this in diagrammatic notation as

\[
\hat{B} = \hat{A}
\]

(4.12)

This Hermitian operator is in

\[
V^{c_d a_1 b_2 a_5} = V^{a_1} \otimes V^{b_2} \otimes V^{a_5} \otimes V^{c_4} \otimes V^{d_6} \otimes V^{c_7}
\]

(4.13)
The operator tensor formulation

Note that we have taken the partial trace over the space associated with $b_3$. We will call the product in (4.11) and (4.12) the circuit trace since, once we expand in terms of fiducials, we are taking the trace over a fiducial circuit consisting of a fiducial preparation operator and a fiducial result operator.

More generally, we can consider expressions such as

$$\hat{A}^{a_1 b_2} \hat{B}^{c_2 a_3} \hat{C}^{b_5} \in \mathcal{V}_{a_6}^{a_1 b_6}. \quad (4.14)$$

Here we have three repeated labels ($b_2$, $c_3$ and $a_4$). Once expanded in terms of fiducial operators each of these repeated labels will correspond to a fiducial operator circuit.

(e) The operator hopping metric

Whenever we wire together operator tensors and then insert the fully decomposed form the operator hopping metric will appear. This is

$$a^g_{a_1} := a^g_{a_1} \hat{X}^{a_1} \hat{X}^{-a_1} \iff \begin{array}{c} \bullet \rightarrow \bullet \end{array} \quad (4.15)$$

Strictly, we should use a different symbol than for the hopping metric deriving from fiducial operations. However, we will be seeking to set them equal in the next section, so we will use the same symbol.

(f) General operator circuit

We can use full decomposability of operators to convert an operator circuit into a duotensor calculation. For example,
This is very similar to the operation case discussed in §3 above where we used full decomposability of operations, the main difference being that we have equality rather than equivalence in the first and the second step. This is because we have equality in the full decomposability of operators (4.7), but only equivalence in the full decomposability of operations (3.22).

5. Operator tensor formulation of quantum theory

(a) Correspondence

We will say that operations correspond to operators if there is a mapping from operations, \( A_{a_1 b_2 \ldots c_3} \), to operators, \( \hat{A}_{a_1 b_2 \ldots c_3} \), such that the probability for any circuit composed of operations is equal to the circuit operator obtained under this mapping. If operations correspond to operators then, for example,

\[
\text{Prob}(A_{a_1 b_2} B_{b_2} C_{a_1 c_3}) = \hat{A}_{a_1 b_2} \hat{B}_{b_2} \hat{C}_{a_1 c_3}.
\]

(5.1)

We can write the same example in diagrammatic notation as

\[
\begin{array}{c}
\text{Prob} \\
\includegraphics[width=2cm]{prob_circuit}
\end{array} = \begin{array}{c}
\includegraphics[width=2cm]{prob_operator}
\end{array}
\]

(5.2)

In fact, if we set up a correspondence from fiducial operations to fiducial operators, then a correspondence from general operations to general operators follows. To see this assume that we have found a correspondence

\[
X_{a_1} \rightarrow \hat{X}_{a_1}
\]

(5.3)

for \( a_1 = 1 \) to \( K_a \) for all types \( a \). Since we have correspondence, it follows that

\[
\text{Prob}(a_1 X_{a_1} X_{a_1}') = a_1 \hat{X}_{a_1} \hat{X}_{a_1}'.
\]

(5.4)

In other words, the hopping metric associated with the operations is equal to the hopping metric associated with the operators for each type. Then, in general, we can say that the operation

\[
A_{a_1 b_2 \ldots c_3}^{d_4 e_5 \ldots f_6} = a_1 b_2 \ldots c_3 X_{a_1}^{d_4} X_{b_2}^{e_5} \ldots X_{c_3}^{f_6}
\]

(5.5)

corresponds to the operator

\[
\hat{A}_{a_1 b_2 \ldots c_3}^{d_4 e_5 \ldots f_6} = a_1 b_2 \ldots c_3 \hat{X}_{a_1}^{d_4} \hat{X}_{b_2}^{e_5} \ldots \hat{X}_{c_3}^{f_6}
\]

(5.6)
Note that we have the same duotensor in each expansion. We can illustrate that this gives us operation–operator correspondence by means of an example. Thus, we have

$$\text{Prob} \left( \begin{array}{c}
A \\
B \\
C
\end{array} \right) = \begin{array}{c}
A \\
B \\
C
\end{array} = \hat{A} \hat{B} \hat{C}$$

(5.7)

Here we are using full decomposability of operations to get from the first to the second expression, and full decomposability of operators to get from the third to the second expression. The fact that we have equal hopping metrics means that we have equality of the first and third expressions (as in (5.2)). Clearly, this will work for any circuit.

(b) Experimentally determining operators

Here we will discuss how to determine experimentally the operator associated with an operation. First we need to set up fiducial sets of preparations, $a_i X^{a_i}$, and fiducial sets of results, $X_a$. This can be done either by having a knowledge of the physics (for example, we know that for a spin-half particle, results corresponding to spin along the $+x$, $+y$, $+z$ and $-z$ directions will suffice), or through exhaustive tomography on all the preparations and results associated with the given system type followed by linear analysis of the results to pick out fiducial sets. Having established these fiducial sets, we can measure the hopping metric by experimentally determining $\text{Prob}(a_i' X^{a_i} X_a)$. Next, by means of appropriate linear algebra, we find sets of fiducial operator preparations and results that have the same hopping metric, i.e.

$$\text{Prob}(a_i' \hat{X}^{a_i} \hat{X}_a) = \text{Prob}(a_i' X^{a_i} X_a)$$

(5.8)

Having obtained the hopping metric and the fiducial preparation and result operators we can determine the operator associated with an operation as follows:

- first we perform local process tomography placing fiducial preparations on all the inputs and fiducial results on all the outputs; the set of probabilities so obtained is equal to the duotensor with all black dots (see §3h);
- next, obtain the inverse of the hopping metric and use this to convert the duotensor to the form having all white dots; and
- finally, calculate the operator tensor by weighting fiducial operators with this all-white dots duotensor as in (4.6) or (4.7).

(c) Physicality of operators

We do not expect all operators to correspond to operations. Thus, the set of operators that are allowed will be restricted in some way. We assume that, for
every type, the set of operators that are associated with operations contains at least the following:

— every rank one projection preparation operator, \( \hat{A}^{a_1} \);
— every rank one projection result operator, \( \hat{C}^{a_1} \); and
— the identity result operator, \( \hat{I}^{a_1} \).

Recall that a type, \( a \), may correspond to a composite system. The identity result operator has the property that it gives 1 when applied to any rank one projection preparation operator (e.g. \( \hat{A}^{a_1} \hat{I}^{a_1} = 1 \)). Thus, it must correspond to the deterministic result (where the set of outcomes is equal to the set of all possible outcomes).

We define \textit{Physical operators}. An operator, \( \hat{B}^{b_2}_{a_1} \), is said to be \textit{physical} if

\[
0 \leq \hat{A}^{a_1g_3}_{a_1} \hat{B}^{b_2}_{a_1} \hat{C}^{b_2g_3}_{b_2} \quad (5.9)
\]

and

\[
\hat{A}^{a_1g_3}_{a_1} \hat{B}^{b_2}_{a_1} \hat{I}^{b_2g_3}_{b_2} \leq 1 \quad (5.10)
\]

for all rank one projection operators \( \hat{A}^{a_1g_7}_{a_1} \) and \( \hat{C}^{d_4g_7}_{d_4} \) and for all types \( g \).

This means that any circuit built out of the given operator sandwiched between the operators we have already admitted (rank one projection preparation and result operators and the identity result operator) will be between 0 and 1 as is necessary for the probability interpretation.

We define the \textit{input transpose} of an operator as the partial transpose in the input space with respect to some given basis. We denote the input transpose of \( \hat{B}^{b_2}_{a_1} \) by \( \hat{B}^{b_2}_{a_1} \). One way to find the input transpose is to write the operator in a fully decomposed form and then take the transpose of the fiducial result operators (as these correspond to the inputs). We note that, if an operator is positive after taking the input transpose with respect one basis, then the input transpose will be positive when taken with respect to any other basis. We can define the \textit{output transpose} in a similar way. More generally, we can consider expressions such as \( \hat{A}^{c_3d_4}_{a_1b_2} \), where we take the partial transpose over some of the spaces. We note a useful result. Namely, if we take the partial transpose in any space over which the circuit trace is taken, then the expression remains unchanged. For example,

\[
\hat{A}^{c_3d_4}_{a_1b_2} \hat{B}^{b_2c_5}_{a_6} = \hat{A}^{c_3d_4}_{a_1b_2} \hat{B}^{b_2c_5}_{a_6} \quad (5.11)
\]

This is simple to prove (see §8.3 of [2]).

We will now prove the following theorem.

\textit{Physicality theorem}. An operator, \( \hat{B}^{b_2}_{a_1} \), is physical if and only if (i) it has positive input transpose, i.e. \( \hat{B}^{b_2}_{a_1} \geq 0 \), and (ii) its output trace is less than or equal to the identity, i.e. \( \hat{B}^{b_2}_{a_1} \hat{I}^{b_2} \leq I_{a_1} \).
To prove this, note that we can write
\[ \hat{A}_{a1g3} = |A_{a1g3}\rangle\langle A_{a1g3}|, \quad \hat{C}_{b2g3} = |C_{b2g3}\rangle\langle C_{b2g3}|. \] (5.12)

We will consider taking the output transpose with respect to the basis \(|V_{a1}[n]\rangle\) \((n = 1\) to \(N_{a}\)). We can write, in the Schmidt decomposed form,
\[ |A_{a1g3}\rangle = \sum_{n} c_n |V_{a1}[n]\rangle |W_{g3}[n]\rangle, \] (5.13)

where the states \(|\hat{W}_{g}[n]\rangle\) constitute an orthonormal basis set for \(\mathcal{H}_{g3}\) allowing this Schmidt decomposition. We can write
\[ \langle C_{b2g3}| = \sum_{n} \langle E_{b2}[n]| \langle W_{g3}[n]|. \] (5.14)

Then
\[ \hat{A}_{a1g3} \hat{C}_{b2g3} = \left( \sum_{m} c_m^{*} |V_{a1}[m]\rangle \otimes |E_{b2}[m]\rangle \otimes \left( c_n \sum_{n} |V_{a1}[n]\rangle \otimes \langle E_{b2}[n]| \right) \right), \] (5.15)

where we have used the fact that we are taking the partial trace over the space associated with \(g_3\) (we have also inserted the \(\otimes\) symbol for clarity). The output transpose of this (in the \(|V_{a1}[n]\rangle\) basis) is
\[ \hat{A}_{a1g3}^{T} \hat{C}_{b2g3} = \left( \sum_{m} c_m^{*} |V_{a1}[m]\rangle \otimes |E_{b2}[m]\rangle \right) \otimes \left( \sum_{n} c_n \langle V_{a1}[n]| \otimes \langle E_{b2}[n]| \right). \] (5.16)

This is proportional to a rank one projection operator. We are free to choose \(c_n\) and \(|E_{b2}[n]\rangle\) as we like (subject only to normalization constraints) and, hence, we can make this proportional to any rank one operator. Now we note that
\[ \hat{A}_{a1g3} \hat{B}_{a1}^{b2} \hat{C}_{b2g3} = \hat{A}_{a1g3}^{T} \hat{C}_{b2g3} \hat{B}_{a1}^{b2} \] (5.17)
since, as pointed out above, such expressions are invariant taking the transpose in any given space over which the partial trace is taken. Since the expression in (5.16) can be made proportional to a rank one operator and since the expression in (5.17) must be non-negative by (5.9), it follows that \(\hat{B}_{a1}^{b2}\) must be positive. This proves the necessity of the first point. The necessity of the second point follows immediately from (5.10), the fact that \(\hat{I}_{b2g3} = \hat{I}_{b2} \hat{I}_{g3}\), and the fact that \(\hat{A}_{a1g3}\) can correspond to any rank one projection operator. It is also clear, by these methods, that sufficiency follows. Hence the theorem is proven.

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We can easily see that any operator circuit composed only of physical operators will be equal to a number between 0 and 1 (as required for the probability interpretation). To illustrate this consider the example

$$\hat{A}^{a_1b_2} \hat{B}^{c_3a_4}_{b_2} \hat{C}^{a_1c_3a_4}_{a_4}$$

(5.18)

(this example is shown diagrammatically on the left of (5.2)). We can foliate this circuit

$$[\hat{A}^{a_1b_2}][\hat{C}^{c_3a_4}_{a_4}]$$

(5.19)

where we have indicated time steps (and hence hypersurfaces of the foliation) by square brackets. We have had to insert the identity transformation, $I^{a_5}_{a_1}$, to allow this foliation as two hypersurfaces intercept the given wire. Now, we take the partial transpose on the spaces intercepted by *alternate* hypersurfaces

$$[\hat{A}^{a_1b_2^T}][\hat{C}^{c_3a_4}_{a_4}]$$

(5.20)

Now any given operator has had either the input or output transpose taken and, since all operators in (5.19) are physical, all the operators in (5.20) are now positive (positivity of input transpose is equivalent to positivity of output transpose). Hence, the expression must be positive. This will work for any circuit, no matter how many hypersurfaces are needed to foliate it, as long as we take the transpose on alternate hypersurfaces. That the operator circuit is less than or equal to 1 follows by proceeding backwards through foliation. Thus, $[\hat{C}^{c_3a_4}_{a_4}]$ is less than $\hat{I}^{a_5c_3a_4}_{a_4}$. Hence, $[\hat{C}^{c_3a_4}_{a_4}]$ is less than $\hat{I}^{a_1b_2}_{a_2}$. Hence, the whole thing is less than or equal to 1. It is interesting that we invoke the possibility of foliating the circuit here. A circuit can be foliated if and only if there are no closed loops [1]. Hence, there is a deep connection between such operator circuits behaving like probabilities (being bounded by 0 and 1) and the lack of such closed loops (which would correspond to closed time-like curves).

We define

A *complete set of physical operators*, $\{\hat{B}^{b_2}_{a_1} | l = 1 \text{ to } L\}$, is one in which each operator, $\hat{B}^{b_2}_{a_1}[l]$, has positive input transpose and, further,

$$\sum_{l=1}^{L} \hat{B}^{b_2}_{a_1}[l] \hat{I}_{b_2} = \hat{I}_{a_1}.$$  

(5.21)

The operators in a complete set of physical operators must each be physical as (5.21) implies $\hat{B}^{b_2}_{a_1}[l] \hat{I}_{b_2} \leq \hat{I}_{a_1}$ (using the fact that $\hat{B}^{b_2}_{a_1}[l] \hat{I}_{b_2} = \hat{B}^{b_2}_{a_1}[l] \hat{I}_{b_2} \geq 0$). Further, (5.21) is equivalent to the condition that

$$\sum_{l=1}^{L} \hat{B}^{b_2}_{a_1}[l] \hat{I}_{b_2}g_3 = 1$$

(5.22)

for any positive operator, $\hat{A}^{a_1g_3}$, having trace equal to one.

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Mathematical axioms for quantum theory

We will now give axioms for quantum theory in the operator tensor formulation. Quantum theory. The following two mathematical axioms specify quantum theory.

Axiom 1. Operations correspond to operators.
Axiom 2. Every complete set of physical operators corresponds to a complete set of operations.

The operators here are understood to act on a complex Hilbert space.

Recall that a complete set of operations is one in which each member is associated with the same apparatus use with the same settings but having disjoint outcome sets whose union is the set of all outcomes for this apparatus use. The first axiom guarantees that we can calculate the probability of a circuit (composed of operations) by replacing each operation by the corresponding operator. The second axiom tells us that every permissible set of operators (i.e. every complete set of physical operators) actually corresponds to a realizable complete set of operations. A more succinct statement is the following.

Quantum theory. Every complete set of physical operators corresponds to a complete set of operations and vice versa.

The vice versa part of this implies axiom 1 although, taken at face value, it is a little stronger than axiom 1.

These axioms are motivated by assuming that certain operators are allowed (rank one projection operators for preparations and results, and the identity operator for results) and seeing what the largest class of operators consistent with this situation is. We get an alternative formulation of quantum theory in this way, which is easily shown to be equivalent to the usual formulation as discussed in §1b (see [2] for more details).

Formalism locality

So far we have considered how to calculate the probability for a circuit. However, we may be interested in doing calculations for some part of a circuit without doing a calculation for the whole circuit. An extreme example would be where we model the entire universe by means of a circuit (let us assume that the universe is finite such that the circuit has a finite number of operations). In this case, we would, for many applications, need to be able to make predictions concerning only a part of the universe. In the circuit framework, an arbitrary space–time region corresponds to a fragment (more accurately, it corresponds to the fragments having some given causal structure that can be placed in a corresponding ‘hole’ in the bigger circuit). These considerations motivate the following definition.

Formalism locality. A formalism for a physical theory is said to have the property of ‘formalism locality’ if we can do calculations pertaining to any region of space–time employing only mathematical objects associated with that region.

Formalism locality is a property of the way a physical theory is formulated rather than, necessarily, being a property of the theory itself. We will show that the operator tensor formulation has this property. Thus, consider a set of fragments, \( A_{a_1b_2\ldots c_3}[n] \), all having the same causal structure (see §2b).
The most general thing we can consider calculating for this situation is the probability ratio
\[
\frac{\text{Prob}(A_{d_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[m])}{\text{Prob}(A_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[n])}.
\]
(5.23)

What does this mean? In particular, in most cases we expect this probability to depend on what is done outside the given space–time region—in other words, we expect that it will, in most cases, depend on what the bigger circuit is. However, this may not always be the case. Thus, what we are seeking is (i) some mathematical condition telling us when this probability ratio is well defined (independent of what happens outside the given space–time region) and (ii) in such situations, we also want to know what this probability ratio is equal to.

If we complete the fragments into a circuit in the same way, then we have
\[
\frac{\text{Prob}(A_{d_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[m]E_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6})}{\text{Prob}(A_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[n]E_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6})} = \frac{\hat{A}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[m]\hat{E}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}}{\hat{A}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[n]\hat{E}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}}.
\]
(5.24)

The only way for the probability ratio in (5.23) to make sense is if the expression in (5.24) is independent of \(\hat{E}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}\). But \(\hat{E}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}\) can span the space of possible Hermitian operators and, hence, the only way to have this independence is if \(\hat{A}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[m]\) and \(\hat{A}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[n]\) are proportional:
\[
\hat{A}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[m] = r \hat{A}_{a_1 b_2 \cdots c_3}^{d_4 e_5 \cdots g_6}[n].
\]
(5.25)

The probability ratio is then equal to the proportionality constant, \(r\). Hence we have formalism locality. Standard formulations of quantum theory do not have this property.

(f) Transforming operator tensors

We can transform an operator tensor in a similar way to the way we would a tensor. We must be sure that any operator circuit remains unchanged under such a transformation (operator circuits are the equivalent of scalars for tensors). Thus, for each system type \(a\), we can write
\[
\hat{X}_{a_1}^{a_l} = \hat{T}_{a_1}^{a_l} \hat{X}_{a_1}^{a_l} = \hat{T}_{a_1}^{a_l} \hat{X}_{a_1}^{a_l},
\]
(5.26)
where, importantly, we require
\[
\hat{T}_{a_1}^{a_1} \hat{T}_{a_1}^{a_2} = \hat{T}_{a_1}^{a_2},
\]
(5.27)
where \(\hat{T}_{a_1}^{a_2}\) corresponds to the identity transformation having the properties that \(\hat{T}_{a_1}^{a_2} \hat{C}_{a_3}^{a_4} = \hat{C}_{a_3}^{a_4}\) and \(\hat{T}_{a_1}^{a_2} \hat{C}_{a_2}^{a_4} = \hat{C}_{a_1}^{a_4}\) for any operator \(\hat{C}_{a_3}^{a_4}\). Hence we have
\[
\hat{X}_{a_1}^{a_l} \hat{X}_{a_1}^{a_l} = \hat{X}_{a_1}^{a_l} \hat{X}_{a_1}^{a_l},
\]
(5.28)
The operator tensor formulation

as this is an operator circuit (it has no open wires). This expression is, in fact, the hopping metric (it is a duotensor) and, consequently, it follows that under such transformations, any operator circuit will remain unchanged.

What transformations, \( \hat{T}_{a_i}^{a_1} \), can we allow? If we are only interested in leaving operator circuits invariant, then any invertible transformation will do. However, we may also be interested in being sure that physical operators transform to physical operators. We started by assuming that the set of rank one projectors corresponds to preparations. It follows from the facts that preparation operators must be positive and have trace less than or equal to one, that such rank one projectors represent pure states and that all pure states are represented by such rank one projectors. Therefore, if we wish to preserve physicality under a transformation, rank one projector preparations must be transformed to rank one projector preparations. By Wigner’s theorem [48], we know that this is only true if we have transformations corresponding to unitary or anti-unitary maps on the underlying Hilbert space (see Peres [49] for a nice discussion of Wigner’s theorem). Consider an operator tensor, \( \hat{T}_{a_i}^{a_1} \), corresponding to a unitary map

\[
\hat{T}_{a_i}^{a_1} = U \hat{A}_{a_1} A^{a_1} U^\dagger. \tag{5.29}
\]

(Here we have not attempted to balance the subscripts and superscripts as the notation on the left-hand side is foreign to the operator tensor notation generally adopted in this paper.) Such transformations will clearly preserve physicality of a general operator tensor. What about the anti-unitary case? Consider a preparation operator \( \hat{A}_{a_1b_2} \) corresponding to a pure entangled state. Any anti-unitary map can be written as complex conjugation followed by a unitary map. At the level of the space \( V^{a_1} \), this corresponds to a transposition transformation followed by a transformation corresponding to a unitary map. Thus, the essential part of the transformation corresponding to an anti-unitary map when applied to one system is partial transposition for that system. If we perform a partial transposition for the system of type \( a \) but perform no transformation for the system of type \( b \), then, after the transformation, the preparation operator will no longer be physical in general (this follows from the work of Peres [50]). Hence, if we include transformations corresponding to anti-unitary maps on the underlying Hilbert space, then we will not preserve physicality.

With standard tensors, we can restrict ourselves to orthogonal transformations such that the coordinate system remains orthogonal, or we can consider general invertible transformations such that we consider general coordinate systems (as in General Relativity). Similarly, with operator tensors we can restrict ourselves to unitary transformations such that the operators remain physical, or we can relax this and consider general invertible transformation and then the operators will become non-physical. For the purposes of this paper, it is better to stick to physicality preserving transformations so that the axioms above apply after a transformation. However, it is possible that for some other applications the freedom to have general transformations (such that we go to non-physical operators) will be important just as the freedom of general coordinate transformations (such that we go to non-orthogonal coordinate systems) was important in formulating General Relativity.
6. Discussion

(a) Time symmetry and asymmetry

The standard formulation of quantum theory requires that we foliate a circuit so that we can evolve a state in time. This means adding extra structure to a circuit that is not part of the physics. The operator tensor formulation does not do this. Rather, it supplies a formulation of quantum theory in which the calculation looks like the description of the circuit. Operations correspond to operators. An operator, $\hat{A}_{a_1b_2}^{c_3d_4}$, for example, must satisfy two conditions: (i) that it has positive input transpose ($\hat{A}_{a_1b_2}^{c_3d_4} a_1^T b_2^T \geq 0$) and (ii) its output trace is less than or equal to the identity ($\hat{A}_{a_1b_2}^{c_3d_4} \hat{I}_{c_3d_4} \leq \hat{I}_{a_1b_2}$). Inputs and outputs define a direction in time. Space, in the circuit framework, is written into the fact that we can have composite systems. The first condition is consistent with time symmetry since positivity of the input transpose is equivalent to positivity of the output transpose (e.g. $\hat{A}_{a_1b_2}^{c_3d_4} a_1^T b_2^T \geq 0$ is equivalent to $\hat{A}_{a_1b_2}^{c_3d_4} c_3^T d_4^T \geq 0$). However, this condition does put space and time on a slightly different footing. This is analogous to the way that time is treated in a slightly different way in relativity (the time coordinate is associated with, say, a minus sign in the metric while the space coordinates are associated with a plus sign). Condition (ii) is equivalent to the condition that $\hat{A}_{a_1g_3}^{a_1} \hat{B}_{b_2}^{b_2} \hat{I}_{b_2g_3} \leq 1$ for any rank one projector $\hat{A}_{a_1g_3}^{a_1}$. The time reversed condition (which we do not demand) would read $\hat{B}_{a_1}^{b_2} \hat{B}_{a_1}^{b_2} \hat{C}_{b_2g_3}^{b_2g_3} \leq 1$ for any rank one projector $\hat{B}_{a_1}^{b_2}$. It is easy to see that $\hat{B}_{a_1}^{b_2}$ is physical. On the other hand, $\hat{B}_{b_2}^{b_2}$ is not physical although it does satisfy the time reversed condition just given. Axiom 2 implies that there exists an operation corresponding to any physical operator. Hence, there is an operation corresponding to $\hat{I}_{a_1}$. There cannot be an operation corresponding to $\hat{I}_{b_2}$, however, as it is non-physical. Thus, we see that this formalism is explicitly time asymmetric and that this asymmetry comes from condition (ii) in the definition of physicality.

In the case where we restrict ourselves only to pure states and unitary transformations, this time asymmetry disappears. However, unitary transformations are not sufficient for covering the cases where we extract non-trivial measurement results (i.e. they fail to cover any non-trivial experiment). It is an important question as to whether this formalism implies a fundamental time asymmetry in nature or whether this is only apparent. In this connection, it is worth noting that the recent formulation of Leifer & Spekkens [12], which shares some features with the present formalism, does not appear to be time asymmetric.

(b) Quantum field theory and quantum gravity

The formalism here pertains to discrete circuits. If we take a region of space–time and cut it up into some number of pieces, then we can place wires between these pieces to form a circuit. Now, if these smaller pieces have only space-like (or null) boundaries, then we can think of the future-facing boundaries as corresponding to outputs and the past-facing boundaries as corresponding to inputs. If some part of the boundary is time-like, then it will correspond to both
The operator tensor formulation

input and outputs (this is like a fragment having inputs and outputs coming out of the side). The challenge of setting up quantum field theory is to work out how to take the limit of this situation to the infinitesimal (rather than discrete) case. However, this framework offers certain advantages as an approach to quantum field theory. Namely, it provides a formulation which is in keeping with the spirit of special relativity without necessary reference to any specific foliation.

This framework might also provide a good stepping stone to a theory of quantum gravity. Formalism locality, as a desirable property, was motivated by considerations from quantum gravity [10]. In standard quantum theory, we use ‘rectangular’ regions of space–time resulting from evolving a state from a state on a past space-like hypersurface to a future space-like hypersurface. However, in a theory of quantum gravity we expect to have indefinite causal structure, so it will be impossible to refer our laws to specially shaped regions of space–time (the notion of ‘space-like’ will not make sense if we have indefinite causal structure). If this reasoning is correct, formalism locality will be a necessary feature of quantum gravity. The limiting case of a theory of quantum gravity in the direction of applicability of quantum theory is likely to be a formulation of quantum theory with the formalism locality property.

One great challenge faced in applying these techniques to quantum field theory and possibly to quantum gravity is to know how to adapt or reproduce that relevant physics which is usually formulated in terms of differential equations using the Turing inspired ideas of computer science.

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