Graph Algebras for Quantum Theory

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Abstract. - We consider algebraic structure of Quantum Theory and provide its combinatorial representation. It is shown that by lifting to the richer algebra of graphs operator calculus gains simple interpretation as the shadow of natural operations on graphs. This provides insights into the algebraic structure of the theory and sheds light on the combinatorial nature and philosophy hidden behind its formalism.

Introduction. – Quantum Theory seen in action is an interplay of mathematical ideas and physical concepts. From the present-day perspective its formalism and structure is founded on theory of Hilbert spaces [1]. According to a few basic postulates physical notions of a system and apparatus, as well as transformations and measurements, are described in terms of operators. In this way algebra of operators constitutes the proper mathematical framework within which quantum theories are built. Structure of this algebra is determined by two operations, addition and multiplication of operators, which lie at the root of all fundamental aspects of Quantum Theory [2].

Physical content of Quantum Theory comes from beyond the abstract mathematical formalism. It is provided by the correspondence rules assigning operators with physical quantities. This is always an ad hoc procedure involving concrete representations of the operator algebra chosen to best reflect physical concepts related with the phenomena under investigation. Physics of the last century developed several such schemes e.g. in terms of matrices (Heisenberg), differential equations (Schrödinger), path integrals (Feynman), phase space (Wigner), etc. Various realizations of the operator algebra invoke different physical ideas, and hence are capable of describing diverse physical situations - the key factor in successful application of abstract mathematical notions in description of the physical world.

Interest in combinatorial representations of mathematical entities stems from a wealth of concrete models they provide. Their convenience comes from simplicity, which being based on elementary notion of enumeration directly appeals to intuition often rendering invaluable interpretations illustrating abstract mathematical constructions. This makes combinatorial perspective particularly attractive to quantum physics in its active pursuit of proper understanding and new viewpoints on fundamental phenomena.

In this Letter we are interested in combinatorial representation of the operator algebra of Quantum Theory which will be recast in the language of graphs. In some respects this draws on the Feynman idea to represent physical processes as diagrams used as a bookkeeping tool in the perturbation expansions in field theory [3]. Combinatorial approach, however, has much more to offer if applied to the overall structure of Quantum Theory seen from the algebraic point of view. We shall show that by lifting to more structured algebra of graphs abstract operator calculus gains straightforward interpretation as the shadow of natural operations on graphs. This not only provides interesting insights into the algebraic structure of a theory but also sheds light on the intrinsic nature and philosophy hidden behind the formalism of Quantum Theory.

Quantum Theory as Algebra of Operators. – General setting for Quantum Theory consists of specifying Hilbert space $\mathcal{H}$ of the system and identifying operators with physically relevant quantities. Operators acting in $\mathcal{H}$ naturally make an algebra with addition and multiplication which we denote by $\mathcal{O}$. Most interesting structures in $\mathcal{O}$ are, of course, those generated by operators having physical interpretation. They usually originate from considering some observable of interest along with operations causing changes in the state of a system.
Accordingly, one takes a hermitian operator, say $N$, representing some observable and sets the basis in $\mathcal{H}$ related to states with definite values of the corresponding physical quantity. Since we shall be interested in eigenvectors, and not the eigenvalues, we take for simplicity $N|n\rangle = n|n\rangle$ numbering the chosen eigenbasis $|n\rangle$ in $\mathcal{H}$ ($n = 0, 1, 2, \ldots$). One is then interested in describing processes changing state of the system e.g. time evolution, interactions or any other transformation. For that purpose it is convenient to introduce annihilation $a$ and creation $a^\dagger$ operators which shift the basis vectors by one, i.e. $[a, N] = a$ and $[a^\dagger, N] = -a^\dagger$. Conventionally, these operators are required to satisfy the canonical commutation relation

$$[a, a^\dagger] = 1,$$  \hfill (1)

being the hallmark of noncommutativity in Quantum Theory. Operators defined above play the role of elementary processes altering the system by changing its state with respect to the chosen physical characteristic, i.e. switching between the eigenvectors $|n\rangle$. In fact, any change of state can be seen as some combination of such creation and annihilation acts, making operators $a$ and $a^\dagger$ convenient building blocks describing transformations of a system.

Creation and annihilation operators can be used to represent elements of the algebra $\mathcal{O}$. Indeed, each operator can be seen as an element of a free algebra generated by $a$ and $a^\dagger$, i.e. written as linear combination of words in generators. This procedure is, however, ambiguous due to commutation relation eq. (1) which yields different representations of the same operator [4]. To solve this problem the order of $a$ and $a^\dagger$ has to be fixed. Conventionally it is done by choosing the normally ordered form in which all annihilators stand to the right of creators [5,6]. Consequently, each operator $A \in \mathcal{O}$ can be uniquely written in the normally ordered form as

$$A = \sum_{r,s} \alpha_{rs} a^\dagger r a^s.$$  \hfill (2)

In this way elements of the operator algebra $\mathcal{O}$ are represented in terms of ladder operators $a$ and $a^\dagger$, and interpreted as combinations of elementary acts of annihilation and creation. Eq. (2) will be the starting point of combinatorial representation of the algebra $\mathcal{O}$.

**Graphs and their Algebra.** – Interested in combinatorial realizations of operator algebras we shall specify two classes of graphs $\mathcal{g}$ and $\mathcal{g}_1$, the latter being the shadow of the former under suitable forgetful procedure. We shall employ the convenient notion of graph composition to show how these structures are naturally made into algebras providing the representation of the algebra $\mathcal{O}$.

**Graphs & Composition.** Graph is a collection of vertices connected by lines with internal structure determined by some construction rules. For the purpose at hand we consider specific class of graphs defined in the following way.

**Vertices & Lines.** Basic building blocks of graphs are vertices (black dots) with attached two sorts of lines, going into and out from the vertex, having loose ends marked with gray and white spots respectively. A generic one-vertex graph $\Gamma^{(r,s)}$ is characterized by two numbers $r$ and $s$ counting ingoing and outgoing lines respectively, see fig. 1a. By $\mathcal{g}$ we shall denote the class comprising of all one-vertex graphs and the void graph (no vertices, no lines). In further construction we shall assume that all lines attached to vertices are distinguishable.

![Fig. 1: a) Generic one-vertex graph $\Gamma^{(r,s)} \in \mathcal{g}_1$. b) Example of a multi-vertex graph (8 vertices and 2 connected components) built of two kinds of vertices $\Gamma^{(2,2)}$ (X shape) and $\Gamma^{(2,1)}$ (Y shape).](image)

**Construction Rules.** Multi-vertex graph $\Gamma$ is a set of vertices with additional structure introduced by joining some of the outgoing lines with the ingoing ones. Requirement that the original direction of lines is preserved results in a directed structure of graphs with natural paths between vertices. We further restrict the class of considered graphs to those without cycles, i.e. exclude graphs with closed paths. Example of a multi-vertex graph is shown in fig. 1b.

Rules specified above define the class of graphs denoted further by $\mathcal{g}$. In a less formal manner we can describe these graphs as having inner structure determined by directed connections between vertices and a characteristic set of outer lines marked with gray and white spots at the ends. Overall picture of a graph makes impression of a kind of process with vertices being intermediate steps transforming gray spots into white ones. This observation can be developed further with help of the convenient notion graph composition.

\footnote{We do not specify limits of summation and constraints on coefficients since it does not affect the algebraic considerations and can be introduced at each step if needed.}
Composition. Two graphs can be composed by joining some of the ingoing lines (gray spots) of the first one with some of the outgoing lines (white spots) of the second one. This operation is inner in $g$ since it preserves direction of the lines and does not introduce cycles. Observe that two graphs can be composed in many ways, i.e. as many as there are possible choices of pairs of lines (gray spots from the first one and white spots from the second one) which are are joined, see fig. 2. Note also that composing graphs in the reverse order yields different results.

Notion of graph composition allows for their iterative definition, i.e. any element of $g$ can be constructed starting from the void graph by successive composition with one-vertex graphs. Consequently, the class of one-vertex graphs $g_1 \subset g$ can be seen as basic processes or events happening one after another and making up a composite process - a multi-vertex graph.

Equivalence of Graphs. In many cases one is not interested in the inner structure of a graph and focuses only on the outer lines. This is equivalent to considering its one-vertex equivalents obtained by replacing all inner vertices and lines by a single vertex and keeping all the outer lines (white and gray spots) untouched, i.e. $g \xrightarrow{\sim} g^{(r,s)}$ where $G$ is the graph with $r$ white and $s$ gray spots. For example in fig. 1b it consists in $G \xrightarrow{\sim} G^{(9,6)}$. The mapping $g \xrightarrow{\sim} g_1$ comes down to forgetting about the inner structure of graphs and introduces the equivalence relation in $g$. Accordingly, two graphs are equivalent $G_1 \sim G_2$ if and only if both have the same number of ingoing and outgoing lines respectively. The simplest choice of representatives of equivalence classes are the one-vertex graphs and so the quotient set $g/\sim$ is isomorphic to the set of one-vertex graphs $g_1$.

There are two characteristic mappings between $g$ and $g_1$: the canonical projection map described above and the inclusion map $g_1 \subset g$, i.e.

$$g \xrightarrow{\sim} g_1$$

In this sense $g_1$ is a shadow of the more structured class $g$. Observe that the arrows in diag. (3) can not be reversed, i.e. once the inner structure of a graph is forgotten it can not be restored.

Algebra of Graphs. Both classes of graphs $g$ and $g_1$ can be endowed with the structure of noncommutative algebra based on the natural concept of graph composition. Algebra requires two operations, addition and multiplication, which are constructed as follows. We define $G$ as the vector space (over $\mathbb{C}$) generated by the basis set $g$, i.e.

$$G = \{ \sum \alpha_i G_i : \alpha_i \in \mathbb{C}, G_i \in g \}.$$

Addition in $G$ has the usual form

$$\sum_i \alpha_i G_i + \sum_i \beta_i G_i = \sum_i (\alpha_i + \beta_i) G_i.$$

Nontrivial part in the definition of algebra $G$ concerns multiplication, which by bilinearity

$$\sum_i \alpha_i G_i \cdot \sum_j \beta_j G_j = \sum_{i,j} \alpha_i \beta_j G_i \cdot G_j,$$

comes down to determining it on the basis set $g$. Recalling the notion of graph composition the definition suggests itself as (compare with fig. 2)

$$G_i \cdot G_j = \sum \text{all compositions of } G_i \text{ with } G_j.$$

Note that all terms in the sum are distinct with coefficients equal to one. Such defined multiplication is noncommutative and makes $G$ into genuine associative algebra with unit (void graph).

Imposing algebraic structure on $g_1$ follows the above scheme only to a certain point. Accordingly, one defines the vector space

$$G_1 = \{ \sum_{i,j} \alpha_{i,j} G^{(i,j)} : \alpha_{i,j} \in \mathbb{C}, G^{(i,j)} \in g_1 \}.$$
with addition defined analogously to eq. (5). Multiplication again comes down to defining it on the basis set \( \mathfrak{g}_1 \), but an obstacle here is that composition pulls out from the class \( \mathfrak{g}_1 \), i.e., produces two-vertex graphs which belong to \( \mathfrak{g} \). This however can be overcome applying the forgetful mapping \( \Gamma \to \Gamma^{(r,s)} \) to the result. Specifically, multiplication of two graphs in \( \mathfrak{g}_1 \) follows the diag. (3) and consists in:

1) treating them as elements of \( \mathfrak{g} \),
2) multiplying according to eq. (7),
3) forgetting the inner structure of the resulting two-vertex graphs in the sum.

Note that, contrary to eq. (7), some of the resulting terms are equal and sum up to nontrivial integer coefficients. Grouping terms with respect to the number of joined lines yields the explicit formula

\[
\Gamma^{(r,s)} \cdot \Gamma^{(k,l)} = \sum_{i=0}^{\min\{k,s\}} \frac{i!}{i! (s-i)! (k-i)!} \Gamma^{(r+k-i,i,s+l-i)}. \tag{9}
\]

For example: \( \Gamma^{(2,1)} \cdot \Gamma^{(2,2)} = \Gamma^{(4,3)} + 2 \Gamma^{(3,2)} \) and \( \Gamma^{(2,1)} = \Gamma^{(4,3)} + 4 \Gamma^{(3,2)} + 2 \Gamma^{(2,1)} \), see fig. 2. In this way, multiplication in the richer structure \( \mathcal{G} \) is naturally projected onto \( \mathfrak{g}_1 \). Such obtained combinatorial algebra \( \mathfrak{g}_1 \) is associative and still noncommutative. Again, similarly as \( \mathfrak{g} \) and \( \mathfrak{g}_1 \) in diag. (3), both algebras are related by

\[
\mathcal{G} \overset{\sim}{\longrightarrow} \mathfrak{g}_1 \tag{10}
\]

Hence, the algebra \( \mathfrak{g}_1 \) is the shadow of the more structured algebra of graphs \( \mathcal{G} \).

**Graph representation of operator algebra.** – Structures described above are genuine examples of algebras having concrete representations based on the natural concept of graph composition. It appears that both are intimately related to the algebra of operators \( \mathcal{O} \). As suggested by similarity of elements in \( \mathcal{O} \) and \( \mathfrak{g}_1 \), see eqs. (2) and (8), we make correspondence of the basis sets

\[
a^{\dagger} r a^s \longleftrightarrow \Gamma^{(r,s)} \tag{11}
\]

establishing the isomorphism of both vector spaces. It would not be so surprising if not the fact that this mapping also preserves multiplication in both algebras. Indeed, multiplication of basis elements in \( \mathcal{O} \) gives

\[
a^{\dagger} r a^s a^{\dagger} k a^l = \sum_{i=0}^{\min\{k,s\}} \frac{i!}{i! (s-i)! (k-i)!} a^{\dagger} r+k-i a^s+l-i, \tag{12}
\]

which is the result of commuting \( a^s a^{\dagger} k \) to the normally ordered form using the commutator \([a^s, a^{\dagger} k] = \sum_{i=1}^{\min\{k,s\}} \frac{i!}{i! (s-i)! (k-i)!} a^{\dagger} k-i a^s-i \). It is enough to compare eqs. (9) and (12) to show that eq. (11) establishes isomorphism between algebras \( \mathcal{O} \) and \( \mathfrak{g}_1 \). In other words both algebras are essentially the same, i.e. have all elements and operations equivalent. We can thus enjoy the advantages of concrete realization of the abstract operator algebra in terms of graphs. For example instead of multiplying operators in \( \mathcal{O} \) one can do it in \( \mathfrak{g}_1 \) just by composing graphs. The crucial role in this procedure is played by the more structured algebra of graphs \( \mathcal{G} \) where all these operations have simple interpretation. Accordingly, diag. (10) can be complemented to

\[
\mathcal{G} \overset{\sim}{\longrightarrow} \mathfrak{g}_1 \overset{1:1}{\longrightarrow} \mathcal{O} \tag{13}
\]

In this way, algebra \( \mathcal{O} \) gains combinatorial representation via \( \mathfrak{g}_1 \) and can be seen as reflecting natural processes taking place in \( \mathcal{G} \).

**Discussion.** – We have emphasized the fundamental role of algebraic structure of Quantum Theory and pointed out convenient representation of operators by normally ordered expressions in ladder operators \( a \) and \( a^{\dagger} \). This allowed for identification of the operator algebra \( \mathcal{O} \) with combinatorial algebra \( \mathfrak{g}_1 \) constructed as the projection of the genuine algebra of graphs \( \mathcal{G} \). The main result of the Letter shows that these combinatorial structures provide simple interpretation of the operator calculus in terms of natural composition of graphs. Accordingly, operator algebra can be seen as the shadow (via \( \mathfrak{g}_1 \)) of the algebra \( \mathcal{G} \) which is the categorified version of the algebra \( \mathcal{O} \) \([7,8]\). In a suggestive way it can be shown by redrawing diag. (13) as

\begin{center}
\begin{tikzpicture}
    \node (G) {\( \mathcal{G} \)};
    \node (G1) [below of=G] {\( \mathfrak{g}_1 \)};
    \node (O) [below of=G1] {\( \mathcal{O} \)};
    \draw[->] (G) -- (G1);
    \draw[->] (G1) -- (O);
\end{tikzpicture}
\end{center}

The diagram indicates existence of the fundamental graph structure \( \mathcal{G} \) of which the realm of Quantum Theory is just the reflection. That is all objects the theory as well as its calculus can be seen via simple inclusion as elements and operations living their life in the richer algebra of graphs described by natural composition rules. Return to the coarser level of algebra of operators is possible at all times just by forgetting about the inner structure of graphs. As a result, the algebra of graphs suggests itself as a deeper layer of Quantum Theory. The described lifting of the theory to the richer structure \( \mathcal{G} \) is motivated by natural interpretation of graphs as processes transforming quantities or objects, which is an attractive concept from the physical point of view. Moreover, the major advantage of the combinatorial representation of the algebra \( \mathcal{O} \) presented above is that the abstract operator calculus can be seen intuitively as straightforward composition of graphs.

Following these lines one can lay the foundation for the combinatorial interpretation and investigate the ensuing perspective on Quantum Theory.
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