Amplitudes for multiphoton quantum processes in linear optics

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Abstract

The prominent role that linear optical networks have acquired in the engineering of photon states calls for physically intuitive and automatic methods to compute the probability amplitudes for the multiphoton quantum processes occurring in linear optics. A version of Wick's theorem for the expectation value, on any vector state, of products of linear operators, in general, is proved. We use it to extract the combinatorics of any multiphoton quantum processes in linear optics. The result is presented as a concise rule to write down directly explicite formulae for the probability amplitude of any multiphoton process in linear optics. The rule achieves a considerable simplification and provides an intuitive physical insight about quantum multiphoton processes. The methodology is applied to the generation of high-photon-number entangled states by interferometrically mixing coherent light with spontaneously down-converted light.

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I. INTRODUCTION

Linear optics is playing a fundamental role in the development of an engineering of photon states for the operation of quantum communication and computing protocols. A linear optics gate that maps all four Bell states into, distinguishable, separable states in a quantum teleportation and entanglement scheme was reported in [1]. Efficient linear optical schemes for quantum computing based in the scalable implementation of photonics qubit operations using unitary optical arrays and post-selection at the output modes have been advanced in [2, 3]. Recently, generation of high-N maximally entangled NOON states by interference of multiphoton and coherent states [4, 5] has been achieved [6] by means of basic linear optical components.

Although the quantum mechanical fundamentals of linear optics are well established [7–9], the prominent role that linear optical networks have acquired in the engineering of quantum systems calls for physically intuitive and really automatic methods to compute the probability amplitudes for the multiphoton processes occurring in linear multiports.

Thus, we focus here our interest on methodological aspects, mainly. We adopt the formal description of a linear optical network by the scattering operator S whose matrix elements are the probability amplitudes for the transitions from occupation indices $(n_1, \ldots, n_K)$ at K inport modes into occupation indices $(N_1, \ldots, N_K)$ at K other outport modes. Such a multiphoton process is denoted $(n_1, \ldots, n_K) \to (N_1, \ldots, N_K)$.

The main point in determining the S matrix element corresponding to a multiphoton process is the calculation of the vacuum expectation value of products of operators which are linear combinations of photon creation and annihilation operators. In any given case, calculations may be carried out without any fundamental difficulty. The standard way to extract the combinatorics in Wick's original method [13] is to reorder the products of creation and destruction operators, using the appropriate commutation relations, into a normal ordering. Nevertheless, in such a straight approach [11, 12] the calculation may become tedious and cumbersome as the number of photons gets moderately large. For a comparisson of several calculational tools to find explicitly normally ordered forms of boson operator functions see [14].

In this article we present a new approach to Wick's theorem that is less involved, technically. A product of n linear operators, $A_1 A_2 \cdots A_n$, is considered and the combinatorics of

Wick contractions stems from Leibniz rule for commutators. In our setup the combinatorial process is very compact and is, thus, much easier to be followed. Furthermore, our version of Wick's theorem is applicable to the expectation value of products of linear operators, in general, and for any vector state. The scope for applicability of our method is not limited to vacuum expectation values of products of creation and anhilation operators.

By a thorough application of our method for Wick's theorem, we derive a concise rule to extract methodically the combinatorics that is involved in the calculation of the interfering alternatives contributing to the probability amplitude for any multiphoton process $(n_1, \ldots, n_K) \to (N_1, \ldots, N_K)$ in a linear network. The result is presented in the form of a procedural rule to write down explicite formulae for the probability amplitude of any multiphoton process.

The rule has a direct and physically intuitive interpretation which is of a mnemonic value. Interfering alternatives contributing to the amplitude for the multiphoton process $(n_1, \ldots, n_K) \to (N_1, \ldots, N_K)$ are in a one-to-one correspondance with the ways of distributing over the outport modes the photons that are available at the inport modes, preserving their number. Even more appealing would be to say that the interfering alternatives represent all possible paths the incoming photons may follow through the network up to the outport modes. We provide a simple device to handle the combinatorics of alternatives, consisting of some "squares of occupation numbers".

Generation of entangled multiphoton states is analyzed with our methodology. Simple linear optical networks have proved useful [6] in the generation of N-photon states that have a de Broglie (interferometric) wave length that shrinks as a function of the number of photons, N, as $1/N$. This feature is desirable, e.g., in applications requiring high precision phase-resolution. Maximally entangled states known as NOON states have this property. A method to generate NOON states with arbitrarily high photon numbers was proposed in [4]. The principle underpinning the method [4–6] is the unitary mixing of a classical coherent state with quantum down-converted light, by means of a standard beamsplitter.

Our methodology not only makes calculations straightforward. It also puts two points of physical interest on the table. First one is a transparent access to the parameters used to blend the mixture as to attain the largest overlap of the superposition of "Schrödinger cat"-like multiphoton states with a target N-photon NOON state. The other point is to demonstrate the N-fold enhanced phase sensitivity achieved by the emerging state.

The paper is organized as to avoid technical details of the proofs obscure the simple intuitive meaning of the methodology. The following Section II introduces the rule for multiphoton amplitudes by placing the emphasis on its physical interpretation. Then the methodology is applied in Section III to analyze the generation of entangled multiphoton states. The formal proofs are supplied in the last two sections. The proof of Wick's theorem in Section IV and the proof of the procedural rule in Section V.

II. THE RULE FOR MULTIPHOTON AMPLITUDES

We consider, with an interest in methodology, a generic linear optical network presenting a set of K inports, supporting each a single mode. For a succinct review of the quantum mechanical description of linear optical networks, concerned with photonic qubits, the reader may turn to reference [10]. Let us here just tell that annihilation operators for the input modes are denoted by a_i, $i = 1, \ldots, K$. Correspondingly, annihilation operators for the output modes are denoted by b_i, $i = 1, \ldots, K$.

The action of the linear optical network is to mix the input modes, unitarily, over the output modes. The mixing is described by the relation

$$b_i = \sum_{j=1}^{K} W_{ik} a_k, \quad i = 1, \ldots K \ . \tag{1}$$

The unitary matrix W, with entries W_{ij} employed in (1), describes the *one-photon* action of the optical network. The probability amplitude for one photon to go through the network from inport j to outport i is W_{ij}. Matrix W also determines the scattering operator $S(W)$ that transforms any multiphoton input state $|in\rangle$ into the output state $|out\rangle = S(W)\,|in\rangle$. To grasp the physical meaning of matrix W and operator $S(W)$ the reader may turn to reference [8] for examples. One more example we deal with in Section III.

In the multiphoton state $|in\rangle = |n_1, \ldots, n_K\rangle$ index $n_i \geq 0$ is the occupation integer for the single mode at the i-th inport. Similarly, the multiphoton state $|out\rangle = |N_1, \ldots, N_K\rangle$ —the one to catch up at the outports— has occupation integer N_i at the single mode of the i-th outport. The multiphoton process $(n_1, \ldots, n_K) \to (N_1, \ldots, N_K)$ has probability amplitude $\langle N_1, \ldots, N_K|\, S(W)\,|n_1, \ldots, n_K\rangle$ to take effect in the linear optical network W. A rule to compute the amplitude is given in this Section, but we postpone its proof until Sections IV and V.

$$
\begin{array}{c|cccc}
n_1 & \ell_{11} & \ell_{12} & \cdots & \ell_{1K} \\
n_2 & \ell_{21} & \ell_{22} & \cdots & \ell_{2K} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
n_K & \ell_{K1} & \ell_{K2} & \cdots & \ell_{KK} \\
\hline
 & N_1 & N_2 & \cdots & N_K
\end{array}
$$

$$
\sqrt{n_1! \cdots n_K!\; N_1! \cdots N_K!}\quad \frac{\prod_{i,j} W_{ij}^{\ell_{ji}}}{\prod_{i,j} \ell_{ij}!}
$$

FIG. 1. A square for the distribution of occupation numbers, satisfying the conditions $n_i = \sum_j \ell_{ij}$ and $N_j = \sum_i \ell_{ij}$. Below the square is its contribution to the amplitude $\langle N_1, \ldots, N_K|\, S(W)\, |n_1, \ldots, n_K\rangle$.

Wick's theorem applied to the amplitude $\langle N_1, \ldots, N_K|\, S(W)\, |n_1, \ldots, n_K\rangle$ in Section V discloses the interfering alternatives contributing to it. They are identified with all of the possible ways to distribute the occupation integers $(n_i)_{i=1}^K$ at the inports over the outports as to get $(N_i)_{i=1}^K$. Each alternative redistribution of occupation integers from the inports to the outports is conveniently represented by a $K \times K$ matrix (or square), having non-negative integer entries ℓ_{ij}.

A square of occupation numbers is displayed in figure 1. Inport integers $(n_i)_{i=1}^K$ are used as labels for the rows of the square while the outport integers $(N_i)_{i=1}^K$ label the columns. The i-th row of integer entries ℓ_{ij}, $j = 1, \ldots, K$, in the square, constitute a way of distributing over the outports the n_i photons that are available at the i-th inport. In the interest of mnemonics we may say that ℓ_{ij} from the n_i incoming photons "follow a path" in the network leading to outport j. The entries in a square of occupation numbers must thus satisfy the inequalities $0 \le \ell_{ij} \le n_i$ and $0 \le \ell_{ij} \le N_j$, as well as the equality $n_i = \sum_j \ell_{ij}$, along every row.

As seen at the outports, the integer entries ℓ_{ij} in the square, that are redistributing the incoming photons over the outports, must add up to the specified occupation number N_j at every outport j: $N_j = \sum_i \ell_{ij}$ along each of the columns $j = 1, \ldots, K$. Thus, every row and every column in a square of occupation integers sum up to the in- and out-occupation numbers as follows

$$n_i = \sum_j \ell_{ij} \quad \text{and} \quad N_i = \sum_j \ell_{ji} \quad \text{for every } i = 1, \ldots, K. \tag{2}$$

Together, these conditions imply the conservation of the total number of photons, $n_1 + \cdots + n_K = N_1 + \cdots + N_K$, as required by the unitary character of the optical network, W.

In summary, the combinatorial aspect in the problem of finding all the interfering alternatives contributing to the amplitude for the multiphoton process $(n_i)_{i=1}^K \to (N_i)_{i=1}^K$ is identified with the problem of finding all ways of distributing the incoming photons over the outport modes. Alternatives are combinatorially dealt with by writing down all possible squares of occupation numbers. The complex amplitude and combinatorial factor that each alternative contributes to the multiphoton process amplitude is computed in Section V. The answer is the formula given at the bottom of figure 1. The important point for the present is that the formula can be retrieved directly from the corresponding square of accupation numbers and the one-photon amplitudes, W_{ij}.

We have the following rule to compute the probability amplitude for any multiphoton process in a linear optical network. First, write down all the squares of occupation numbers, figure 1, for the labels given by the in- and out-occupation numbers, $(n_1, \cdots, n_K)$ and $(N_1, \ldots, N_K)$, verifying that every row and every column add up to the values in the corresponding labels, i.e., conditions (2). The combinatorial exercise once accomplished, then proceed to translate squares to formulae following the prescription in figure 1. The amplitude we produce

$$\langle N_1, \ldots, N_K |\, S(W) \,| n_1, \ldots, n_K \rangle \;=\; \sqrt{n_1! \cdots n_K!\; N_1! \cdots N_K!} \sum_{\text{squares}} \frac{1}{\prod_{i,j} \ell_{ij}!} \;\prod_{i,j} W_{ij}^{\ell_{ji}} \tag{3}$$

is the sum over all the interfering alternatives, represented by the squares.

III. LINEAR GENERATION OF HIGH-N ENTANGLED STATES

An important piece of quantum linear optics is the generatation of NOON states with arbitrarily high photon numbers [6] by the method that was advanced in [4, 5]. The key element is to prepare an interferometric mixture of a classical coherent state with quantum down-converted light. The first experimental realization was reported in [6]. A schematics of the setup is shown in figure 2. The beam splitter W has matrix entries $W_{11} = W_{12} =$

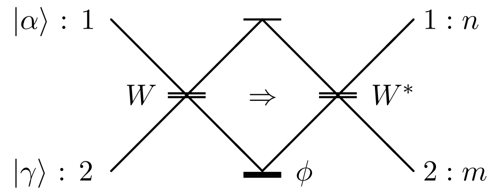

FIG. 2. Preparation of high-N NOON photon states and interferometer for the confirmation of the N-fold enhanced phase sensitivity.

$W_{22} = 2^{-1/2}$ and $W_{21} = -2^{-1/2}$ and the corresponding multiphoton scattering operator is denoted by $S(W)$.

We proceed to analyze the process by applying the method of previous Section II. What we want is state $|\text{NOON}\rangle := (\,|N,0\rangle + |0,N\rangle\,)/\sqrt{2}$ to emerge from beam splitter W in figure 2. Then, at its inports, labeled 1 and 2, we must supply the state

$$|\Phi : N\rangle := S(W)^* \,|\text{NOON}\rangle = \sum_k |k, N-k\rangle\, \langle k, N-k|\, S(W)^*\, |\text{NOON}\rangle \;, \tag{4}$$

where the hermitian conjugate operator $S(W)^* \equiv S(W^*)$ represents the time-reversed action of the first beam splitter on the NOON state. For state $|\text{NOON}\rangle$ the amplitudes involved in (4),

$$\langle k, N-k|\, S(W)^*\, |\text{NOON}\rangle = \frac{1}{\sqrt{2}}\big(\, \langle k, N-k|\, S(W)^*\, |0,N\rangle + \langle k, N-k|\, S(W)^*\, |N,0\rangle\,\big) \;,$$

are computed by a straightforward application of rule (3). For the in-out distribution of occupation numbers in the process $(0,N) \to (k, N-k)$ there is one square only,

$$\langle k, N-k|\, S(W)^*\, |0,N\rangle \quad = \quad \begin{array}{c|cc} 0 & 0 & 0 \\ N & k & N-k \\ \hline & k & N-k \end{array} \quad = \quad \sqrt{\frac{N!}{k!(N-k)!}}\, \Big(\frac{1}{\sqrt{2}}\Big)^{N-2k} \;,$$

and for $(N,0) \to (k, N-k)$ there is one too,

$$\langle k, N-k|\, S(W)^*\, |N,0\rangle \quad = \quad \begin{array}{c|cc} N & k & N-k \\ 0 & 0 & 0 \\ \hline & k & N-k \end{array} \quad = \quad \sqrt{\frac{N!}{k!(N-k)!}}\, (-1)^{N-k} \Big(\frac{1}{\sqrt{2}}\Big)^{N-2k} \;.$$

The squares of occupation numbers were translated to the formulae for amplitudes following the prescription in figure 1. We just had to provide the beam splitter matrix entries $W_{11} =$

$W_{12} = W_{22} = 2^{-1/2}$ and $W_{21} = -2^{-1/2}$. Thence, the reverse-scattered NOON state (4), the one required at the inports of W, is

$$|\Phi : N\rangle = \sum_{k=0}^{N/2} \sqrt{\frac{N!}{(2k)!(N-2k)!}} \left(\frac{1}{\sqrt{2}}\right)^{N-1} |N-2k\rangle_1 |2k\rangle_2 \ . \tag{5}$$

Just by construction, as the two modes of state (5) are mixed up by the first beam splitter W in the setup of figure 2, a pure N-photon NOON state emerges at the outports of W.

The key remark in reference [4] is that the product state $|\alpha\rangle_1 |\gamma\rangle_2$, of a coherent state $|\alpha\rangle$ and the squeezed vacuum state $|\gamma\rangle$, includes N-photon components that may be tuned-up to be quite similar to (5). The states $|\alpha\rangle_1$ and $|\gamma\rangle_2$ at the inports of the array in figure 2 are defined by the equations $(a_1 - \alpha)|\alpha\rangle = 0$ and $(a_2 + a_2^* \gamma)|\gamma\rangle = 0$, where α and γ are the complex amplitudes of the coherent light and of pair generation, respectively. The reader will get assistance in solving these equations in references [15] and [9], respectively. The N-photon component of the input product state $|\alpha\rangle_1 |\gamma\rangle_2$ is

$$|\eta : N\rangle = Z \sum_{k=0}^{N/2} \frac{1}{k!} \sqrt{\frac{N!(2k)!}{(N-2k)!}} \left(\frac{\eta}{2N}\right)^k |N-2k\rangle_1 |2k\rangle_2 \ , \tag{6}$$

where Z is a normalization constant and $\eta = N\gamma/\alpha^2$ is the natural tuning parameter introduced in [4].

Our aim on state (6) is to blend the mixing of coherent and down-converted lights that it involves, such that the state $|\eta : \text{NOON}\rangle := S(W)|\eta : N\rangle$, emerging from W, is as close to the maximally entangled "true" $|\text{NOON}\rangle$ state as possible [4]. The similarity of the target and trial N-photon states is sized up by the overlap $|\langle \eta : \text{NOON}|\text{NOON}\rangle|^2$ which we compute as $|\langle \eta : N|\Phi : N\rangle|^2$, by using the states in (5) and (6). The values of the tuning η that produce the largest values of the overlap are plotted in figure 3 for values of N up to $N = 20$. The corresponding values of the optimal overlap are plotted too in figure 3. They are very close to 100% fidelity [4].

In order to confirm, in an experimental situation, that the input state $|\alpha\rangle |\gamma\rangle$ makes emerge an almost-perfect N-photon NOON component (if the value of η is chosen as in figure 3), the state at the outports of W is made to interfere in a subsequent beam splitter W^*. The signature of the NOON state is a N-fold enhanced phase sensitivity in the interference fringes, related to a de Broglie wave length reduced by the factor $1/N$. The interferometer in figure 2 is intended to disclose it. In an ideal situation the n–m coincidence fringes are

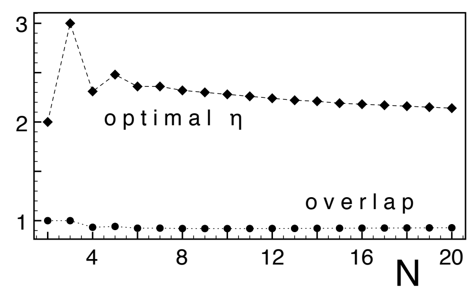

FIG. 3. Optimal overlap $|\langle\eta:\mathrm{NOON}|\mathrm{NOON}\rangle|^2$ and corresponding optimal value of η (square boxes) versus the total number of photons, N.

proportional to the probability

$$P(n;m|\eta:N) = |\langle n;m|\,S(M)\,|\eta:N\rangle|^2 \tag{7}$$

to detect n photons at outport 1 in coincidence with $m = N - n$ photons at outport 2. In (7), matrix M and the corresponding operator $S(M)$ describe the scattering produced by the Mach-Zehnder interferometer ($W \Rightarrow W^*$) in figure 2.

Before we can apply rule (3) to calculate the amplitude involved in (7) we must expand state $|\eta:N\rangle$ as in (6),

$$\langle n;N-n|\,S(M)\,|\eta:N\rangle = \sum_{k=0}^{N/2} C_k\,\langle n;N-n|\,S(M)\,|N-2k\,;2k\rangle \;\;, \tag{8}$$

where the coefficients introduced by the expansion (6) are denoted by C_k. The amplitudes in (8) are ready for rule (3). The combinatorial part of the job tells us that each amplitude is the following sum over squares

$$\langle n;N-n|\,S(M)\,|N-2k;2k\rangle = \sum_{\ell=\ell_{min}}^{\ell_{max}} \begin{array}{c|cc} N-2k & \ell & N-2k-\ell \\ 2k & n-\ell & 2k+\ell-n \\ \hline & n & N-n \end{array} \;, \tag{9}$$

with $\ell_{min} = \max\{0, n-2k\}$ and $\ell_{max} = \min\{n, N-2k\}$. The extreme values for ℓ are a consequence of the conditions that all the entries of the square in (9) are not negative and are not greater than the number of photons that are available at the inports.

The squares of occupation numbers in (9) are translated to formulae by just applying the prescription in figure 1. The W-amplitudes involved are the entries of the unitary matrix, $M = W^*\Phi W$, describing the mixing action of the Mach-Zehnder interferometer, the one

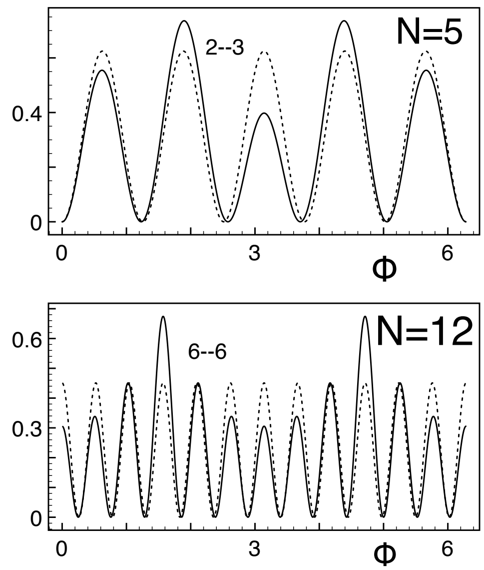

FIG. 4. Probability for n–m $(m = N - n)$ coincidence outcomes, as a function of the phase control ϕ, for the approximate NOON states produced by the mixture of a coherent state and a squeezed vacuum state. For comparison, the n–m fringes produced by true NOON states are shown in dotted lines.

shown in figure 2. The matrix entries are $M_{11} = M_{22} = \cos(\phi/2)$ and $M_{12} = M_{21} = -i\sin(\phi/2)$. Hence, a direct application of the rule in figure 1 yields

$$\begin{array}{r|cc} N-2k & \ell & N-2k-\ell \\ 2k & n-\ell & 2k+\ell-n \\ \hline & n & N-n \end{array} \quad = \quad \frac{\sqrt{(N-2k)!\ (2k)!\ n!\ (N-n)!}}{\ell!\ (n-\ell)!\ n!\ (N-n)!} \quad \times$$

$$\cos(\phi/2)^{2k+2\ell-n}\,(-i\sin(\phi/2))^{N+n-2k-2\ell}$$

for the squares in (9). The probability for n–m coincidences (7) may now be computed by using (8), (9) and the formulae for the squares of occupation numbers.

Results of the numerical calculation of the probability $P(n, m|\eta{:}N)$ in (7) are shown in Figure 4 for $N = 5$ and $N = 12$, demonstrating the N-fold enhanced sensitivity of the N-photon components of the state that is emerging from the interfering mixture of a coherent state with a squeezed vacuum [4–6]. For comparison, the n–m fringes produced by true NOON states are shown in Figure 4 as dotted lines.

IV. WICK'S THEOREM FOR EXPECTATION VALUES

Wick's original method [13] is based in a technique to handle the process of normal ordering the products of creation and destruction operators first, and proceeds thereafter to evaluate the expectation value in the vacuum state.

Here we consider instead products of n linear operators, $A_1^n := A_1 A_2 \cdots A_n$, in general. Combinatorics of Wick contractions stems from Leibniz rule for commutators. As a result, the combinatorics is much easier to be followed than in the original normal-ordering procedure. Furthermore, our version of Wick's theorem is not restricted to expectation values for the vacuum state. The technique is applicable to calculate expectation values in any vector state $|x\rangle$, not necessarily the vacuum state.

The departing step is to define the positive A^+ and negative A^- components of A, relative to state vector $|x\rangle$, by

$$A^+ := (1 - \mathbb{1}_x) A \mathbb{1}_x \quad \text{and} \quad A^- := (A - \langle A \rangle)(1 - \mathbb{1}_x) \; ,$$

where $\langle A \rangle := \langle x| A |x\rangle$ is the expectation value of operator A for the vector state $|x\rangle$ and $\mathbb{1}_x = |x\rangle \langle x|$ is the orthogonal projection along vector $|x\rangle$. Notice that by definition, we have the nice properties $\langle x| A^+ = 0$ and $A^- |x\rangle = 0$, implying that $\langle A^+ \rangle = \langle A^- \rangle = 0$. These properties are well known for creation and annihilation operators acting on the vacuum state. The definitions of A^+ and A^- are quite useful because any operator A admits the following decomposition.

Lemma IV.1 *$A = \langle A \rangle + A^- + A^+$.*

Proof. Let us start from the obvious identity

$$A = \mathbb{1}_x A \mathbb{1}_x + A(1 - \mathbb{1}_x) + (1 - \mathbb{1}_x) A \mathbb{1}_x = \mathbb{1}_x A \mathbb{1}_x + A(1 - \mathbb{1}_x) + A^+ \; , \tag{10}$$

where we have used the definition of the positive component A^+ of A. Next, consider the operator $A^0 := \mathbb{1}_x A \mathbb{1}_x + \langle A \rangle (1 - \mathbb{1}_x)$ and any two vectors $|y\rangle$ and $|y'\rangle$ taken from an orthonormal basis containing $|x\rangle$. Then, it is not difficult to prove that $\langle x| A^0 |y\rangle = \langle y| A^0 |x\rangle = \langle y| A^0 |y'\rangle = 0$ and that $\langle y| A^0 |y\rangle = \langle x| A^0 |x\rangle = \langle A \rangle$. We have thus proved that

$$\mathbb{1}_x A \mathbb{1}_x + \langle A \rangle (1 - \mathbb{1}_x) \equiv \langle A \rangle \mathbb{1}.$$

Using this result in (10) we have that $A = \langle A\rangle + (A - \langle A\rangle)(1 - \mathbb{1}_x) + A^+ = \langle A\rangle + A^- + A^+$.
$\square$

From now on we assume all operators are "displaced" operators, $A \leftarrow A - \langle A\rangle$, such that $\langle A\rangle = 0$. Lemma IV.1 tells us that every displaced operator is the sum of a positive and a negative component, $A = A^+ + A^-$.

We are ready to expose the combinatorics implied in the expectation value $\langle A_1 A_2 \cdots A_n\rangle$, on the basis of a recursive method that expands it in terms of the simplest non-trivial expectation values $\langle A_j A_k\rangle$, of pairs of operators. The implication of Lemma IV.1 is that such basic building blocks are provided by commutation rules as follows.

Lemma IV.2 $\langle AB\rangle = \langle [A^-, B^+]\rangle$

Proof. For any two displaced operators, A and B, we have that $A = A^+ + A^-$ and that $B = B^+ + B^-$. By definition, we have that $\langle x|\, A^+ = 0$ and that $B^- \,|x\rangle = 0$. Then, it follows that $\langle A^+ B^-\rangle = \langle A^- B^-\rangle = \langle A^+ B^+\rangle = 0$, such that $\langle AB\rangle = \langle [A^-, B^+]\rangle$. $\square$

The relevance of Lemma IV.2 relies on the fact that, in many important cases, the operator $[A^-, B^+]$ is proportional to the identity operator, $\mathbb{1}$. For such cases, let $[A^-, B^+] = \Delta\mathbb{1}$, where $\Delta \equiv \overbracket{AB}$ is a given complex number, referred to as a *Wick contraction.* The expectation value of the product operator AB is then given by $\langle AB\rangle = \overbracket{AB}$. Recall that the positive and negative components of operators are relative to vector $|x\rangle$ such that $\overbracket{AB}$ is a function of $|x\rangle$. Most of the optical measurements involve the vacuum ($|x\rangle = |0\rangle$) expectation values of products of creation and annihilation operators. For a discrete set of optical modes all we need to know is that $\overbracket{a_i a_j^*} = \delta_{ij}$. For spatial modes with a finite spectral width $\overbracket{a_i(\nu) a_j^*}(\omega) = \delta_{ij}\delta(\omega - \nu)$ are the needed contractions.

Lemma IV.2 is the root of an inductive procedure that returns the expectation value of a product of operators $A_1 A_2 ... A_{n-1} A_n$, of arbitrary length $n > 1$, in terms of elementary contractions $\overbracket{A_j A_k}$. The assumptions are that the A_i operators have been displaced already, $A_i \leftarrow A_i - \langle A_i\rangle$, and that every commutator $[A_i^-, A_j^+] = \Delta_{i,j} \equiv \overbracket{A_i A_j}$ is just a complex number.

In order to work the inductive step out, it is convenient to adopt the notational convention for products: $A_k^\ell = A_k A_{k+1} \cdots A_\ell$ whenever $k \le \ell$, while $A_k^\ell = \mathbb{1}$, otherwise. Then, Wick's theorem follows right after the next two lemmas. First one is Leibniz rule for commutators.

Lemma IV.3 $[A_1^n, B] = \sum_{k=1}^n A_1^{k-1}\ [A_k, B]\ \ A_{k+1}^n$.

Proof. We know that $[A_1^{n-1}A_n, B] = [A_1^{n-1}, B]A_n + A_1^{n-1}[A_n, B]$. Then, assuming the result holds for $[A_1^{n-1}, B]$ we have that $[A_1^n, B] = \sum_{k=1}^{n-1} A_1^{k-1}[A_k, B]A_{k+1}^{n-1}A_n + A_1^{n-1}[A_n, B] = \sum_{k=1}^{n} A_1^{k-1}[A_k, B]A_{k+1}^{n}$. □

Next, we apply Leibniz rule to the expectation value of the product of n operators to express it as the sum of $n-1$ expectation values of the same products with all possible contractions of the right-most operator A_n with all of the others.

Lemma IV.4 $\langle A_1A_2\cdots A_n\rangle = \sum_{k=1}^{n-1}\langle A_1^{k-1}A_kA_{k+1}^{n-1}A_n\rangle = \sum_{k=1}^{n-1}\langle A_1^{k-1}A_{k+1}^{n-1}\rangle\Delta_{k,n}$.

Proof. The point is to notice that $\langle A_1^n\rangle = \langle A_1^{n-1}A_n\rangle = \langle[A_1^{n-1}, A_n^+]\rangle$. Then, by Lemma IV.3 we have that $[A_1^{n-1}, A_n^+] = \sum_{k=1}^{n-1} A_1^{k-1}[A_k, A_n^+]A_{k+1}^{n-1} \equiv \sum_{k=1}^{n-1} A_1^{k-1}A_kA_{k+1}^{n-1}A_n$. The result follows since we are considering operators such that every commutator $[A_i, A_j^+] = [A_i^-, A_j^+]$ is the c-number A_iA_j. □

Recall that we are assuming that every operator has a null expectation value, $\langle A_k\rangle = 0$. Thus, we have the following direct consequence of Lemma IV.4.

Corollary IV.1 $\langle A_1A_2\cdots A_{2n+1}\rangle = 0$.

Theorem IV.1 (Wick) *Let A_i, $i = 1, \ldots, 2n$, be linear operators such that for every i and every j, we have that $\langle A_i\rangle = 0$ and that the commutator $[A_i^-, A_j^+] \equiv \Delta_{ij}$ is a c-number. Then,*

$$\langle A_1A_2\cdots A_{2n}\rangle = \sum_{\text{pairings}} \Delta_{i_1,j_1}\Delta_{i_2,j_2}\cdots\Delta_{i_n,j_n}\ ,$$

where the sum is over all pairings by contractions $\cdots A_{i_k}\cdots A_{j_k}\cdots \equiv \cdots\Delta_{i_k,j_k}\cdots$, each contraction subjected to the condition that $i_k < j_k$.

Proof. By Lemma IV.4 we have that $\langle A_1A_2\cdots A_{2n}\rangle = \sum_{k=1}^{2n-1}\langle A_1^{k-1}A_{k+1}^{2n-1}\rangle A_kA_{2n}$. The induction hypothesis implies then that

$$\langle A_1A_2\cdots A_{2n}\rangle = \sum_{k=1}^{2n-1}\Big(\sum_{\text{pairings'}}\Delta_{i_1,j_1}\Delta_{i_2,j_2}\cdots\Delta_{i_{n-1},j_{n-1}}\Big)\,\Delta_{k,2n}\ , \tag{11}$$

where the first (innermost) sum is over pairings' of the product $A_1,\ldots,A_{k-1}A_{k+1}\cdots A_{2n-1}$ $\big(A_k$ and A_{2n} being excluded, as indicated by the apostrophe$\big)$. The last factor $\Delta_{k,2n}$ in (11) represents a contraction of the last factor A_{2n} with each one of the other $2n-1$ operators on its left-hand side (i.e., the second sum on k). For each contraction A_kA_{2n}, all pairings of the remaining $2n-2$ operators are inserted in (11) by the innermost sum (between the big parentheses). $\square$

Let $P(2n)$ denote the number of pairings of the product $A_1A_2\cdots A_{2n}$. As we noticed in the proof of Theorem IV.1 already, the last factor in the product, A_{2n}, is contracted with everyone of the $2n-1$ other operators on its left side. Each such contraction factorizes as a complex number and we are left, for each contraction, with all of the $P(2n-2)$ pairings of the remaining product of $2n-2$ operators. Thus, for the number of pairings on a product of $2n$ operators we have the recursion $P(2n) = (2n-1)P(2n-2)$, with initial value $P(2) = 1$. The solution for the number of pairings for the product operator in Theorem IV.1 is then $P(2n) = (2n-1)!!$, although some of them might of course be zero.

Optical measurements deal with the vacuum expectation value of products of operators of the form $a^{n_1}a^{*m_1}a^{n_2}a^{*m_2}\cdots a^{n_L}a^{*m_L}$, with positive exponents n_i and m_i, and Wick contractions $\overbrace{aa^*} = 1$, $\overbrace{a^*a} = -1$, $\overbrace{aa} = 0$ and $\overbrace{a^*a^*} = 0$. Theorem IV.1 implies that such an expectation value does not vanish if, and only if, $S_k := \sum_{i=0}^{k}(m_{L-i} - n_{L-i}) \geq 0$ for each $k = 0, \ldots L-2$ while for $k = L-1$ the sum should vanish, $S_{L-1} = \sum_i^L (m_i - n_i) = 0$. By a direct counting of Wick pairings we find that

$$\langle a^{n_1}a^{*m_1}a^{n_2}a^{*m_2}\cdots a^{n_L}a^{*m_L}\rangle = \frac{m_L!}{S_0!}\cdot\frac{(S_0+m_{L-1})!}{S_1!}\cdot\frac{(S_1+m_{L-2})!}{S_2!}\ \cdots\ \frac{n_1!}{0!}\,, \tag{12}$$

result that includes the special case $\langle a^n a^{*n}\rangle = n!$.

V. PROOF OF THE RULE

The generic optical setup for the amplitude $\langle N_1,\ldots,N_K|\,S(W)\,|n_1,\ldots,n_K\rangle$ was described already in Section II. Here, we just provide the proof of the rule for amplitudes. The in and out states involved in an ampmlitud are constructed by applying (a and b) photon creation operators on the vacuum state. The annihilation b-operators are linear superpositions of a-operators as specified by the unitary transformation (1). Thence, the amplitude takes the form

$$\langle N_1,\ldots,N_K|\,S(W)\,|n_1,\ldots,n_K\rangle = \frac{1}{\sqrt{n_1!\cdots n_K!\;N_1!\cdots N_K!}} \times \langle 0|\,\Big(\sum_{i=1}^{K} W_{K,i}a_i\Big)^{N_K}\cdots\Big(\sum_{i=1}^{K} W_{1,i}a_i\Big)^{N_1} a_1^{*n_1}\cdots a_K^{*n_K}\,|0\rangle\,. \tag{13}$$

The alternatives implied by each of the vacuum expectation values in (13), including their combinatorial weights, are extracted by a direct application of Wick's theorem IV.1. We follow the conventions established in the proof we gave in Section IV. To proceed with the expansion of (13) we need the Wick contractions $\overbracket{a_i a_j^*} = \delta_{i,j}$, $i, j = 1, \ldots K$.

The involved part in the calculation of the vacuum expectation values stems from the product of polynomials in W_{ij} of degree N_j, which action (1) introduced in the amplitude (13). To help the reader cope with the calculations in the proof for arbitrary values of K, we present the proof for $K = 2$ inports first.

A. Arrays with two inports

For $K = 2$, the amplitude (13) includes two binomials only, of degrees N_1 and N_2. Given that $[a_1, a_2] = 0$, we are allowed to use the commutative binomial expansion in (13),

$$\begin{aligned} \langle N_1, N_2 |\, S(W)\, | n_1, n_2 \rangle \; = \; & \frac{1}{\sqrt{n_1! n_2! N_1! N_2!}} \sum_{k=0}^{N_1} \sum_{l=0}^{N_2} \binom{N_1}{k} \binom{N_2}{l} W_{11}^{k} W_{12}^{k'} W_{21}^{l} W_{22}^{l'} \quad \times \\ & \langle 0 |\, a_1^{k+l} a_2^{k'+l'} a_1^{*n_1} a_2^{*n_2} \,| 0 \rangle \;\; , \end{aligned} \tag{14}$$

with polynomial degrees $N_1 = k + k'$ and $N_2 = l + l'$. To apply Wick's theorem to the expectation value in (14), notice first that the only non-vanishing Wick contractions are $\overbracket{a_1 a_1^*} = \overbracket{a_2 a_2^*} = 1$. Consequently, the expectation value in (14) vanishes unless $n_1 = k + l$ and $n_2 = k' + l'$. For these values of occupation numbers, since non-null contractions are just 1, we have that

$$\langle 0 |\, a_1^{n_1} a_2^{n_2} a_1^{*n_1} a_2^{*n_2} \,| 0 \rangle \; = \sum_{a_1\text{-pairings}} \; \sum_{a_2\text{-pairings}} 1 \; = \; n_1!\, n_2! \; .$$

For the details, see Section IV, p.14. Thus,

$$\langle 0 |\, a_1^{k+l} a_1^{*n_1} a_2^{k'+l'} a_2^{*n_2} \,| 0 \rangle \; = n_1!\, n_2!\; \delta_{n_1, k+l}\; \delta_{n_1+n_2, N_1+N_2} \; . \tag{15}$$

There is an overall Kronecker δ that accounts for the conservation $n_1 + n_2 = N_1 + N_2$. Substituting this result in the amplitude (14), the other δ reduces the two sums in (14) to one, e.g., on k. Then, using the equality

$$\frac{n_1!\; n_2!}{\sqrt{n_1!\; n_2!\; N_1!\; N_2!}} \binom{N_1}{k} \binom{N_2}{n-k} \quad = \quad \frac{\sqrt{n_1!\; n_2!\; N_1!\; N_2!}}{k!\; k'!\; l!\; l'!}$$

the recipe in (3), for the simplest case $\langle N_1, N_2|\, S(W)\, |n_1, n_2\rangle$, follows.

Representing each alternative as the following square of occupation numbers

$$\begin{array}{c|cc} n_1 & k & l \\ n_2 & k' & l' \\ \hline & N_1 & N_2 \end{array} \quad = \quad \frac{\sqrt{n_1!\; n_2!\; N_1!\; N_2!}}{k!\; l!\; k'!\; l'!}\, W_{11}^{k}\, W_{12}^{k'}\, W_{21}^{l}\, W_{22}^{l'}$$

a probability amplitude is assigned to every distribution of the (n_1, n_2) photons —available at the inports— that makes them appear as (N_1, N_2) photons at the two outports. The overall conservation $n_1 + n_2 = N_1 + N_2$ is implicit and the complete amplitude (14) is the sum over all squares distributing the occupation numbers $(n_1, n_2) \to (N_1, N_2)$.

B. Arrays presenting multiple inports

For an arbitrary number K of inports the amplitude (13) has a product of K multinomials in W_{ij} of degrees N_j. The commutative multinomial expansion of each factor in the product is

$$\Big(\sum_{i=1}^{K} W_{j,i} a_i\Big)^{N_j} = \sum_{\ell_{1j},\ell_{2j},\ldots,\ell_{Kj}} \binom{N_j}{\ell_{1j}, \ell_{2j}, \ldots, \ell_{Kj}} {W_{j,1}}^{\ell_{1j}} {W_{j,2}}^{\ell_{2j}} \cdots {W_{j,K}}^{\ell_{Kj}} \quad \times$$
$${a_1}^{\ell_{1j}} {a_2}^{\ell_{2j}} \cdots {a_K}^{\ell_{Kj}} \;, \qquad (16)$$

with $j = 1, \ldots, K$. The sum in the expansion (16) runs over sets of non-negative integers $\{\ell_{1j}, \ldots, \ell_{Kj}\}$ such that

$$\ell_{1j} + \ell_{2j} + \cdots + \ell_{Kj} = \sum_k \ell_{kj} = N_j \qquad (17)$$

and the multinomial coefficient is given by

$$\binom{N}{\ell_{1j}, \ell_{2j}, \ldots, \ell_{Kj}} := \frac{N!}{\ell_{1j}!\; \ell_{2j}!\; \cdots\; \ell_{Kj}!} \;.$$

The description above applies for each multinomial, from $j = 1$ to K.

In the product of annihilation operators in (16) there appears the factor $a_k^{\ell_{kj}}$, $k = 1 \ldots K$. In the product of all the multinomials appearing in (13), $j = 1$ to K, there is the factor $a_k^{\ell_{k1}} a_k^{\ell_{k2}} \cdots a_k^{\ell_{kK}} = a_k^{M_k}$, where $M_k = \sum_j \ell_{kj}$ for a given value of k. Considering all values of k, from 1 to K, we get the vacuum expectation value $\langle 0|\, {a_K}^{M_K} \cdots {a_1}^{M_1} a_1^{*n_1} \cdots {a_K^*}^{n_K}\, |0\rangle$, appearing in each term in the expansion of (13).

The expectation value is not null only when $M_k = n_k$. For these values of occupation numbers the sum over pairings in Wick's theorem amounts to $\langle 0| \, {a_K}^{n_K} \cdots {a_1}^{n_1} a_1^{*n_1} \cdots {a_K^*}^{n_K} \, |0\rangle = n_1! \cdots n_K!\,$. Thus, every term in the expansion of (13) includes the factor

$$\langle 0| \, {a_K}^{M_K} \cdots {a_1}^{M_1} a_1^{*n_1} \cdots {a_K^*}^{n_K} \, |0\rangle \; = n_1! \cdots n_K! \; \delta_{n_1,M_1} \cdots \delta_{n_K,M_K} \;, \tag{18}$$

where the deltas impose the condition

$$M_j \equiv \ell_{j1} + \ell_{j2} + \cdots + \ell_{jK} = n_j \tag{19}$$

on the sum (16). Taken as a whole, for every $j = 1, \ldots, K$, we conclude that the only sets of indices $\{\ell_{ij}\}$ contributing to the sums in the multinomial expansion of (13) are those satisfying the conditions (17) and (19), simultaneously. Conditions that we have represented graphically as the square of occupation numbers in figure 1.

The corresponding contribution to the amplitude (13) consists, first, of the combinatorial factor

$$\frac{1}{\sqrt{\big(n_1! \cdots n_K!\big)\big(N_1! \cdots N_K!\big)}} \binom{N_1}{\ell_{11}, \ell_{21}, \ldots, \ell_{K1}} \cdots \binom{N_K}{\ell_{1K}, \ell_{2K}, \ldots, \ell_{KK}} n_1! \cdots n_K! = \sqrt{\big(n_1! \cdots n_K!\big)\big(N_1! \cdots N_K!\big)} \quad \frac{1}{\prod_{i,j} \ell_{ij}!} \tag{20}$$

where each multinomial coefficient stems from the expansion of the corresponding multinomial in (13) and the last factor $n_1! \cdots n_K!$ is contributed by the vacuum expectation value (18). The other factor is the product of mixing parameters

$$\big(W_{1,1}^{\ell_{11}} \, W_{1,2}^{\ell_{21}} \, \cdots \, W_{1,K}^{\ell_{K1}}\big) \cdots \big(W_{K,1}^{\ell_{1K}} \, W_{K,2}^{\ell_{2K}} \, \cdots \, W_{K,K}^{\ell_{KK}}\big) = \prod_{ij} W_{ij}^{\ell_{ji}} \tag{21}$$

stemming from the multinomials (16) too.

The net contribution is the product of the factors in (20) and (21). In the interest of an intuitive mnemonic rule, we identify this contribution with the square in figure 1. The amplitude (13) is said to be computed as the sum over all squares for the given occupation numbers, $(n_1, \ldots, n_K)$ and $(N_1, \ldots, N_K)$, as was stated in (3).

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