On the inequivalence of the CH and CHSH inequalities due to finite statistics

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Abstract
Different variants of a Bell inequality, such as CHSH and CH, are known to be equivalent when evaluated on nonsignaling outcome probability distributions. However, in experimental setups, the outcome probability distributions are estimated using a finite number of samples. Therefore the nonsignaling conditions are only approximately satisfied and the robustness of the violation depends on the chosen inequality variant. We explain that phenomenon using the decomposition of the space of outcome probability distributions under the action of the symmetry group of the scenario, and propose a method to optimize the statistical robustness of a Bell inequality. In the process, we describe the finite group composed of relabeling of parties, measurement settings and outcomes, and identify correspondences between the irreducible representations of this group and properties of outcome probability distributions such as normalization, signaling or having uniform marginals.

Keywords: Bell inequalities, nonlocality, device-independent quantum information, symmetries

(Some figures may appear in colour only in the online journal)

1. Introduction

The structure of physical systems can be probed by observing relations between the measurement outcomes of their subsystems. When the subsystems are spacelike separated, special relativity forbids faster-than-light communication; then the outcome probability distributions obey the linear nonsignaling constraints [1–3]. Additionally, when subsystems obey the locality principle, the outcome probability distributions respect linear constraints known as Bell inequalities [4]. The CHSH [5] and CH [6] Bell inequalities were introduced by Clauser et al along with experimental proposals to test the violation of the locality principle by quantum
mechanics. Later on, the CHSH and the CH inequalities were shown to be equivalent [7, 8] provided the outcome probability distributions satisfy the nonsignaling constraints.

Quantum systems respect the nonsignaling constraints; thus, in theory, the CHSH and CH inequalities should be equivalent. However, in practice, experimental probability distributions are estimated using a finite set of samples, and the nonsignaling constraints are only satisfied approximately due to statistical fluctuations. Thus, supposedly equivalent Bell inequalities exhibit differing statistical properties, as hinted by Knill et al [10] and Gill [11]. In particular, the standard deviation of the reported Bell inequality violation is affected, as shown in figure 1 for the CHSH and CH inequalities. With this observation, we can look for the optimal variant of a given Bell inequality. To do so, we decompose the inequality into a nonsignaling subspace (left untouched) and a signaling subspace to be optimized. While several ways to decompose a Bell inequality have already been proposed [3, 12, 13], we show the existence of a unique decomposition that satisfies the requirements of the device-independent framework [14–16].

Expanding on our earlier investigations [13], our method rests on the study of the symmetries of Bell scenarios. In the device-independent approach, nonlocal behaviors are studied without attributing a particular meaning to the parties, the measurement settings and the outcomes, which are, for all purposes, abstract labels—no assumptions are made about the inner workings of devices. Likewise, the set of Bell inequalities is defined up to the relabeling of parties, settings and outcomes [17, 18]. Quite naturally, the symmetry group of those relabelings collects Bell inequalities into families [13, 19–23]. However, in the current work, we assume that we already selected the representative of a Bell inequality to be violated in an experimental setup, and merely optimize its signaling subspace.

The required decomposition of the inequality coefficients into subspaces follows straightforwardly from the structure of the action of the relabeling group: for example, a nonsignaling probability distribution stays nonsignaling after an arbitrary relabeling. The same phenomenon holds for other properties, such as being properly normalized or having uniformly random marginals. These three properties correspond to invariant subspaces of the probability distribution coefficients; a complete list of these subspaces is given by the irreducible representations of the relabeling group.

The present paper has two goals. First, we present a practical method to optimize the Bell inequality variant used in an experiment. Second, we enumerate all the irreducible representations of the relabeling group present in outcome probability distributions and associate them to physical properties. Accordingly, we organize our paper as follows. In section 2, we introduce the relabeling equivalence principle motivating our decomposition. We describe our optimization process in section 3 and illustrate it with simulations of two recent loophole-free Bell experiments. Together, these two sections form a self-contained description of our optimization method. In section 4, we list all the invariant subspaces appearing in the outcome probability distributions of a bipartite scenario with binary settings and outcomes.

11. Definitions used through out the present work

A Bell scenario is described by the triple \((n, m, k)\), where \(n\) is the number of parties, each with \(m\) measurement settings and \(k\) measurement outcomes per settings [24]. We write \((x, y, ...)\) the measurement settings used by the parties, and \((a, b, ...)\) the obtained measurement outcomes. In a Bell scenario, a setup is a concrete or gedanken experiment, whose behavior is described by the joint conditional probability distribution \(P_{ab \mid xy}\). Using a suitable enumeration of the coefficients, this distribution can be written as a vector \(\vec{P} \in \mathbb{R}^d\), where \(d = (mk)^n\).
When a quantum setup can be modeled precisely, the distribution \( p_{ab|xy} \) is exactly given by the Born rule. In experimental situations, however, the distribution \( \vec{P} \) is estimated by an experimental run recording the outcomes of a certain number of trials in the counts \( N(ab\ldots xy\ldots) \). From these counts, the outcome probability distribution \( \vec{P} \) is approximated using the relative frequencies \( p_{ab|xy} \approx N(ab\ldots xy\ldots)/N(xy\ldots) \). A recent example is given by the loophole-free Bell test of Shalm et al. [9] (Supplemental Material): in the scenario (2, 2, 2), the authors present the event counts of six experimental runs, each run collecting approximately \( 2 \cdot 10^8 \) trials.

2. The label equivalence principle and representations

We first derive a general principle from the device-independent framework which motivates our introduction of elements of representation theory in the study of nonlocality. For simplicity, in this paper, we will restrict ourselves to the (2, 2, 2) scenario in which the CHSH inequality is tested. Our results generalizes straightforwardly [25]. In that scenario, the behavior of a setup is described by the distribution \( p_{ab|xy} \) with \( a, b = 0, 1 \) and \( x, y = 0^*, 1^* \) (the asterisk is purely cosmetic to distinguish settings and outcomes). The same probability distribution is interchangeably written as the vector \( \vec{P} \in V = \mathbb{R}^{d=16} \).

However, to write the probability distribution \( p_{ab|xy} \) above, a certain labeling convention has to be used, deciding who is Alice (\( a, x \)) and Bob (\( b, y \)), and which measurement setting (respectively measurement outcome) corresponds to 0* and 1* (respectively 0, 1). The transformation between labeling conventions is given by the relabeling group \( G_{nmk} \), written \( G \) when no confusion is possible. It is fully described in appendix C and contains the relabelings of the parties, the settings, and the outcomes: a specific relabeling is given in figure 2. In a given scenario, the labels of parties, settings, and outcomes are purely abstract and have no physical meaning. This leads to the following principle:
Definition 1 (Label equivalence principle). In the study of nonlocality and device-independent protocols, all labeling conventions are equivalent.

This principle is already present in all study of nonlocality. As an example, let us consider the constraints satisfied by nonsignaling probability distributions. All probability distributions are nonnegative:

$$\forall a, b, x, y, \quad p_{ab|xy} \geq 0,$$

and normalized:

$$\forall x, y, \sum_{ab} p_{ab|xy} = 1.$$  \hspace{1cm} (2)

In addition, the nonsignaling probability distributions satisfy:

$$\forall x, y, a, \sum_b p_{ab|xy} = p_{a|x} \text{ and } \forall x, y, b, \sum_a p_{ab|xy} = p_{b|y}.$$  \hspace{1cm} (3)

Taken as sets of constraints, each of equations (1)–(3) satisfy the label equivalence principle.

To understand the deeper phenomenon at play here, let us make an analogy. In special relativity, the Lorentz group specifies the transformations between reference frames, and in turn, the physics of a relativistic system is contained in the representations of the Lorentz group. Similarly, a natural description of quantum behaviors should be given by the representations of the relabeling group $G$. Already, $V \ni \vec{P}$ is a representation of $G$, as the linear action of $G$ is to permute the coefficients of the probability distribution $p_{ab|xy}$. We then decompose $V$ into the invariant subspaces corresponding to irreducible representations of $G$ [26], and match the resulting subspaces to physical properties. Some of these properties are readily identified: under $G$, properly normalized distributions stay normalized and nonsignaling distributions stay nonsignaling. The full decomposition of $V$ into irreducible representations is presented in section 4. To achieve our goal of optimizing the coefficients of a Bell inequality, a coarser-grained decomposition into three orthogonal subspaces is sufficient: the first subspace corresponds to the normalization conditions equation (2), the second to nonsignaling content.
3. Constructing the optimal variant of a Bell inequality

Having motivated our decomposition of $\vec{P} \in V$ into normalization, nonsignaling and signaling subspaces, we look to optimize the statistical properties of a given Bell inequality. We consider a bipartite nonsignaling setup. This setup can be either a classical or quantum experiment, or even a gedanken experiment simulated on a computer. Because we study the nonlocal properties of the setup, we immediately forget about the description of the physical system and measurements to only remember the probabilities $p_{ab|xy}$ that define it. As the distribution $p_{ab|xy}^\text{setup}$ is nonsignaling, it satisfies equations (1)–(3).

When the setup exhibits nonlocality, the probability distribution $p_{ab|xy}^\text{setup}$ violates a Bell inequality. This Bell inequality can be written using coefficients $\beta_{abxy}$ along with a local bound $u$ such that

$$I = \sum_{abxy} \beta_{abxy} p_{ab|xy} = \vec{\beta} \cdot \vec{P}^\text{local} \leq u,$$

is satisfied when the distribution $p_{ab|xy}^\text{setup}$ is local. In the above equation, we also write $\beta_{abxy}$ as a vector $\vec{\beta} \in V = \mathbb{R}^d$ such that the computation of the inequality value is an inner product. Our method is based on the following proposition, which is a simplified version of the theorem presented in section 4:

**Proposition.** $V$ splits into three orthogonal subspaces $V = V_{\text{NO}} \oplus V_{\text{NS}} \oplus V_{\text{SI}}$ invariant under $G$. Accordingly, the coefficient vectors of probability distributions $\vec{P}$ and Bell inequalities $\vec{\beta}$ can be decomposed into orthogonal vectors:

$$\vec{P} = \vec{P}_{\text{NO}} + \vec{P}_{\text{NS}} + \vec{P}_{\text{SI}}, \quad \vec{\beta} = \vec{\beta}_{\text{NO}} + \vec{\beta}_{\text{NS}} + \vec{\beta}_{\text{SI}}.$$ (5)

In this decomposition, $\vec{P}_{\text{NO}}$, $\vec{P}_{\text{NS}}$ and $\vec{P}_{\text{SI}}$ correspond to the normalization, the nonsignaling content and the signaling content of the probability distribution $\vec{P}$, with the following relations:

(i) $\vec{P}_{\text{NO}} = \frac{1}{d} \vec{1}$ for all probability distributions, where $\vec{1} = (1, 1, ..., 1)^\top$ (normalization),

(ii) $\vec{P}_{\text{SI}} = \vec{0}$ for all nonsignaling probability distributions.

**Proof.** See section 4 and appendix C. $\square$

This decomposition can also be deduced from section 2. Indeed, the equations (2) and (3) are linear conditions on $\vec{P}$, which can be directly translated into equations about a projection of $\vec{P}$. Here equations (2) and (3) respectively correspond to (i), over projection

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3 Let us make a side remark. What is the most fundamental object in the study of nonlocality? On the one hand, we can argue that $p_{ab|xy}^\text{setup}$ is the fundamental object. The composition of the relabeling group $G$ follows from the nonsignaling constraints: nonnegativity equation (1) prescribes a permutation representation on $\vec{P} \in V = \mathbb{R}^d$, so that $G$ is isomorphic to a subgroup of the symmetric group $S_d$. The exact subgroup is the one preserving the normalization equation (2) and nonsignaling equation (3) constraints, recovering $G$. On the other hand, the relabeling group $G$ can be taken as the fundamental object, whose irreducible representations provide directly the components of $\vec{P}$ respecting the nonsignaling principle. However, there are other irreducible representations of $G$ that do not appear in the decomposition of $V \supset \vec{P}$. It is an open question whether they play a role in the study of nonlocality.
\( P_{\text{NO}} \) and (ii), over projection \( P_{\text{SI}} \). The last component \( P_{\text{NS}} \), which is not constrained by normalization and nonsignaling (and then contains all the physical information), is defined as 
\( P_{\text{NS}} = P - P_{\text{NO}} - P_{\text{SI}} \).

Using that proposition and the orthogonality relations, we rewrite the scalar product equation (4):
\[
I = \vec{\beta} \cdot \vec{P} = (\vec{\beta}_{\text{NO}} \cdot \vec{P}_{\text{NO}}) + (\vec{\beta}_{\text{NS}} \cdot \vec{P}_{\text{NS}}) + (\vec{\beta}_{\text{SI}} \cdot \vec{P}_{\text{SI}}) = \text{cte} \quad \text{local} \leq u,
\]

enabling the following transformations of a Bell inequality:

- The local bound \( u \) of the inequality can easily be translated by modifying the coefficients \( \vec{\beta}_{\text{NO}} \),
- The inequality can be rescaled by multiplying both \( \vec{\beta} \) and \( u \) by the same positive factor.
- The coefficients \( \vec{\beta}_{\text{SI}} \) can be set to an arbitrary value.

We see from the first two transformations that a comparison of the violation \( I \) across Bell inequality variants is only possible if the variants are first rescaled such that each of their local and quantum bounds match. Such a rescaling has no physical meaning and is pure convention.

What happens with the third transformation is more surprising. In experiments, the standard deviation \( \sigma \) of the violation \( I_{\text{exp}} = \vec{\beta} \cdot \vec{P}_{\text{exp}} \) has a dependence on \( \vec{\beta}_{\text{SI}} \), and thus the component \( \vec{\beta}_{\text{SI}} \) can be optimized.

3.1. Spurious signaling due to finite statistics

In an experimental run, the distribution \( P_{\text{setup}}^{\text{ab|xy}} \) is estimated by repeating measurements for a certain number \( N \) of trials. For each trial, a setting pair \( (x, y) \) is selected and the outcomes \( (a, b) \) of the corresponding measurements are recorded. Writing \( N(abxy) \) the number of events corresponding to settings \( (x, y) \) and outcomes \( (a, b) \), we estimate:
\[
P_{\text{run}}^{\text{ab|xy}} = \frac{N(abxy)}{N(xy)}; \quad (7)
\]

We saw that \( P_{\text{SI}}^{\text{setup}} = 0 \). However, because \( P_{\text{run}} \) is estimated using a finite number of samples, statistical fluctuations lead to signaling outcome probability distributions: for a particular run, we generally have \( P_{\text{run}}^{\text{SI}} \neq 0 \).

By the central limit theorem, \( P_{\text{run}} \) is well approximated by a multivariate normal distribution \( N(\vec{\mu}, \Sigma) \), where the mean vector \( \vec{\mu} = P_{\text{setup}}^{\text{SI}} \) and the covariance matrix \( \Sigma_{\text{abxya'b'x'y'}} \) could be computed from the multinomial distribution. In practice, the Monte-Carlo estimation of \( \Sigma \) performs well.

For each run, we can compute the Bell violation \( I_{\text{run}} = \vec{\beta} \cdot \vec{P}_{\text{run}} \). If we were to perform infinitely many trials in each run, the average value \( \langle I_{\text{run}} \rangle \) of the Bell inequality would be given by \( I_{\text{setup}} \), as the average signaling component \( \langle P_{\text{run}}^{\text{SI}} \rangle \) would be zero. However, a run is composed of a finite number of trials, creating statistical fluctuations. The variance \( \sigma \) of the Bell violation \( I_{\text{run}} = \vec{\beta} \cdot \vec{P}_{\text{run}} \) is given by \( \sigma^2 = \vec{\beta}^\top \Sigma \vec{\beta} \); it depends on \( \vec{\beta}_{\text{SI}} \), which can be optimized.

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\( ^4 \) Some papers report the ratio \( s = (I_{\text{exp}} - u)/\sigma \) representing the magnitude of the violation as the number of standard deviations above the local bound. This ratio \( s \) is invariant under translation and scaling.
3.2. Construction of the optimal variant

Finding the optimal variant of a Bell inequality boils down to the minimization of $\sigma$ over the variables $\vec{\beta}_S$. We prove in appendix D.1 that the variant of the inequality $\vec{\beta}^*$ whose value has minimal variance is given by:

$$\vec{\beta}^* = \left( \bar{\Pi} - \Pi \left( \Pi \Sigma \Pi + \bar{\Pi} \right)^{-1} \Pi \Sigma \bar{\Pi} \right) \vec{\beta},$$

(8)

where $\Pi$ is the orthogonal projection over the signaling space $V_S$ (given in appendix D.1 and table C4) and $\bar{\Pi} = \mathbb{I} - \Pi$. If the matrix $(\Pi \Sigma \Pi + \bar{\Pi})$ is not invertible, the inverse can be replaced by the Moore-Penrose pseudo-inverse.

Note that the implementation of equation (8), which is the solution to a minimization problem of a quadratic function (standard problem in optimization), can be done easily and efficiently.

3.3. Implementation on simulated loophole-free Bell experiments

To illustrate the impact of our method, we study the robustness the CH, CHSH and Eberhard inequalities to the effects of finite statistics. Then, we derive the optimal Bell inequality. The original expressions have been shifted and rescaled so that the local bound is at 0 and the maximal quantum violation at $2(\sqrt{2} - 1)$. Specifically:

- The CHSH inequality ([27]) is shifted by $-\frac{1}{8} \vec{1}$. We consider $\vec{\beta}^{CHSH} = \vec{\beta}^{CHSH}_{[27]} - \frac{1}{8} \vec{1}$.

$\vec{\beta}^{CHSH} = \begin{pmatrix} 0.5 & -1.5 & 0.5 & -1.5 \\ -1.5 & 0.5 & -1.5 & 0.5 \\ 0.5 & -1.5 & -1.5 & 0.5 \\ -1.5 & 0.5 & 0.5 & -1.5 \end{pmatrix}$

- The CH inequality ([6]) has its marginal terms $p_{a|x}$ and $p_{b|y}$, interpreted as $p_{a|x} = \sum_b p_{ab|x0}$ and $p_{b|y} = \sum_a p_{ab|y0}$, respectively. To obtain the same maximal violation, the inequality is scaled by: $\vec{\beta}^{CH} = 4\vec{\beta}^{CH}_{[6]}$.

$\vec{\beta}^{CH} = \begin{pmatrix} -4 & -4 & 4 & 0 \\ -4 & 0 & 0 & 0 \\ 4 & 0 & -4 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$

- The EH inequality ([9]) corresponds to the CH inequality with marginal terms interpreted as $p_{a|x} = \sum_b p_{ab|x1}$ and $p_{b|y} = \sum_a p_{ab|y1}$, It is scaled by $\vec{\beta}^{EH} = 4\vec{\beta}^{EH}_{[9]}$.

$\vec{\beta}^{EH} = \begin{pmatrix} 0 & 0 & 0 & -4 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -4 & 0 & 0 & -4 \end{pmatrix}$

5 Our convention is $\beta = \left( \begin{array}{cccc} \beta_{00'0'} & \beta_{00'1'} & \beta_{01'0'} & \beta_{01'1'} \\ \beta_{10'0'} & \beta_{10'1'} & \beta_{11'0'} & \beta_{11'1'} \\ \beta_{00''0'} & \beta_{00''1'} & \beta_{01''0'} & \beta_{01''1'} \\ \beta_{10''0'} & \beta_{10''1'} & \beta_{11''0'} & \beta_{11''1'} \end{array} \right)$.
To illustrate our method, we simulate two types of experiments. The first simulation is inspired by the experiment described in [27]. We suppose that the source deterministically provides pairs of entangled photons. In this configuration, the vacuum component is negligible. For the second case, we assume that the source is based on the spontaneous parametric down conversion process, as employed in [9]. In this last case, the vacuum component is predominant. As described in appendix A, we use the features given in [9, 27] to generate the following probability distributions:

\[
\vec{P}(1) = \begin{pmatrix}
0.39 & 0.09 & 0.35 & 0.13 \\
0.08 & 0.44 & 0.12 & 0.40 \\
0.39 & 0.09 & 0.10 & 0.38 \\
0.08 & 0.44 & 0.37 & 0.15
\end{pmatrix}
\]

\[
\vec{P}(2) = \begin{pmatrix}
1 - 4.0 \times 10^{-5} & 1 \times 10^{-5} & 1 - 9.8 \times 10^{-5} & 8.7 \times 10^{-6} \\
9.7 \times 10^{-6} & 2.0 \times 10^{-5} & 6.7 \times 10^{-5} & 2.2 \times 10^{-5} \\
1 - 9.8 \times 10^{-5} & 6.8 \times 10^{-7} & 8.3 \times 10^{-7} & 8.9 \times 10^{-7} \\
8.3 \times 10^{-7} & 2.2 \times 10^{-5} & 8.9 \times 10^{-7} & 4.7 \times 10^{-7}
\end{pmatrix}
\]

To see the effect of the finite number of trials on the violation, we performed a Monte-Carlo type simulation. Given a number of trials, the algorithm returns a simulated number of detection events for the sixteen combinations of settings and outcomes.

Figure 3. a. Violation of Bell inequality for \(\vec{P}(1)\) ([27]). We observe same average violation \(\langle I \rangle = 0.302\) but different standard deviation \(\sigma_{\text{CHSH}} = 0.211\) and \(\sigma_{\text{CH}} = 0.464\). b. Violation of Bell inequality for \(\vec{P}(2)\) ([9]). We observe same average violation \(\langle I \rangle = 1.25 \times 10^{-5}\) but different standard deviation \(\sigma_{\text{CHSH}} = 5.65 \times 10^{-6}, \sigma_{\text{CH}} = 1.20 \times 10^{-5}, \sigma_{\text{EH}} = 3.72 \times 10^{-6}\) and \(\sigma_{\text{opt}} = 2.60 \times 10^{-6}\). In both cases, we renormalized the inequalities such as the bound for the violation is 0 (and not 2 for CHSH) and such as the maximal quantum violation is the same.

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9.7 \times 10^{-6} & 2.0 \times 10^{-5} & 6.7 \times 10^{-5} & 2.2 \times 10^{-5} \\
1 - 9.8 \times 10^{-5} & 6.8 \times 10^{-7} & 8.3 \times 10^{-7} & 8.9 \times 10^{-7} \\
8.3 \times 10^{-7} & 2.2 \times 10^{-5} & 8.9 \times 10^{-7} & 4.7 \times 10^{-7}
\end{pmatrix}
\]

To see the effect of the finite number of trials on the violation, we performed a Monte-Carlo type simulation. Given a number of trials, the algorithm returns a simulated number of detection events for the sixteen combinations of settings and outcomes.

The histogram distributions obtained for the two experiments after 200 000 simulated runs are given in figure 4. The figure 4(a) shows the violation distribution obtained when we perform 245 steps with the probability distribution \(\vec{P}(1)\) given in equation (9). The CHSH and CH inequalities give the same amount of violation in average without the same standard deviation. As CHSH and CH only differs on their signaling component, this clearly show the influence of the signaling part on the statistical fluctuations around the mean violation. In this case, because the distribution obeys a particular symmetry (up to experimental imperfections), the inequality variant with minimal variance is CHSH (see appendix D.2).

We also observe this effect with a non-maximally entangled photon pair source described by the probability distribution \(\vec{P}(2)\) given in equation (9). figure 4(b) shows the violation distributions obtained for \(176 \times 10^{6}\) steps. As before, we obtain for the three inequalities, CHSH, CH, and EH, the same amount of violation in average with different standard deviations. Moreover, by using equation (8), we found an inequality that exploits the noise correlation between the probabilities to reduce the influence of the statistical error. This optimal inequality is:
As expected, we see in figure 4(b) that this inequality gives the same average violation with an improved standard deviation. This upgrades the violation, from $1.0 \sigma$ with CH and $3.4 \sigma$ with EH (considered in [9]) to $4.8 \sigma$ with the optimal inequality.

4. Physical properties of scenarios naturally emerge from the symmetry group

We saw in section 2 that the description $\vec{P}$ of a device-independent setup is made using an arbitrary labeling convention. Moreover, there exists a group $G$ of transformations, the relabelings, between those conventions and $V \ni \vec{P}$ is a representation of that group. In the following, we decompose it into irreducible components and identify each irreducible component with a corresponding physical property. By construction, those properties are independent from the labeling convention in use (for an introduction to representation theory, see appendix B).

**Theorem.** In the scenario $(2, 2, 2)$, the representation $V$ of $G$ is reducible, with orthogonal irreducible nonequivalent components:

$$V = V_{NO1} \oplus V_{NO2} \oplus V_{NO3} \oplus V_{marg} \oplus V_{corr} \oplus V_{SI} \oplus V_{SI}^{coarse} \oplus V_{NO} \oplus V_{NS} \oplus V_{SI},$$

(11)

where the subspaces have their bases and associated physical meanings given in table 1. This decomposition is unique as the finest decomposition that preserves the group structure. Any vector $\vec{P}$ can be decomposed as:

$$\vec{P} = \vec{P}_{NO1} \oplus \vec{P}_{NO2} \oplus \vec{P}_{NO3} \oplus \vec{P}_{marg} \oplus \vec{P}_{corr} \oplus \vec{P}_{SI}^{coarse} \oplus \vec{P}_{NO} \oplus \vec{P}_{NS} \oplus \vec{P}_{SI},$$

(12)

such that for any $g \in G$, we have $\vec{P}^g = \vec{P}_{NO1}^g \oplus \vec{P}_{NO2}^g \oplus \vec{P}_{NO3}^g \oplus \vec{P}_{marg}^g \oplus \vec{P}_{corr}^g \oplus \vec{P}_{SI}^g$ with $\vec{P}_{LBL}^g, \vec{P}_{LBL}^g \in V_{LBL}$ for all subspace labels $LBL$. In particular, $\vec{P}_{LBL}^g \neq 0$ is independent from the labeling convention. This can be seen as a confirmation of our intuition: ‘the setup contains the physical property $LBL$’ is an assertion which is independent from the labeling convention.
The same decomposition applies to the coefficient vector $\vec{\beta}$ of a Bell inequality.

**Proof.** The irreducible decomposition of $V$ is constructed step by step in appendix C. □

We now interpret the elements that appear in the decomposition, identifying them to intuitive physical properties. We illustrate it with setups whose behavior $\vec{P}$ contain specific physical behavior (table 2):

- **Normalization subspace $V_{\text{NO}}$**:
  
  This subspace corresponds to the physical property ‘$\vec{P}$ is properly normalized’, corresponding to the four normalization conditions (2). For any normalized outcome distribution, $\vec{P}_{\text{NO1}} = \frac{1}{4}$ and $\vec{P}_{\text{NO2}} = \vec{P}_{\text{NO3}} = 0$.
  
  In the setup UNI (table 2), Alice and Bob throw two unbiased coins for any setting. This results in the uniform distribution $\vec{P}_{\text{UNI}} \in V_{\text{NO}}$.

- **Marginals subspace $V_{\text{marg}}$**:
  
  This subspace corresponds to the marginals of Alice and Bob respectively independent from Bob and Alice choice of setting. We further split it into $V_{\text{marg}} \equiv V_{\text{marg}}^A + V_{\text{marg}}^B$ by discerning the roles of Alice and Bob, otherwise mixed by the group. The physical property ‘Alice and Bob have uniform marginals’ ($p_{a|x} = p_{b|y} = 1/2$) is preserved under relabelings and corresponds to $\vec{P}_{\text{marg}} = 0$. In the correlator notation [3], it corresponds to
  
  \[
  \langle A_x \rangle = \frac{1}{2} \sum_{ab} (-1)^a p_{a|b} \quad \text{and} \quad \langle B_y \rangle = \frac{1}{2} \sum_{ab} (-1)^b p_{a|b} \] (providing that the distribution of measurement settings is itself unbiased for signaling setups).
  
  In the setup BIAS (table 2), Alice throws a fair coin and Bob a $1/4$ biased coin for any setting. We observe that $\vec{P}_{\text{BIAS}} = \vec{P}_{\text{NO}} + \vec{P}_{\text{marg}}$.

- **Correlation subspace $V_{\text{corr}}$**:
  
  This subspace corresponds to the correlation between Alice and Bob outcomes, i.e. whether $a = b$. Outcomes distributions $\vec{P} = \vec{P}_{\text{NO}} + \vec{P}_{\text{corr}}$ are symmetric under relabeling of all outcomes ($a \rightarrow 1 - a$ and $b \rightarrow 1 - b$), and are optimally tested by CHSH (see appendix D.2). In the correlator notation, it corresponds to the elements $\langle A_x B_y \rangle = \sum_{ab} (-1)^{ab} p_{a|b}$.

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**Table 1.** Irreducible components appearing in the probability distributions of bipartite Bell scenarios with their dimension and basis ($Q_{ijkl}(ab|xy) = \vec{P}^i_j k^l$ for $i, j, k, l = \pm 1$, see table C4).

| Vector subspace | Basis | Physical meaning | Dim |
|-----------------|-------|------------------|-----|
| $V_{\text{NO}} \equiv V_{\text{NO1}} \oplus V_{\text{NO2}} \oplus V_{\text{NO3}}$ | $\vec{Q}^{+++}$ | Normalization | 4 |
| $V_{\text{NO1}}$ | $\vec{Q}^{+++}$ | Normalization | 1 |
| $V_{\text{NO2}}$ | $\vec{Q}^{+++}$ | Normalization | 2 |
| $V_{\text{NO3}}$ | $\vec{Q}^{+++}$ | Normalization | 1 |
| $V_{\text{NS}} \equiv V_{\text{marg}} \oplus V_{\text{corr}}$ | | Nonsignaling | 8 |
| $V_{\text{marg}}(\equiv V_{\text{marg}}^A + V_{\text{marg}}^B)$ | $\vec{Q}^{+++}$ | Marginals | 4 |
| $V_{\text{corr}}$ | $\vec{Q}^{+++}$ | Bob marginals | 2 |
| $V_{\text{corr}}$ | $\vec{Q}^{+++}$ | Correlations | 4 |
| $V_{\text{SI}}(\equiv V_{\text{SI}}^{\rightarrow A} + V_{\text{SI}}^{\rightarrow B})$ | | Signaling | 4 |
| $V_{\text{SI}}^{\rightarrow A}$ | $\vec{Q}^{+++}$ | Signaling $A \rightarrow B$ | 2 |
| $V_{\text{SI}}^{\rightarrow B}$ | $\vec{Q}^{+++}$ | Signaling $B \rightarrow A$ | 2 |
In the setup BW (table 2), an object with color either black or white (with equal probability \(\frac{1}{2}\)) is cut it in two parts which are sent to Alice and Bob. The outcome measured by Alice and Bob attributes a number \(0, 1\) and \(b = 0, 1\) to the colors. The resulting distribution, \(\vec{p}_{\text{BW}} = \vec{p}_{\text{NO}} + \vec{p}_{\text{corr}}\), contains correlations but is nonsignaling with uniform marginals.

- **Signaling subspace** \(V_{\text{SI}}\):

  This subspace corresponds to the physical property ‘the outcome distribution is signaling’. As for \(V_{\text{marg}}\), we discern the roles of Alice and Bob to split \(V_{\text{SI}} \equiv V_{\text{SI}}^B + V_{\text{SI}}^A\), representing respectively the signaling from Alice to Bob (when \(\vec{p}_{\text{SI}}^B \neq 0\)) and from Bob to Alice (when \(\vec{p}_{\text{SI}}^A \neq 0\)). To be more explicit, \(\vec{p}_{\text{SI}}^A\) contains strictly the information about the dependence of Alice’s outcome on Bob’s choice of setting.

  In the setup SIG (table 2), Alice measurement setting is Bob outcome and Alice throws an unbiased coin. It contains only signaling from Alice to Bob. The resulting distribution is purely signaling: \(\vec{p}_{\text{SIG}} = \vec{p}_{\text{NO}} + \vec{p}_{\text{SI}}^A\).

  Table 2 also contains the setup OPTQ corresponding to the optimal quantum violation of CHSH and the setup PRBOX corresponding to the PR-box [2]. Neither setup has marginal or signaling term. Their correlation terms \(\vec{p}_{\text{corr}}\) are collinear, with PRBOX more correlated than OPTQ. The last line NOISE gives the decomposition of the statistical fluctuations present when \(\vec{p}_{\text{corr}}\) is estimated using a finite number of samples. In general, there is noise in each of \(V_{\text{marg}}, V_{\text{corr}}\) and \(V_{\text{SI}}\).

  This theorem, whose generalization to all \((n, m, k)\) scenarios will be given in a future note [25], is a direct proof of the unicity of the decomposition made in [13]. In this work, Rosset \textit{et al} defined a projection on the nonsignaling subspace that commutes with the relabelings. As shown here for the scenario \((2, 2, 2)\), this projection is unique.

5. Conclusion

The study of quantum nonlocality in the device-independent framework considers the labeling of parties, measurement settings and outcomes as pure convention. Transformations between labeling conventions are given by the relabeling group. We explored the structure of this

| Name     | Nonzero components | \(p_{ab|xy}\) | \(\vec{p}\) |
|----------|--------------------|---------------|-------------|
| UNI      | \(V_{\text{NO}}\) | \(\frac{1}{4}\) | \(\frac{1}{4}\vec{Q}_{+++}\) |
| BIAS     | \(V_{\text{NO}}, V_{\text{marg}}\) | \(\frac{1}{4} (\frac{1}{2}\delta_{a=0} + \frac{1}{2}\delta_{a=1})\) | \(\frac{1}{4}\vec{Q}_{+++} - \frac{1}{4}\vec{Q}_{++-}\) |
| SIG      | \(V_{\text{NO}}, V_{\text{SI}}^B\) | \(\frac{1}{4}\delta_{a=b}\) | \(\frac{1}{4}\vec{Q}_{+++} + \frac{1}{4}\vec{Q}_{++-}\) |
| BW       | \(V_{\text{NO}}, V_{\text{corr}}\) | \(\frac{1}{4}\delta_{a=b}\) | \(\frac{1}{4}\vec{Q}_{+++} + \frac{1}{4}\vec{Q}_{++-}\) |
| PRBOX    | \(V_{\text{NO}}, V_{\text{corr}}\) | \(\frac{1}{4}\delta_{a+b=xy}\) | \(\frac{1}{4}\vec{Q}_{+++} + \frac{1}{4}\sum_{kl} \tau_{kl} \vec{Q}_{+-kl}\) |
| OPTQ     | \(V_{\text{NO}}, V_{\text{corr}}\) | \(\vec{p}^ {\text{exp}}_{ab|xy}\) | \(\frac{1}{4}\vec{Q}_{+++} + \frac{1}{4}\sum_{kl} \tau_{kl} \vec{Q}_{+-kl}\) |
| NOISE    | \(V_{\text{marg}}, V_{\text{corr}}, V_{\text{SI}}\) | \(\epsilon_{ab|xy} = p^ {\text{exp}}_{ab|xy} - p^ {\text{corr}}_{ab|xy}\) | \(\epsilon_{\text{marg}}, \epsilon_{\text{corr}}, \epsilon_{\text{SI}}\) |
relabeling group and of some of its representations. In particular, the decomposition of the coefficient space of a Bell inequality singles out the normalization and signaling subspaces. Arbitrarily many variants of a Bell inequality can be generated by changing the vector components corresponding to these subspaces; however, if the obtained inequalities are equivalent on nonsignaling distributions, their statistical properties differ in experimental use. We showed how to construct the inequality with minimal variance, which optimizes the number of standard deviations above the local bound in experimental works. We simulated the outcome distributions coming from two recent experiments [9, 27] and discussed the optimality of variants such that CHSH, CH or Eberhard inequalities compared to our method.

Recently, several authors [28, 29] introduced formal statistical tests to reject the locality hypothesis with a certain $p$-value threshold. These tests are heavily dependent on the inequality variant considered. We leave the generalization of our method to these tests as an open question.

To our knowledge, this work represents the first application of the representation theory of finite groups to the relabeling group of Bell scenarios. Here, we described the decomposition of the representation space corresponding to $\rho_{ab, |xy\ldots|}$. We leave the study of the other irreducible representations to future work. If, as we conjecture, the relabeling group is a fundamental object in the study of device-independent protocols, its representations should play a major role in other protocols.

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Appendix A. Generation of the probability distributions

A.1. Deterministic entangled state sources

The probability distribution for the deterministic entangled state source is calculated from the experimental parameters given in [27]. In this experiment, the authors entangled two NV centers using the electronic spin as a two dimensional system with basis states denoted as $|\uparrow\rangle$ and $|\downarrow\rangle$. They aim to prepare the two spins in a maximally entangled state of the form $|\psi^-\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2}$, but due to imperfections in the state preparation, they generate a partially entangled state $\rho$ described by the density matrix:

$$\rho = \frac{1}{2} \begin{pmatrix} \lambda & 0 & 0 & 0 \\ 0 & 1 - \lambda & V & 0 \\ 0 & V & 1 - \lambda & 0 \\ 0 & 0 & 0 & \lambda \end{pmatrix},$$  \hspace{1cm} (A.1)

with $\lambda = 0.022$ and $V = 0.873$.

The measurement apparatuses perform an imperfect projection along the Z axis. To take into account the measurement imperfections the projectors are defined by:
\[ \Pi_0' = \eta_a' \Pi_+ + (1 - \eta_a') \Pi_- , \quad \Pi_1' = (1 - \eta_a') \Pi_+ + (\eta_a') \Pi_- , \]  
where \( \Pi_{\pm} = (1 \pm \sigma_z)/2 \). The readout fidelities are equal to \( \eta_a' = 0.954, \eta_a = 0.994, \eta_b = 0.939 \), and \( \eta_b = 0.998 \) for the measurement apparatuses of Alice and Bob. The outcome probabilities are then \( p_{a|x} = \text{Tr} \left[ (\Pi_a' \otimes \Pi_b') R(\theta_a', \theta_b', \rho R(\theta_a', \theta_b')^\dagger) \right] \) where \( R(\theta_a', \theta_b') \) is the rotation operator with respect to \( Z \) applied on the two spins. The authors found that the maximal violation of the CHSH inequality is obtained for the angles \( \theta_a = 0, \theta_a = \pi/2, \theta_b = -3\pi/4 - \epsilon \), and \( \theta_b = 3\pi/4 + \epsilon \), with \( \epsilon = 0.026\pi \). With this parameter we obtained the probability distribution given in equation (9). As expected, this probability distribution gives the same violation (2.30) of the CHSH Bell inequality than the one they mention (corresponding to the shifted value 0.30 = 2.30 – 2 given in figure 4(a)).

### A.2. Nondeterministic entangled state sources

The nondeterministic entangled state source was inspired by [9], where two spontaneous parametric down conversion processes are used to generate polarization entangled photon pairs of the form \( |\psi \rangle = 0.961 |HH\rangle + 0.276 |VV\rangle \). Here, the main difference with the previous approach is that the source is based on a spontaneous processes. This means that most of the time no photons are generated and rarely one or several pairs are. The nonlinear photon-pair generation nonlinear process with a large number of modes is described by the operator:

\[ C_i(\mu) = e^{-\mu} \sum_{n=0}^{4} \mu^{|n|/2} n!^{1/2} (a_i^† b_i^†)^n , \]  

where \( \mu \) is the mean number of photon pairs in the spatial modes \( a \) and \( b \): the former is given to Alice, the latter to Bob. To properly define the density matrix measured by the authors, we need to take into account all the photon losses, which can be applied to mode \( a \) via the loss operator: \( L_a(\eta) = \sum_{n=0}^{4} (1 - \eta)^{n/2} \eta^{n/2} |n\rangle \langle n| \otimes \mathbb{1} \). where \( \eta \) is the transmission probability. The complete source, i.e. with the two nonlinear processes and all the losses over all the modes, is depicted by the density matrix of the form \( \rho = S(0|0\rangle \langle 0|S^\dagger \) with \( S(\mu_H, \mu_V, \eta_A, \eta_B) = L_{b_y}(\eta_B)L_{b_y}(\eta_B)L_{a_y}(\eta_A)L_{a_y}(\eta_A)C_H(\mu_H)C_V(\mu_V) \). To simulate the source proposed in [9], we used the parameters \( \eta_A = 0.747, \eta_B = 0.756, \mu_V = \mu_V^{1.2} \), and \( \mu_H = \mu_H^{1.2} \) with \( r = 0.288 \) and \( \mu = 4 \times 10^{-4} \).

For the detection, only one non-photon-number-resolving detector is used on each side to measure the photons in the \( H \) mode. The detection events correspond to outcome 1 and the non-detection to an outcome 0. The measurement apparatus (written here for Alice) is described by the operators:

\[ \Pi_a^1 = (\mathbb{1} - |0\rangle \langle 0|_{a_H} \otimes \mathbb{1}_{a,V,H}, \quad \text{and} \quad \Pi_a^0 = |0\rangle \langle 0|_{a_H} \otimes \mathbb{1}_{a,V,H} . \]  

The probabilities given in equation (9) are obtained by \( p_{a|x} = \text{Tr} \left[ (\Pi_a^1 \Pi_b^0) R(\theta_a', \theta_b', \rho R(\theta_a', \theta_b')^\dagger) \right] \) for the polarization measurement angles \( \theta_a = -4.2^\circ, \theta_a = 25.9^\circ, \theta_b = -4.2^\circ \), and \( \theta_b = 25.9^\circ \).

### Appendix B. Introduction to representation theory

Here, we give a brief introduction to the theory of finite group representations and its main results we use. For a more complete introduction, we adress the reader to [26].
A group of symmetries $G$ corresponds to a finite set of transformations $g$ with an algebraic group structure: identity, inverse, composition in $G$.

In our case, these symmetries will be built from permutations of the settings, outputs and parties.

While group $G$ contains the abstract structure of the transformations, its concrete effects are seen on a representation of $G$ on a vector space $V$, for which any $g \in G$ is associated with a linear invertible transformation of $V (v \in V \mapsto v^g \in V)$ where this association preserves the structure of $G$.

For example, imagine we are interested in the Bell scenario ‘Alice tosses a coin’, i.e. $(1, 1, 2)$. $G$ is the group of transformations from one arbitrary labeling (e.g. Heads = 0, Tails = 1) of the result to any possible labeling $(G = \mathfrak{S}_2 = \{\text{Id}, \rho\}$, where $\text{Id}$ is the identity map and $\rho$ exchanges 0 and 1). Then $G$ acts on $V = \mathbb{R}^2$ by: $\text{Id}$ does nothing and $\rho$ exchanges the coordinates (this is called the natural representation).

$W \subset V$ is said to be invariant by $G$ if for any $w \in W, g \in G$, we always have $w^g \in W$. Then, if the only subspaces $W \subset V$ invariant by $G$ are $\{0\}$ and $V$, we say that this representation is irreducible and write: ‘$V$ is an irreducible representation of $G$’.

Back to Alice and her coin, it is easy to see that the representation is not irreducible: $v = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is a counter example as $v^\rho = \rho v = v$.

We then have the following result, at the foundation of representation theory:

**Theorem.** If $G$ is finite, there is a finite number of irreducible representations $(W_1, W_2, \ldots)$. Any representation $V$ of $G$ can be uniquely decomposed as an orthogonal sum of irreducible representations $V = W_1 \oplus \ldots \oplus W_r$.

At the level of the vectors, any $v \in V$ can be uniquely decomposed as $v = w_1 + \ldots + w_p$ with $w_k \in W_k$. Then $\forall g \in G, v^g = w_1^g + \ldots + w_p^g$ with $w_k^g \in W_k$.

This result, which looks quite technical, has an important physical meaning. If our formalism describes the physical reality in a vector space $V$, if this description is redundant and if $G$ contains the transformations between the different descriptions of the same physical reality, then our formalism contains some degeneracy (being the choice of some specific $g \in G$). Decomposing $V$ into irreducible representations is a way to remove this degeneracy. Most properties of $v \in V$ are not universal. For example, ‘first coordinate of $v$ is 0’ is often an arbitrary property, as it usually depends on the choice of $g \in G$ (in our case, the choice of labeling). However, some properties of the $w_k$ components are universal: ‘$w_1 = 0$’ is independent of the choice of $g \in G$.

We adopt this notation: If $V$ decomposes into $W_1$ and $W_2$ under $G$, we write $V = W_1 \oplus W_2$.

With a $(1, 1, 2)$ Bell scenario, there are two irreducible representations of dimension one, $W_1 = t$ (trivial irreducible representation) and $W_2 = s$ (sign irreducible representation), with $\rho$ acting as $\text{Id}$ over $t$ and as $-\text{Id}$ over $s$. Here $V = t \oplus s$, with $t$ generated by $\epsilon_+ = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $s$ generated by $\epsilon_- = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. The two physical properties are the norm ($t$) and the bias of the coin ($s$).

In the following, we apply these results to our specific case. The symmetry group is $G$, the group of relabelings. We are then interested in the ‘relabeling-independent’ physical properties of a Bell setup. As we will see, there are only four such properties: the norm, the marginals, the correlations and the signaling contribution.
Appendix C. Step by step construction of the (2, 2, 2) scenario along with its symmetries

We prove here the theorem of section 4 by constructing the scenario, the symmetry group and its representation. As presented in figure C1, the construction is done piece by piece, adding successively outcomes, settings and parties, while keeping track of the decomposition of the representation into irreducibles. We start with the scenario (1, 1, 2) with two outcomes, then add the settings to obtain the scenario (1, 2, 2) and lastly add parties, obtaining the full (2, 2, 2) scenario. We give here the main ingredients of the proof, insisting on its physical meaning. For more technical details and a complete inventory of the irreducible representations of wreath products groups, see [30].

Let us first recall our theorem:

**Theorem.** In the scenario (2, 2, 2), the representation $V$ of relabeling group $G$ given by its action on $\vec{P}$ is reducible, with orthogonal irreducible nonequivalent components:

$$V = V_{\text{NO}} \oplus V_{\text{NO}} \oplus V_{\text{NO}} \oplus V_{\text{marg}} \oplus V_{\text{corr}} \oplus V_{\text{St}},$$

(C.1)

where the subspaces have their bases given in table 1.

As proved in the following, a basis for the above subspaces is given by the vectors $\vec{Q}_{ijkl}$, defined as

$$\vec{Q}_{ijkl}(ab|xy) = i^{a}j^{b}k^{c}l^{d}p_{ab},$$

(i, j, k, l = ±1).

(C.2)

Any distribution $\vec{P}$ writes:

$$\vec{P} = \sum_{ijkl=\pm1} \alpha_{ijkl} \vec{Q}_{ijkl}, \quad \alpha_{ijkl} = \frac{1}{16} \sum_{abxy} i^{a}j^{b}k^{c}l^{d}p_{ab}p_{xy}.$$

(C.3)

While the individual basis vectors $\vec{Q}_{ijkl}$ are arbitrary, the subspaces themselves are uniquely specified by the action of the relabeling group.

C.1. First step: scenario (1, 1, 2)

We first start with a (1, 1, 2) Bell scenario, which corresponds to a physical device that outputs □ or ☐, as represented in figure C1 (a). We choose an arbitrary labeling, e.g. ☐ ≡ 0 and □ ≡ 1, to define the probability $p_{a}$ of obtaining the result 0 or 1. Then the probability vector is given by:

$$\vec{P} = \sum_{a} p_{a} e_{a} = \begin{pmatrix} p_{0} \\ p_{1} \end{pmatrix} \in V_{112} \equiv \mathbb{R}^{2},$$

(C.4)

with $e_{0} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $e_{1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ the canonical basis of $\mathbb{R}^{2}$. As represented in table C1, the symmetry group is $G_{112} \equiv S_{2} = \{ \text{Id}, \rho \}$, where Id is the identity and $\rho$ exchanges 0 and 1, i.e. exchanges $e_{0}$ and $e_{1}$.

We now show how to express $\vec{P}$ in a more convenient way by giving the decomposition of $V_{112}$ into irreducible representations under $G_{112}$. Defining $e_{\pm} = e_{0} \pm e_{1}$, one can write $\vec{P}$ as $\vec{P} = \vec{P}_{\text{NO}} + \vec{P}_{\text{corr}}$, where $\vec{P}_{\text{NO}} = \alpha_{+} e_{+}$ is the normalization part of $\vec{P}$ (with $\alpha_{+} = \frac{1}{2}(p_{0} + p_{1})$) and $\vec{P}_{\text{corr}} = \alpha_{-} e_{-}$ is the physical part of $\vec{P}$ (with $\alpha_{-} = \frac{1}{2}(p_{0} - p_{1})$). $\vec{P}_{\text{corr}}$ is just the bias between the two outcomes. The action of the elements of $G_{112}$ over $\vec{P}$ is then very easy to compute: Id does nothing, and $\rho$ changes the sign of $\vec{P}_{\text{corr}}$. Then, we write
\[ V_{112} = t \oplus s, \] where \( t \) (respectively \( s \)) is the vector space generated by \( \{ \epsilon_+ \} \) (respectively \( \{ \epsilon_- \} \)). The important properties of \( t \) and \( s \) are that they are stable under the action of elements of \( G_{112} \). More precisely, \( t \) (the trivial irreducible representation of \( G_{112} \)) is left invariant by any element of \( G_{112} \) and \( s \) (the sign irreducible representation of \( G_{112} \)) is such that \( \rho \) acts as \( -\text{Id} \).

**C.2. Second step: scenario (1, 2, 2)**

As represented in figure C1 (b), we extend our scenario to a (1, 2, 2) Bell scenario by adding two measurement settings (e.g. with the arbitrary labeling \( \bullet \equiv 0 \) and \( \Box \equiv 1 \)). When we label the experiment, we may decide on the labeling of the outcomes depending on the choice of measurement settings, which leads to eight possible labelings. After the labeling is chosen, we can define the probability \( p_{a|\{x\}} \) to obtain an outcome \( a \) given the setting \( x \):

\[
\vec{\beta} = \sum_{a} p_{a|x} e_a \otimes e_x^* \in V_{122} = \mathbb{R}^2 \otimes \mathbb{R}^2^* \cong \mathbb{R}^4,
\]

where \( \{ e_a \}_{a=0,1} \) (respectively \( \{ e_x^* \}_{x=0,1} \)) is the canonical basis of \( \mathbb{R}^2 \) (respectively \( \mathbb{R}^2^* \)). Note that we changed the usual convention for the tensor product enumeration, changing the value of subscript \( a \) first. Again, we use an asterisk for the inputs, to distinguish them from the outputs. An element of \( G_{122} \) is defined by one permutation of the setting \( x \), and two permutations of the outcomes (one for each setting): two elements can be seen in table C2. More formally, \( G_{122} = S_2 \wr S_2^* \) is the wreath product (written \( \wr \)) of \( G_{112} \) (permutation of the settings) with \( \mathbb{R}_2 \) (permutation of the outcomes) of \( G_{112} \).
S (permutation of the outcomes) and V_{122} is the imprimitive representation constructed from V_{112} (see appendix E).

In order to decompose V_{122} into irreducible representations, we can first decompose it under the action of G_{112} \subset G_{122} only:

$$R_2 \otimes R_2^* \oplus \mathcal{G}_{112} = (t \oplus s) \otimes R_2^* \oplus \mathcal{G}_{112} = (t \otimes 0^*) \oplus (t \otimes 1^*) \oplus (s \otimes 0^*) \oplus (s \otimes 1^*),$$

(C.6)

where t ⊗ x^* and s ⊗ x^* are generated by \(\epsilon_+ \otimes \epsilon_+^*\) and \(\epsilon_- \otimes \epsilon_-^*\), respectively. Then, to decompose under the full group G_{122}, one has to take into account all possible permutations of the setting. Finally, we find:

$$R_2 \otimes R_2^* \overset{\mathcal{G}_{122}}{\cong} T \oplus S^* \oplus \phi,$$

(C.7)

where T ≡ t ⊗ t^*, S^* ≡ t ⊗ s^* and \(\phi \equiv s \otimes 0^* + s \otimes 1^*\) are generated by \{\(\epsilon_+ \otimes \epsilon_+^*\), \(\epsilon_+ \otimes \epsilon_-^*\}\} and \{\(\epsilon_- \otimes \epsilon_+^*\), \(\epsilon_- \otimes \epsilon_-^*\}\}, respectively. As expected, these three spaces are globally unchanged by any element \(\rho \in G_{122}\).

In this decomposition, \(\mathcal{P}\) can be written as \(\mathcal{P} = \mathcal{P}_{NO1} + \mathcal{P}_{NO2} + \mathcal{P}_{phy}\) where \(\mathcal{P}_{NO1} = \alpha_+ \epsilon_+ \otimes \epsilon_+^* \in T\) and \(\mathcal{P}_{NO2} = \alpha_- \epsilon_- \otimes \epsilon_-^* \in S^*\) are the normalization parts and \(\mathcal{P}_{phy} = \alpha_+ \epsilon_+ \otimes \epsilon_+^* + \alpha_- \epsilon_- \otimes \epsilon_-^* \in \phi\) is the physical part (with \(\alpha_+ = \frac{1}{4} \sum_{k=1}^{N} \rho_{kl} \rho_{lk}\)). Here \(\alpha_+\) represents the bias in the settings which is 0 for normalized probability vectors. In the physical part, \(\alpha_-\) is the sum of the outcome biases for the two possible settings while \(\alpha_-\) is the difference of the outcome biases for the two possible settings.
To extend to a (2, 2, 2) Bell scenario, we consider two parties arbitrarily labeled as Alice and Bob, as represented in figure C1(c). The symmetry group \( G_{222} \) of this scenario is composed of 128 ways to relabel the setup: a specific element is represented in table C3. For a specific setup, we can define the probability \( p_{ab|x,y} \) of obtaining the outcomes \((a, b)\) given that the settings are \((x, y)\). The associated probability vector is given by:

\[
\vec{p} = \sum_{a,b} p_{ab|x,y} e_a^A \otimes e_x^X \otimes e_b^B \otimes e_y^Y = \begin{pmatrix}
p_{00|0,0} \\
p_{10|0,0} \\
\vdots \\
p_{01|1,1} \\
p_{11|1,1}
\end{pmatrix} \in V_{222} = (\mathbb{R}^2 \otimes \mathbb{R}^2^*)_A \otimes (\mathbb{R}^2 \otimes \mathbb{R}^2^*)_B \cong \mathbb{R}^{16}.
\]

(Here again, similarly to equation (C.5), we chose a subscript enumeration different from the usual one). More formally, \( G_{222} \) is a wreath product: \( G_{222} = G_{122} \wr \mathcal{S}_{AB}^2 = \mathcal{S}_2 \wr \mathcal{S}_2 \wr \mathcal{S}_2 \wr \mathcal{S}_2 \) and \( V_{222} \) is the primitive representation constructed from \( V_{122} \). In order to decompose \( V_{222} \) into irreducible representations, we can first decompose independently each \((\mathbb{R}^2 \otimes \mathbb{R}^2^*)_A \otimes (\mathbb{R}^2 \otimes \mathbb{R}^2^*)_B\) under \( G_{122} \):

\[
V_{222} = (\mathbb{R}^2 \otimes \mathbb{R}^2^*)_A \otimes (\mathbb{R}^2 \otimes \mathbb{R}^2^*)_B
\]

\[
G_{222}^A(T \oplus S^* \oplus \phi)_A \otimes (T \oplus S^* \oplus \phi)_B
\]

\[
G_{222}^B(T_A \otimes T_B) \oplus (T_A \otimes S_B^*) \oplus (S_A^* \otimes T_B) \oplus (S_A^* \otimes S_B^*) \\
\oplus (T_A \otimes \phi_B) \oplus (\phi_A \otimes T_B) \oplus (\phi_A \otimes \phi_B) \oplus (\phi_A \otimes S_B^*)
\]

\( G_{222} \) recombines those components by allowing the exchange between A and B. Thus, we obtain:

\[
\]
\[
V_{222} \cong (T_A \otimes T_B) \oplus (T_A \otimes S_B^1 + S_A^1 \otimes T_B) \oplus (S_A^1 \otimes S_B^T)
\]
\[
\oplus (T_A \otimes \phi_B + \phi_A \otimes T_B) \oplus (\phi_A \otimes \phi_B) \oplus (S_A^1 \otimes \phi_B + \phi_A \otimes S_B^A)
\]

(C.9)

figure C2 illustrates all the possible permutations of the six irreducible representations. Those irreducible representation are clearly nonequivalent. In this decomposition, \( \vec{P} \) can be written as:

\[
\vec{P} = \vec{P}_{NO1} + \vec{P}_{NO2} + \vec{P}_{NO3} + \vec{P}_{marg} + \vec{P}_{corr} + \vec{P}_{SI}.
\]

(C.10)

Defining \( \hat{Q}_{ijkl} = \epsilon_{ij} A \otimes \epsilon_{k}^* B \otimes \epsilon_{l}^* A \otimes \epsilon_{B} \) and \( \alpha_{ijkl} = \frac{1}{16} \sum_{abxy} \hat{p}_{ijkl} k_j^a p_{ab|xy} \), we have:

\[
\vec{P} = \sum_{ijkl} \alpha_{ijkl} \hat{Q}_{ijkl},
\]

(C.11)

The correspondence between equations (C.10) and (C.11) is direct and can be read in table 1.

C.4. Physical interpretation of the irreducible representations

We now interpret the subspaces of the theorem present in the decomposition (C.10).

- Normalization subspace \( V_{NO} \):
  
  Let \( \vec{P}_{NO} \in V_{NO} \) be the component of \( \vec{P} \) over the first three subspaces \( V_{NO1}, V_{NO2} \) and \( V_{NO3} \). As said in section 4, it is easy to see that \( \vec{P}_{NO} \) is fixed by the four normalization conditions on \( \vec{P}, \sum_{ab} p_{ab|xy} = 1 \), which impose \( \alpha_{++++} = \frac{1}{4} \) and \( \alpha_{++++} = \alpha_{++-} = \alpha_{+-+} = \alpha_{++-} = 0 \). Then \( \vec{P}_{NO} \) characterizes the normalization of \( \vec{P}_{NO} \) only.

  This can also be deduced from the way elements of \( G \) act over \( V_{NO} \). For \( M = A, B \), \( T_M = (t \otimes t^*)_M \) and \( S_M^T = (t \otimes s^*)_M \) contain \( t \), the trivial representation of the outcomes: the subspaces containing only \( T_M \) and \( S_M^T \) are not affected by any relabeling of the outcomes. Therefore they correspond to a property of \( \vec{P} \) which can be known even by someone who has no access to the outcomes, so \( \vec{P}_{NO} \) can only be about the normalization of \( \vec{P} \).

- Marginal subspace \( V_{marg} \):
  
  \( V_{marg}^B = T_A \otimes \phi_B \) contains \( T_A = t_A \otimes t_A^* \). It is unchanged by any relabeling (setting or outcome) on Alice’s side. Hence it corresponds to a property of \( \vec{P} \) which can be known given Bob if he does not communicate with Alice. This is known as Bob’s marginals. We call \( \vec{P}_{marg}^B \) the projection of \( \vec{P} \) over this subspace. Likewise, \( V_{marg}^A = \phi_A \otimes T_B \) corresponds to Alice’s marginals. In terms of coefficients, we have \( \vec{P}_{marg}^A = \alpha_{++++} \hat{Q}_{++++} + \alpha_{++-} \hat{Q}_{++-} + \alpha_{+-+} \hat{Q}_{+-+} + \alpha_{++-} \hat{Q}_{++-} + \alpha_{++-} \hat{Q}_{++-} + \alpha_{++-} \hat{Q}_{++-} \).

- Correlation subspace \( V_{corr} \):

\[9\]

Those three components have an interpretation when this decomposition is directly applied to the statistics of the experiment \( \tilde{N} = \{N_{ab|xy}\} \), before the normalization equation (7). In this case, they give information about the \( N_{ab|xy} \), \( t_A \otimes t_B \) is about the total number of steps \( N = \sum_{ab} N_{ab|xy} \), \( S_A^1 \otimes T_B \) the bias on Alice’s setting \( \sum_{ab} (-1)^N_{ab|xy} \), \( S_B^T \otimes T_B \) the bias on Bob’s setting \( \sum_{ab} (-1)^N_{ab|xy} \) and \( S_A^1 \otimes S_B^T \) the correlations of the two biases \( \sum_{ab} (-1)^{n+n} N_{ab|xy} \).
\( \bar{P}_{\text{corr}} \) contains the same information as the usual correlators. Indeed, the correlators \( \langle A_i B_j \rangle \) corresponds to the new orthogonal basis \( \bar{E}_{ij} = \sum_{k \in I} k^2 \bar{Q}_{ik} \). In this basis, we have:

\[
\bar{P}_{\text{corr}} = \sum_{xy} E_{xy} \bar{E}_{xy},
\]

where \( E_{xy} = \langle A_i B_j \rangle \).

Looking at the way elements of \( G \) act over \( V_{\text{corr}} \), we can show that it must correspond to correlations. Let us consider the relabeling of outputs \( \rho \in G_{122} \) of only one party (which exchange 0 and 1). This defines two relabelings of the \( (2, 2, 2) \) scenario, \( \rho_A \) (respectively \( \rho_B \)), which acts on Alice’s (respectively Bob’s) side only. Hence, \( \phi_A \circ \phi_B \) has the property of transforming the same way for \( \rho_A \) and \( \rho_B \): if \( \bar{P}_{\text{corr}} \) is the component of \( \bar{P} \) over \( V_{\text{corr}} \), we have \( \bar{P}_{\text{corr}}^\rho_B = \bar{P}_{\text{corr}} \). Now, as \( \rho = \rho^{-1} \) (with two settings/outcomes), \( (\bar{P}_{\text{corr}}^\rho)^n = \bar{P}_{\text{corr}} \). Then \( \bar{P}_{\text{corr}} \) corresponds to a property of \( \bar{P} \) where the relationship between Alice’s and Bob’s outcome is important, but the result of Alice by itself is not; this is the correlation part.

- **Signaling subspace** \( V_{\text{SI}} \):

\( V_{\text{SI}} \) is the component of \( \bar{P} \) that acts on Alice’s side only. Hence, \( \bar{P}_{\text{SI}} = \bar{P}_{\text{corr}} \). We have \( \bar{P}_{\text{SI}} = \alpha_{+} + \bar{Q}_{+} \) and \( \bar{P}_{\text{SI}} = \alpha_{-} + \bar{Q}_{-} \).

**Appendix D. Optimal form of a Bell inequality**

**D.1. Derivation**

Here, we prove formula equation (8). Remember that \( \Pi \) is the projector over the signaling subspace, directly given by \( \Pi = \frac{1}{\tau} \sum_{ij} \bar{Q}_{ijkl} \bar{Q}_{ijkl} \), where the \( \bar{Q}_{ijkl} \) are given in table C.4. We saw in section 3.1 that the mean of \( \langle \bar{P} \rangle = \bar{P}_{\text{corr}} \) is given by \( \langle \bar{P} \rangle = 1_{\text{setup}} \). We continue here with the computation of the variance \( \sigma^2 \):

\[
\sigma^2 = \bar{\beta}^T \Sigma \bar{\beta} = \bar{\beta}_{\text{NOS}}^T \Sigma \bar{\beta}_{\text{NOS}} + \bar{\beta}_{\text{SI}}^T \Sigma \bar{\beta}_{\text{SI}} + 2 \bar{\beta}_{\text{NOS}}^T \Sigma \bar{\beta}_{\text{SI}},
\]

where \( \bar{\beta}_{\text{NOS}} = \bar{\beta}_{\text{NO}} + \bar{\beta}_{\text{NS}} \). With \( \Pi \) the orthogonal projector over \( V_{\text{SI}} \) and \( \Pi = 1 - \Pi \), we have \( \bar{\beta}_{\text{SI}} = \Pi \bar{\beta} \) and \( \bar{\beta}_{\text{NOS}} = \bar{\beta}_{\text{NO}} + \bar{\beta}_{\text{NS}} \). Now, we search the Bell inequality variant with the minimal variance \( \sigma^2 \). This corresponds to finding the minimum \( \bar{\beta}_{\text{SI}} \) of the following function \( f \) over the space \( V_{\text{SI}} \):

\[
f(\bar{\beta}_{\text{SI}}) = \sigma^2 = \bar{\beta}_{\text{NOS}}^T \Sigma \bar{\beta}_{\text{NOS}} + \bar{\beta}_{\text{SI}}^T \Sigma \bar{\beta}_{\text{SI}} + 2 \bar{\beta}_{\text{NOS}}^T \Sigma \bar{\beta}_{\text{SI}}.
\]

As the covariance matrix \( \Sigma \) is positive semidefinite by construction, the minimum is obtained by \( \nabla_{\bar{\beta}_{\text{SI}}} \) null over \( V_{\text{SI}} \). We obtain \( \Pi \Sigma \bar{\beta}_{\text{SI}} + \Pi \Sigma \bar{\beta} = 0 \). Then:

\[
\bar{\beta}_{\text{SI}} = -\Pi (\Sigma \Sigma + \Pi)^{-1} \Pi \Sigma \bar{\beta}.
\]
from which the optimal variant of the inequality can be reconstructed: \( \vec{\beta}^* = \vec{\beta}_{\text{NOS}} + \vec{\beta}_{\text{SI}}^* \), which leads to equation (8). In all our tests, the matrix \((\Pi \Sigma \Pi + \overline{\Pi})\) was invertible; when this is not the case, there are subspaces in \( V_{\text{SI}} \) that do not contribute to the variance, and \((\Pi \Sigma \Pi + \overline{\Pi})^{-1}\) can replaced by the pseudoinverse.

### D.2. Optimality of CHSH for symmetric setups

We prove here that in the case of a \((2, 2, 2)\) setup physically symmetric in the two outputs (such as the setup used in [27] in its noiseless idealization), we have, for any Bell inequality \( \vec{\beta} \) equivalent to CHSH:

\[
\vec{\beta}^T_{\text{NOS}} \Sigma \vec{\beta}_{\text{SI}} = 0. \tag{D.4}
\]

Then, the optimal solution to minimize \( \vec{\beta}_{\text{SI}}^T \Sigma \vec{\beta}_{\text{SI}} \) is to set \( \vec{\beta}_{\text{SI}}^T = 0 \), ie CHSH is the optimal inequality.

Let \( \rho \) be the symmetry which exchanges 0 and 1 on Alice’s and Bob’s sides. As usual, it can be seen as a relabeling of the outputs, ie a linear map \( \vec{\beta}_{\text{NOS}} \overset{\rho}{\rightarrow} \vec{\beta}_{\text{NOS}}; \vec{\beta}_{\text{SI}} \overset{\rho}{\rightarrow} \vec{\beta}_{\text{SI}}^* \). It can also be seen as a transformation of the experimental setup itself: this time, we apply the transformation over the physical setup, transforming the physical state and the measurement operators. This

\[
\begin{array}{cccccccccccc}
\vec{Q} & i & j & k & l & a & b & x & y \\
0000 & + & + & + & + & + & + & + & + \\
1000 & + & + & + & + & + & + & + & + \\
0100 & + & + & + & + & + & + & + & + \\
1100 & + & + & + & + & + & + & + & + \\
0010 & + & + & + & + & + & + & + & + \\
1010 & + & + & + & + & + & + & + & + \\
0110 & + & + & + & + & + & + & + & + \\
1110 & + & + & + & + & + & + & + & + \\
0001 & + & + & + & + & + & + & + & + \\
1001 & + & + & + & + & + & + & + & + \\
0101 & + & + & + & + & + & + & + & + \\
1101 & + & + & + & + & + & + & + & + \\
0011 & + & + & + & + & + & + & + & + \\
1011 & + & + & + & + & + & + & + & + \\
0111 & + & + & + & + & + & + & + & + \\
1111 & + & + & + & + & + & + & + & + \\
\end{array}
\]

Table C4. Coordinates of the orthogonal basis \( \vec{Q}_{ijkl} \) and corresponding subspaces, as detailed in equations (C.2) and (C.3). In this basis, \( \vec{B} = \sum_{ijkl} \alpha_{ijkl} \vec{Q}_{ijkl} \) with \( \alpha_{ijkl} = \frac{1}{16} \sum_{abxy} \beta_i^j \beta_k^l \beta_{\text{abxy}} \). Here ‘+’ corresponds to ‘1’ and ‘−’ corresponds to ‘−1’.

\[
\begin{array}{cccccccccccc}
\vec{Q} & i & j & k & l & a & b & x & y \\
0000 & + & + & + & + & + & + & + & + \\
1000 & + & + & + & + & + & + & + & + \\
0100 & + & + & + & + & + & + & + & + \\
1100 & + & + & + & + & + & + & + & + \\
0010 & + & + & + & + & + & + & + & + \\
1010 & + & + & + & + & + & + & + & + \\
0110 & + & + & + & + & + & + & + & + \\
1110 & + & + & + & + & + & + & + & + \\
0001 & + & + & + & + & + & + & + & + \\
1001 & + & + & + & + & + & + & + & + \\
0101 & + & + & + & + & + & + & + & + \\
1101 & + & + & + & + & + & + & + & + \\
0011 & + & + & + & + & + & + & + & + \\
1011 & + & + & + & + & + & + & + & + \\
0111 & + & + & + & + & + & + & + & + \\
1111 & + & + & + & + & + & + & + & + \\
\end{array}
\]
transforms the covarient matrix $\Sigma \rightarrow \Sigma'$. Thus, we have $\beta_{\text{NOS}}^T \Sigma \beta_{\text{SI}}^T = \beta_{\text{NOS}}^T \Sigma' \beta_{\text{SI}}^T$. Moreover, we can show the following:

(i) For any Bell inequality $\beta$ equivalent to CHSH (i.e. equal over the nosignaling subspace), we have $\beta_{\text{NOS}} = -\beta_{\text{NOS}}$ and $\beta_{\text{SI}} = -\beta_{\text{SI}}$.

**Proof.** We consider the decomposition given in the theorem to decompose $\beta_{\text{NOS}} = \beta_{\text{NO}} + \beta_{\text{Marg}} + \beta_{\text{Corr}}$. As $\beta$ is equivalent to CHSH, we have $\beta_{\text{Marg}} = \beta_{\text{Marg}} = 0$. Section 4 gives that for any party $M$, $\rho$ is Id over $T_M, S_M$ and $-\text{Id}$ over $\phi_M$. Then, considering figure C2, we see that $\beta_{\text{NOS}} = \beta_{\text{NO}} + \beta_{\text{Corr}} = \beta_{\text{NO}} + \beta_{\text{Corr}} = \beta_{\text{NOS}}$ and $\beta_{\text{SI}} = -\beta_{\text{SI}}$. \hfill \square

(ii) For any Bell setup symmetric in the two outputs, we have $\Sigma' = \Sigma$.

**Proof.** No matter what physical formalism is used to describe the Bell setup (classical, quantum, etc), the transformation $\rho$ must have a meaning over the physical setup. The first setup is associated to a covarient matrix $\Sigma$, and the transformed one to $\Sigma'$. If this transformation lets the setup invariant (which is the case in the idealized noise-less setup [27]), we must have $\Sigma = \Sigma'$.

\hfill \square

**Appendix E. Wreath product groups**

Any given setup of a Bell scenario is represented by a vector $P \in V$, which is a representation of a finite group $G$ associated to the scenario. As we will see in the next section, this group is built from an operation over groups, the wreath product $\wr$. Indeed, $G$ is the wreath product of the three groups of permutations of the outcomes, settings and parties: $G = \mathfrak{S}_{\text{outcomes}} \wr \mathfrak{S}_{\text{settings}} \wr \mathfrak{S}_{\text{parties}}$. The vector space $V$ is a representation of this group. More precisely, it is the natural representation of the wreath product of the primitive representation of the $\mathfrak{S}_{\text{outcomes}}$-natural representation of the $\mathfrak{S}_{\text{settings}}$-primitive representation of the $\mathfrak{S}_{\text{parties}}$-primitive representation.

Here, we will briefly introduce the notions of wreath product and primitive/imprimitive representations in the case of permutation groups. Those structures are used in appendix C.

If $\mathfrak{S}_p$ and $\mathfrak{S}_q$ are two permutation groups, their wreath product is a finite group $G = \mathfrak{S}_p \wr \mathfrak{S}_q$. Any element $g \in G$ is defined by:

- an element $\rho \in \mathfrak{S}_q$,
- for each $0 \leq k^* \leq q - 1$, an element $\sigma_k^* \in \mathfrak{S}_p$.

From now, we will focus on the case $q = 3$ and $p = 2$ (generalization are straightforward). Then, $g \equiv (\rho, (\sigma_0^*, \sigma_1^*, \sigma_2^*))$. The internal product in $G$ may be expressed formally. However, here we introduce it by its most convenient interpretation, where elements of $G$ are seen as transformations of a tree. We consider a two level tree, the first level having three nodes (labeled $0^*, 1^*, 2^*$) and each of these nodes having two leaves (labeled 0, 1). Then, any $g \in G$ transforms the tree as follows:

- it permutes the first level with $\rho^*$,
- for each node number $k^* \in \{0^*, 1^*, 2^*\}$, it permutes its leaves according to $\sigma_k^*$.

\footnote{For a usual quantum Bell test, it corresponds to a transformation of the setting state and a transformation of the measurement operators. In this case, the probabilities are given by $P_{\text{class}} = \text{Tr} \left[ (\Pi^{0}_a \otimes \Pi^{0}_b) R(\phi^{0}_{a}, \phi^{0}_{b}) (\rho(\phi^{0}_{a}, \phi^{0}_{b}) \right]$ and $\rho$ is a transformation of $\rho$ and the measurement operators $\Pi^{m}_{M}$ (with $M = A, B$ and $m = a, b$). For the idealized [27], this expression is unchanged by application of $\rho$.}
Then, the product of \( g, g' \in G \) is \( g'' \), the transformation which result in the same tree than the one obtained after successive map of the tree by \( g' \) and \( g \) and the inverse can be defined in the same way. This gives a group structure. A simple example \( g_0 \), with its tree representation, is given in table E1.

### Table E1. Example of tree representation of an element \( g_0 \) of \( S_2 \wr S_3^* \).

| \( g_0 \in S_2 \wr S_3^* \) | Transformation of |
|-----------------------------|------------------|
| 0* 1* 2*                   | 1* 0* 2*         |
| 0 1 0 1 0 1               | 0 1 1 0 1 0     |

Then, the product of \( g, g' \in G \) is \( g'' \), the transformation which result in the same tree than the one obtained after successive map of the tree by \( g' \) and \( g \) and the inverse can be defined in the same way. This gives a group structure. A simple example \( g_0 \), with its tree representation, is given in table E1.

### E.1. Primitive and imprimitive representations

There are two natural ways to create representations of wreath product groups, the primitive and the imprimitive representations. Again, the most convenient is to use the tree representation.

- For the imprimitive representation, we consider that each path from the root of the tree to a leaf is associated to some vector. Such a path can be labeled with two numbers \( j^* \) and \( i \), and is associated to a vector \( e_i \otimes e_{j^*} \). The basis vectors span \( V_{\text{prim}} \cong \mathbb{R}^2 \otimes \mathbb{R}^* \). Then, we apply \( g \) to the tree and obtain a new vector. This gives the action of \( g \) over any basis vector of \( V_{\text{prim}} \). One can easily find that the basis vector \( e_1 \otimes e_{0^*} \) is mapped to \( e_0 \otimes e_{1^*} \) by \( g_0 \).

- For the primitive representation, we consider the eight possible choices of the position of one leaf in each of the three groups of two leaves. Then, such a choice can be labeled with three numbers \( i_0^*, i_1^*, i_2^* \), and is associated to a basis vector \( e_{i_0^*} \otimes e_{i_1^*} \otimes e_{i_2^*} \). The basis vectors span \( V_{\text{prim}} \cong \mathbb{R}^2 \otimes \mathbb{R}^2 \). Then, we apply \( g \) to the tree and obtain a new vector. This gives the action of \( g \) over any basis vector of \( V_{\text{prim}} \). One can easily find that the basis vector \( e_1 \otimes e_0 \otimes e_0 \) is mapped to \( e_0 \otimes e_0 \otimes e_1 \) by \( g_0 \).
Mathematically, an element $(\rho, (\sigma_0^\ast, \sigma_1^\ast, \sigma_2^\ast)) \in S_2 \wr \mathbb{S}_3^*$ acts on the basis as 

$$e_1 \otimes e_0 \otimes e_0 \rightarrow e_{\sigma_0^\ast - 1(1,0)} \otimes e_{\sigma_1^\ast - 1(1,0)} \otimes e_{\sigma_2^\ast - 1(1,0)}.$$ 

These two natural representations are not irreducible.

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