Generalized Probabilistic Description of Noninteracting Identical Particles

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We investigate an operational description of identical noninteracting particles in multiports. In particular, we look for physically motivated restrictions that explain their bunching probabilities. We focus on a symmetric 3-port in which a triple of superquantum particles admitted by our generalized probabilistic framework would bunch with a probability of $\frac{3}{4}$. The bosonic bound of $\frac{2}{3}$ can then be restored by imposing the additional requirement of product evolution of certain input states. These states are characterized by the fact that, much like product states, their entropy equals the sum of entropies of their one-particle substates. This principle is, however, not enough to exclude the possibility of superquantum particles in higher-order multiports.

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Introduction.—Although quantum mechanics is a well established theory, its foundations still lack a satisfactory explanation. This is in stark contrast to special relativity, where all the predictions can be traced back to the invariance of the physical laws in inertial systems and the constant speed of light for all observers. To deepen our understanding of the quantum theory, we need to discover the underlying principles.

This quest has been undertaken in two ways. The first, the *device-independent* approach, consists of restricting the conditional probability distributions of some black boxes with information-theoretic principles. For example, in their seminal paper [1] Popescu and Rohrlich proposed a principle which guarantees that a box cannot be used for superluminal communication. This restriction, called no-signaling, was, however, not enough to exclude all stronger-than-quantum correlations. Soon, more fundamental principles were discovered, including macroscopic locality [2], local orthogonality [3], and many others [4–6], but none of them was fully successful in restoring the quantum theory.

The other approach, known under the umbrella term *generalized probabilistic theory* (GPT), aims to single out the quantum formalism from information-theoretic principles. It defines the notions of systems, states, transformations, and measurements and then narrows them down with additional axioms until Hilbert spaces, density matrices, and the Born rule appear. Some notable works written in this spirit include Refs. [7–11].

In this Letter, we employ elements of the GPT formalism to provide an operational description of linear optical interferometric experiments with bosons and fermions. Our framework consists of input and output probability distributions of states linked with a transformation matrix. This matrix captures two important features of optical multiports. First, the particles do not interact; therefore, each particle evolves individually and the differences in measured probability distributions stem solely from the particle statistics and interference [12–19]. To reflect this, we impose a consistency condition which constrains transformations of probability distributions. This condition is analogous to no-signaling and states that the distribution of an individual particle, or a subset of particles, cannot depend on the total number of particles. Second, the entropy of the probability distribution does not decrease, which is implemented by requiring that the transformation matrix be doubly stochastic [20].

These restrictions are obeyed by quantum particles; however, we show that they allow for the existence of hypothetical particles whose grouping tendencies, commonly known as bunching, are stronger than in the case of bosons. This example can be considered as an analog of a Popescu-Rohrlich (PR) box within the realm of identical particles. Finally, we provide an additional principle which rules out the superbunching particles on a tritter (symmetric 3-port). It consists of requiring that states whose entropy equals the sum of the entropies of their substates undergo a product evolution. Such states resemble product states, which are significant components of many GPTs (see, for instance, Refs. [9–11]). Interestingly, this principle is not enough to exclude superquantum particles in higher-order multiports.

The motivation for our research is twofold. First, we would like to contribute to the search for general rules underlying the foundations of quantum theory [1–11]. In particular, our goal is to describe the fundamental properties of systems consisting of more than two identical particles. Second, indistinguishability was recognized as a resource for quantum computation [21]; therefore, its deeper understanding can result in future practical applications.

General framework.—Every experiment has three stages. The first stage is a preparation of a system in some initial state. Due to various reasons, the state need not be exactly determined. Therefore, the most general state description is given by a set of probability distributions over the values of measurable properties. In the next stage, the system undergoes an evolution, and its state changes. The description of this change is given by a set of allowable transformations on the set of probability distributions. Finally, in the last stage, some properties of the system are measured.

In this Letter, we consider a system of N noninteracting identical particles which can be distributed over K different modes. The state is determined by a set of particle occupation numbers for each mode, $s = \{n_1, n_2, \ldots, n_K\}$. The number of particles is conserved; therefore $\sum_{i=1}^{K} n_i = N$. The total number of different states is $d = (K + N - 1)!/[N!(K - 1)!]$. Since the description need not be deterministic, we consider d-dimensional probability vectors $\mathbf{\Pi}$ over all states. We will refer to these vectors as distributions.

The model is simple—we prepare an initial probability distribution $\mathbf{\Pi_i}$ which is transformed into a final distribution $\mathbf{\Pi_f}$. The transformation is given by a stochastic matrix $\mathbb{S}$, i.e., $\mathbf{\Pi_f} = \mathbb{S}\mathbf{\Pi_i}$. The distribution $\mathbf{\Pi_f}$ describes the statistics of detection events which can be registered by particle counters.

In order to illustrate the above idea, let us consider a well-known example of $N = 2$ and $K = 2$ corresponding to noninteracting bosons on a symmetric beam splitter (BS). There are three possible states, which we denote as $\{2, 0\}$, $\{1, 1\}$, and $\{0, 2\}$. The probability vector is of the form $\mathbf{\Pi} = (p(2,0), p(1,1), p(0,2))^T$. The transformation reads

$$\mathbb{S}_{BS} = \begin{pmatrix} 1/4 & 1/2 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/2 & 1/4 \end{pmatrix}. \qquad (1)$$

Before we proceed, we need to make one important comment. One may question that the above approach does not allow us to describe transformations on all physically accessible initial states. For example, our generalized probabilistic framework does not consider quantum superpositions of the states $\{2, 0\}$, $\{1, 1\}$, and $\{0, 2\}$. The model assumes that we only deal with mixtures over states with well-defined occupation numbers. However, note that any quantum superposition can be obtained from such states by a proper transformation. This pretransformation can be included in the main transformation. For example, before the particles go into the BS, they can go through another device which will prepare a superposition. In a similar way, one may question that this approach does not allow us to measure all states. However, just like with preparation, any measurement basis can be transformed into the occupation number basis, and this post-transformation can be also included in the main transformation.

Consistency condition.—Let us focus on how to encode the lack of interaction into our framework. We start with an observation regarding a BS transformation made by two of the authors previously in Ref. [22]. Namely, the transformation of a single-particle distribution does not depend on the presence of the other particle. Here, we generalize this property to arbitrary transformations and arbitrary subsets of particles.

In order to do that, we investigate the relationship between the N- and $(N - 1)$-partite probability distributions $\mathbf{\Pi}^{(N)}$ and $\mathbf{\Pi}^{(N-1)}$. In essence, $\mathbf{\Pi}^{(N-1)}$ should be consistent with a probability distribution obtained from $\mathbf{\Pi}^{(N)}$ by randomly removing one particle. This can be described as $\mathbf{\Pi}^{(N-1)} = \mathbb{D}^{(N)}\mathbf{\Pi}^{(N)}$, where $\mathbb{D}^{(N)}$ is a rectangular stochastic matrix. Its entries D_{ij} correspond to probabilities of transition between an N-partite state s_j and an $(N - 1)$-partite state s'_i. Such a transition is possible if and only if deleting a single particle from some mode k of a state s_j gives a state s'_i. Let $n_{k(i,j)}$ be the occupation number of the mode that we delete a particle from in s_j to achieve the transition. Then $D_{ij} = n_{k(i,j)}/N$ if this state transition is possible and 0 otherwise.

For example, in the case of $N = 2$ and $K = 2$, the transition from a bipartite distribution to a single-partite distribution (supported on states $\{1, 0\}$ and $\{0, 1\}$) is given by the 2×3 matrix

$$\mathbb{D}^{(2)} = \frac{1}{2}\begin{pmatrix} 2 & 1 & 0 \\ 0 & 1 & 2 \end{pmatrix}. \qquad (2)$$

Finally, we can construct matrices allowing us to transform N-partite into M-partite distributions via simple multiplication $\mathbb{D}^{(N\to M)} = \mathbb{D}^{(M+1)} \ldots \mathbb{D}^{(N-1)}\mathbb{D}^{(N)}$.

Now we introduce constraints on transformations $\mathbb{S}$. We start with a transformation of a single particle $\mathbb{S}^{(1)}$. This transformation is the primitive of our model, since with no interactions, single-particle transformation must be the basis for the evolution of an arbitrary number of particles. For example, in the case of a symmetric BS, this transformation is given by

$$\mathbb{S}^{(1)}_{BS} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \qquad (3)$$

The bipartite transformation $\mathbb{S}^{(2)}$ can be chosen in an arbitrary way, provided that the following constraint is fulfilled for all bipartite probability vectors $\mathbf{\Pi_i}^{(2)}$:

$$\mathbb{D}^{(2)}\mathbb{S}^{(2)}\mathbf{\Pi_i}^{(2)} = \mathbb{S}^{(1)}\mathbb{D}^{(2)}\mathbf{\Pi_i}^{(2)}. \qquad (4)$$

In simple words, the above means that if we first transform a bipartite distribution and then reduce it to a single-partite distribution, we would get the same result as if we first reduced a bipartite distribution to a single-partite distribution and then transformed it. This can be easily generalized to an arbitrary number of particles

$$\mathbb{D}^{(N\to 1)}\mathbb{S}^{(N)}\mathbf{\Pi_i}^{(N)} = \mathbb{S}^{(1)}\mathbb{D}^{(N\to 1)}\mathbf{\Pi_i}^{(N)}. \qquad (5)$$

Moreover, this constraint should hold at the level of all the M-partite subsets

$$\mathbb{D}^{(N\to M)}\mathbb{S}^{(N)}\mathbf{\Pi_i}^{(N)} = \mathbb{S}^{(M)}\mathbb{D}^{(N\to M)}\mathbf{\Pi_i}^{(N)}, \qquad (6)$$

where M is an arbitrary integer $M < N$. We will call Eq. (6) the *consistency condition*.

To illustrate this restriction, let us once more consider the example of a symmetric BS. Equations (2), (3), and (4) imply $\mathbb{D}^{(2)}\mathbb{S}^{(2)}\mathbf{\Pi_i}^{(2)} = (1/2, 1/2)^T$ for any distribution $\mathbf{\Pi_i}^{(2)}$. This means that the final distribution must satisfy

$$\begin{pmatrix} p(2,0) + 1/2p(1,1) \\ p(0,2) + 1/2p(1,1) \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}. \qquad (7)$$

Note that the above is obeyed by bosons, fermions, and distinguishable particles as well.

Double stochasticity.—Additionally, we would like the entropy of the probability distribution not to decrease. This property can be encoded in the transformation matrix $\mathbb{S}$ by requiring it to be doubly stochastic; i.e., the sum of its entries in each row and column equals 1 [20]. The extra condition captures the fact that for quantum multiport experiments, the entropy of $\mathbf{\Pi_f} = \mathbb{S}\mathbf{\Pi_i}$ is never smaller than the entropy of $\mathbf{\Pi_i}$. This is because the multiport transformation is unitary, and the measurement of the particle number is modeled by a decoherence in the particle-number basis. Neither of these processes can decrease the entropy.

For instance, in the case of an asymmetric beam splitter followed by the particle-number measurement, the transformation matrix $\mathbb{S}$ is given by

$$\mathbb{S}^{(1)}_{aBS} = \begin{pmatrix} T & R \\ R & T \end{pmatrix}, \qquad (8)$$

where $T + R = 1$.

Although every unitary quantum multiport transformation and the particle-number measurement can be represented by a doubly stochastic matrix, not all doubly stochastic matrices correspond to a quantum process. In this Letter, we consider a general class of doubly stochastic transformations which obey the consistency condition discussed above. In particular, we show that it is possible to find such transformations that allow for stronger bunching than in the case of quantum bosons.

Beyond quantum theory.—Multipartite quantum states are expressed in terms of operators $a_i^\dagger$ which create a particle in mode i. For our purposes, we do not need to go into detail about the underlying particle statistics to show that the consistency condition is obeyed in quantum theory. It is enough to observe that due to lack of interaction, creation operators evolve independently $a_i^\dagger \to a_i'^\dagger$. Therefore, Eq. (6) is automatically satisfied. Moreover, we have already argued that in the quantum case, the entropy of the probability distributions does not decrease.

Interestingly, the two requirements still allow for a more general description of transformations. Although the quantum theory admits perfect bunching and antibunching in the $N = 2$ and $K = 2$ scenario, for $N > 2$ or $K > 2$ one can propose some more extreme behaviors. Here, we discuss the case $N = 3$ and $K = 3$.

Let us first consider a quantum description of a symmetric 3-port, commonly known as a tritter. Its quantum properties have been studied in great details—see, for example, the work by Campos [15]. There are three input modes described by creation operators $a_i^\dagger$ and three output modes described by $a_i'^\dagger$ ($i = 1, 2, 3$). The transformation is given by a unitary mapping $a_i'^\dagger = \sum_j U_{ij} a_j^\dagger$, where $U_{ij} = (1/\sqrt{3})\omega^{\delta_{ij}}$, δ_{ij} is the Kronecker delta and ω is the third root of unity.

The quantum tritter transformation applied to the three-boson state $\{1,1,1\}$ produces the states $\{3,0,0\}$, $\{0,3,0\}$, and $\{0,0,3\}$ with a probability of 2/9 each and the state $\{1,1,1\}$ with a probability of 1/3. Interestingly, unlike $N = 2$ and $K = 2$, the quantum probability of bunching B_Q does not saturate the algebraic bound of 1:

$$B_Q = p^{(111)}_{300} + p^{(111)}_{030} + p^{(111)}_{003} = \frac{2}{3} < 1, \qquad (9)$$

where $P^{(y)}_x$ denotes the probability of transforming the state y into state x. Although we do not provide a proof of this statement, by the end of this work we will show that the value of 2/3 is implied by a fundamental principle obeyed by the quantum theory.

At this point, one may wonder if some hypothetical particles, which obey the consistency and the double stochasticity conditions, can have greater tripartite-bunching properties than bosons. The answer is positive. Consider, for example, the three-particle transformation $\mathbb{S}^{(3)}_T$

$$\begin{array}{c|c|c|c} & \begin{smallmatrix} 3&0&0 \\ 0&3&0 \\ 0&0&3 \end{smallmatrix} & \begin{smallmatrix} 2&2&1&1&0&0 \\ 1&0&2&0&2&1 \\ 0&1&0&2&1&2 \end{smallmatrix} & \begin{smallmatrix} 1 \\ 1 \\ 1 \end{smallmatrix} \\ \hline \begin{smallmatrix} 3&0&0 \\ 0&3&0 \\ 0&0&3 \end{smallmatrix} & 0 & \frac{1}{8} & \frac{1}{4} \\ \hline \begin{smallmatrix} 2&1&0 \\ 2&0&1 \\ 1&2&0 \\ 1&0&2 \\ 0&2&1 \\ 0&1&2 \end{smallmatrix} & \frac{1}{8} & \frac{5}{48} & 0 \\ \hline \begin{smallmatrix} 1&1&1 \end{smallmatrix} & \frac{1}{4} & 0 & \frac{1}{4} \end{array}, \qquad (10)$$

where the blocks are schematically denoted by a single element which is the same for all its entries. The above transformation has a bunching probability $B_S = \frac{3}{4}$. One can easily verify that $\mathbb{S}_T^{(3)}$ is doubly stochastic. It remains to be shown that it also follows the consistency condition. In order to do that, note that from the point of view of our generalized probabilistic description, the single-partite tritter transformation is given by

$$\mathbb{S}_T^{(1)} = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}. \tag{11}$$

Then, for all the possible initial states we indeed have $\mathbb{D}^{(3\to1)}\mathbb{S}_T^{(3)}\mathbf{\Pi_i}^{(3)} = \mathbb{S}_T^{(1)}\mathbb{D}^{(3\to1)}\mathbf{\Pi_i}^{(3)}$.

Recovering the quantum bound on the bunching probability.—The above example can be considered as an identical-particle analog of the PR box [1]. Note that in the case of the PR boxes, the no-signaling principle does not recover quantum theory. In our case, the conditions imposed by our framework do not recover quantum theory either. However, here we find an additional physical restriction that allows for the recovery of bosonic behaviour on a tritter.

Let us first observe that the average two-particle bunching probability bounds the three-particle one from above.

$$B \leq \frac{p_{200}^{(110)} + p_{200}^{(101)} + p_{200}^{(011)} + \cdots + p_{002}^{(101)} + p_{002}^{(011)}}{3}. \tag{12}$$

This follows from the consistency condition applied to the general form of the transformation of state $\{1,1,1\}$. Since the transformation matrix needs to be doubly stochastic, the above expression can be written as

$$B \leq 1 - \frac{p_{200}^{(200)} + p_{200}^{(020)} + p_{200}^{(002)} + \cdots + p_{002}^{(020)} + p_{002}^{(002)}}{3}. \tag{13}$$

The goal is therefore to show that the right-hand side of (13) is bounded from above by $\frac{2}{3}$. To do that, we propose a restriction on the possible transformations of states in which all particles occupy the same mode.

Let us first motivate it by drawing a parallel with product states. If a product state describes noninteracting subsystems, each subsystem evolves independently. In this case, the evolution of the whole is given by the product of evolutions of the parts.

We focus on a two-partite case, which is the most relevant to our considerations. If we denote the two independent subsystems in a product state by A and B, their entropies satisfy the relation

$$H(A,B) = H(A) + H(B). \tag{14}$$

A similar condition can be written for the probability distributions of two particles:

$$H(\mathbf{\Pi}^{(2)}) = 2H(\mathbf{\Pi}^{(1)}) = 2H(\mathbb{D}^{(2\to1)}\mathbf{\Pi}^{(2)}). \tag{15}$$

The above states that the entropy of the whole probability distribution is the same as the sum of entropies of its two one-particle marginals. It is easy to verify that the only state of two particles that satisfies Eq. (15) is of the form $\{2,0,0\}$. As a side note, observe that in the first quantization, these are the only states of identical particles that can be written in a product form. Consequences of that fact have been studied in Refs. [23,24].

Because of this analogy with the product states, and because of the general assumption that particles do not interact, we propose that states in which all particles are in the same mode should evolve as a product of single-particle evolutions. In the two-particle case, this principle means that a system described by a probability distribution $\mathbf{\Pi}^{(2)}$ evolves as

$$\mathbb{S}^{(2)}\mathbf{\Pi}^{(2)} = \mathbb{S}^{(1)}\mathbf{\Pi}^{(1)} \times \mathbb{S}^{(1)}\mathbf{\Pi}^{(1)}, \tag{16}$$

where states of the type $a \times b$ are treated as equivalent to $b \times a$ because of the indistinguishability of particles. For instance, we have $\{0,1,1\} \equiv \{0,1,0\} \times \{0,0,1\} \equiv \{0,0,1\} \times \{0,1,0\}$, so the two-particle vector space shrinks to six dimensions. Formula (16) means that for a tritter we have $p_{200}^{(200)} = p_{020}^{(200)} = p_{002}^{(200)} = \frac{1}{9}$. Since the same reasoning holds for the states $\{0,2,0\}$ and $\{0,0,2\}$, inequality (13) simplifies to $B \leq \frac{2}{3}$, which is the quantum bound for a three-partite bunching on a tritter.

Finally, we would like to note that our approach can be applied to any system, not only the tritter. For instance, two particles on an N-port have the average quantum bunching probability B equal to

$$B = 2\frac{p_{20\ldots0}^{(11\ldots0)} + \cdots + p_{0\ldots02}^{(0\ldots011)}}{N(N-1)} = \frac{2}{N}, \tag{17}$$

which is also the upper bound on bunching in our model. On the other hand, some additional restrictions are required to recover quantum behavior for $N > 3$ and $K > 3$. For example, we have considered the case $N = 4$ and $K = 4$ and observed that the following transformation admits superquantum bunching while satisfying all the restrictions of our model:

$$
\begin{array}{c|c|c|c|}
 & \begin{smallmatrix} 3 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 3 \end{smallmatrix} & \begin{smallmatrix} 2 & \cdots & 0 \\ 1 & \cdots & 0 \\ 0 & \cdots & 1 \\ 0 & \cdots & 2 \end{smallmatrix} & \begin{smallmatrix} 1 & \cdots & 0 \\ 1 & \cdots & 1 \\ 1 & \cdots & 1 \\ 0 & \cdots & 1 \end{smallmatrix} \\
\hline
\begin{smallmatrix} 3 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 3 \end{smallmatrix} & \frac{3}{32} & \frac{3}{64} & \frac{1}{64} \\
\hline
\begin{smallmatrix} 2 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 1 & 2 \end{smallmatrix} & \frac{1}{96} & \frac{13}{192} & \frac{7}{192} \\
\hline
\begin{smallmatrix} 1 & 1 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & 1 & 1 \end{smallmatrix} & \frac{1}{8} & 0 & \frac{1}{8} \\
\end{array} \tag{18}
$$

Perhaps an extended version of the product state argument is needed to explain all but the simplest cases.

Conclusions and outlook.—We have proposed an operational description of the evolution of noninteracting indistinguishable particles. The model is particularly related to linear optical experiments with multipartite interference of bosons or fermions. Our approach explores bunching in generalized theories. In particular, we show that our framework admits exotic bunching probabilities. The superquantum symmetric 3-port (tritter) we present could be considered a PR-box counterpart in the realm of particle statistics. In this case an additional principle, governing the evolution of a certain class of states, is enough to recover the bosonic bounds. However, it is not sufficient in higher-order multiports. There are a few possibilities for why this happens. First, our principle may need extension to include more general classes of states, not only those in which all the particles are in the same mode. Moreover, symmetric quantum n-ports (for $n > 3$) have more than one inequivalent representation [25]. For example, a 4-port can be described by a discrete Fourier transform, but also by a Groover-like unitary matrix. The two representations generate different output probability distributions. Nevertheless, they both lead to the same maximal bunching probabilities, which suggest that fundamental laws behind bosonic behavior go beyond the subtleties of particular evolutions (see the Supplemental Material [26] for details).

This work fits into the very lively field of research on explaining elements of the quantum mechanics with intuitive principles. Investigation of particle statistics admitted by superquantum theories is of general interest, as it might lead to new tests of quantum foundations. We hope that our results will be a stimulating contribution to this endeavor.

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