Sets of Marginals and Pearson-Correlation-based CHSH Inequalities for a Two-Qubit System

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Abstract—Quantum mass functions (QMFs), which are tightly related to decoherence functionals, were introduced by Loeliger and Vontobel [IEEE Trans. Inf. Theory, 2017, 2020] as a generalization of probability mass functions toward modeling quantum information processing setups in terms of factor graphs.

Simple quantum mass functions (SQMFs) are a special class of QMFs that do not explicitly model classical random variables. Nevertheless, classical random variables appear implicitly in an SQMF if some marginals of the SQMF satisfy some conditions; variables of the SQMF corresponding to these “emerging” random variables are called classicable variables. Of particular interest are jointly classicable variables.

In this paper we initiate the characterization of the set of marginals given by the collection of jointly classicable variables of a graphical model and compare them with other concepts associated with graphical models like the sets of realizable marginals and the local marginal polytope.

I. INTRODUCTION

Graphical models like factor graphs [1]–[3] have been used to represent various statistical models. In the following, we will call a factor graph consisting only of non-negative real-valued local functions a standard factor graph (S-FG). S-FGs have many applications, in particular in communications and coding theory (see, e.g., [4, 5]) and statistical mechanics (see, e.g., [6]). In these applications, factor graphs frequently represent the factorization of the joint probability mass functions (PMFs) of all the relevant random variables. Quantities of interest can then be obtained by exactly or approximately computing marginals of this joint PMF and suitably processing these marginals.

Factor graphs have also been used to represent quantum-mechanical probabilities [7, 8]. In contrast to S-FGs, these factor graphs consist of complex-valued local functions satisfying some constraints. In the following, we will call such factor graphs quantum-probability factor graphs (Q-FGs). A Q-FG is typically used to represent the factorization of the joint quantum mass function (QMF) as introduced in [7].

In this paper, we first discuss similarities and differences between PMFs and QMFs. Some of the features of QMFs will then motivate the study that is carried out in the rest of this paper.

II. PMFs vs. QMFs

In this section, we highlight some similarities and crucial differences between PMFs and QMFs. First, we consider a classical setup. In particular, we assume that we are interested in a graphical model representing the joint PMF $P_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n)$, where $Y_1,\ldots,Y_n$ are some random variables of interest taking values in some alphabets $Y_1,\ldots,Y_n$ (in a typical application, we might have observed $Y_1 = y_1,\ldots,Y_{n-1} = y_{n-1}$ and would like to estimate $Y_n$ based on these observations.) In most applications, the PMF $P_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n)$ does not have a “nice” factorization in terms of simple factors. However, frequently, with the introduction of suitable auxiliary variables $x_1,\ldots,x_m$ taking values in some alphabets $X_1,\ldots,X_m$, respectively, there is a function $p(x,y)$, where $x := (x_1,\ldots,x_m)$ and $y := (y_1,\ldots,y_n)$, such that

$$p(x,y) \in \mathbb{R}_{\geq 0} \quad \text{(for all } x, y \text{),}$$

$$\sum_{x,y} p(x,y) = 1,$$

$$\sum_x p(x,y) = P_Y(y) \quad \text{(for all } y \text{),}$$

and such that $p(x,y)$ has a “nice” factorization. (For example, in a hidden Markov model, the joint PMF of the observations does not have a “nice” factorization, but the joint PMF of the hidden state process and the observations has a “nice” factorization.) Note that the function $p(x,y)$ can, thanks to its properties, be considered as a joint PMF of some random variables $X_1,\ldots,X_m,Y_1,\ldots,Y_n$.

Second, we consider a quantum-mechanical setup. We assume, again, that we are interested in a graphical model representing the joint PMF $P_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n)$, where $Y_1,\ldots,Y_n$ are some random variables of interest taking values in some alphabets $Y_1,\ldots,Y_n$. Such random variables can, for example, represent the measurements obtained when running some quantum-mechanical experiment, and we might be interested in estimating $Y_n$ based on the observations.

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1 For simplicity, in the following all alphabets will be finite.
where $Y_1 = y_1, \ldots, Y_{n-1} = y_{n-1}$. As in the classical case, the PMF $P_{Y_1, \ldots, Y_n}(y_1, \ldots, y_n)$ usually does not have a “nice” factorization in terms of simple factors. Moreover, standard physical modeling of quantum-mechanical systems shows that introducing a function $p(x, y)$ as defined above does usually not help toward obtaining a function with a “nice” factorization. However, in many quantum-mechanical setups of interest, with the introduction of suitable auxiliary variables $X_1, X_2, \ldots, X_m$ taking values in some alphabets $\mathcal{X}_1, \mathcal{X}_2, \ldots, \mathcal{X}_m$ (with $\mathcal{X}_i = \mathcal{X}$, $i \in \{1, \ldots, m\}$), there is a function $q(x, x', y)$, called quantum mass function (QMF) \([7]\), such that
\[
q(x, x', y) \in \mathbb{C} \quad \text{(for all } x, x', y) \\
\sum_{x, x', y} q(x, x', y) = 1.
\]
and such that $q(x, x', y)$ has a “nice” factorization. The major difference between $p(x, y)$ and $q(x, x', y)$ is that the former takes values in $\mathbb{R}_{\geq 0}$, whereas the latter takes values in $\mathbb{C}$. In particular, $\sum_y q(x, x', y)$ is in general not a PMF over $(x, x')$, thereby showing that $x, x'$ cannot be considered as random variables. (See \([7]\) for more details.)

In \([8]\), the authors discussed an approach to QMFs where $y$ does not appear explicitly anymore, but “emerges” from a QMF. More precisely, they first introduced a simple quantum mass function (SQMF) $q(x, x')$ that satisfies
\[
q(x, x') \in \mathbb{C}_{\geq 0} \quad \text{(for all } x, x') \\
\sum_{x, x'} q(x, x') = 1, \\
q(x, x') \text{ is a PSD kernel in } (x, x').
\]

Afterwards, they defined “classicable” variables.

**Definition 1.** Let $\mathcal{I}$ be a subset of $\{1, \ldots, m\}$ and let $\mathcal{I}^c := \{1, \ldots, m\} \setminus \mathcal{I}$ be its complement. The variables $x_\mathcal{I}$ are called jointly classicable if the function
\[
q(x_\mathcal{I}, x'_\mathcal{I}) := \sum_{x_\mathcal{I} \in \mathcal{I}, x'_\mathcal{I} \in \mathcal{I}^c} q(x, x')
\]
is zero for all $(x_\mathcal{I}, x'_\mathcal{I})$ satisfying $x_\mathcal{I} \neq x'_\mathcal{I}$.\(^3\)

Note that if $x_\mathcal{I}$ are jointly classicable, then one can define the function $p(x_\mathcal{I}) := q(x_\mathcal{I}, x_\mathcal{I})$, for which it is straightforward, thanks to the properties of SQMFs, to show that it is a PMF. It is in this sense that random variables $y_1, \ldots, y_n$ that were omitted when going from QMFs to SQMFs can “emerge” again.\(^4\)

\(^3\)It would be more precise to call this function $q_\mathcal{I}$. However, for conciseness, we drop the index $\mathcal{I}$ as it can be inferred from the arguments.

\(^4\)A similar observation is at the origin of the so-called “single-framework” rule in the consistent-histories approach to quantum mechanics.\(^5\)

**Example 3.** Consider the Q-FG $N_3$ in Fig.\(\text{4}\) whose global function is an SQMF. In that Q-FG, the matrix $\rho$ represents a PSD matrix and the matrices $U_1, U_2$ are unitary matrices. One can show that for all choices of $\rho$, $U_1$, and $U_2$, the collection $K$ can be chosen to contain the sets $\{1, 2\}$, $\{1, 4\}$, $\{2, 3\}$, and $\{3, 4\}$.

Interestingly enough, the collection of functions $\{p(x_\mathcal{I})\}_{\mathcal{I} \in K}$ is usually such that there is no PMF $p(x)$ such that for every $\mathcal{I} \in K$, the function $p(x_\mathcal{I})$ can be obtained as a marginal of $p(x)$.\(^5\) In general, we can only guarantee that for two sets $\mathcal{I}_1, \mathcal{I}_2 \in K$ the following consistency constraint holds:
\[
\sum_{x_\mathcal{I}_1 \cap \mathcal{I}_2} p(x_\mathcal{I}_1) = \sum_{x_\mathcal{I}_2 \cap \mathcal{I}_1} p(x_\mathcal{I}_2) \quad \text{(for all } x_\mathcal{I}_1 \cap \mathcal{I}_2).\]

Let us comment on these special properties of $\{p(x_\mathcal{I})\}_{\mathcal{I} \in K}$:

- It turns out that these special properties of $\{p(x_\mathcal{I})\}_{\mathcal{I} \in K}$ are at the heart of quantum mechanical phenomena like Hardy’s paradox \([12]\) and the Frauchiger–Renner paradox \([13]\). In fact, the Q-FG $N_3$ in Fig.\(\text{4}\) can be used to analyze Hardy’s paradox. On the side, note that $N_4$ also captures the essence of Bell’s game \([13]\).

- Interestingly, these special properties of $\{p(x_\mathcal{I})\}_{\mathcal{I} \in K}$ are very similar to the properties of the beliefs in the local marginal polytope of an S-FG (see, e.g., \([15]\))\(^6\).

The above observations motivate the systematic study of the collection $\{p(x_\mathcal{I})\}_{\mathcal{I} \in K}$ for a given SQMF. Indeed, one key contribution of this paper is to study this collection for the Q-FG $N_4$ in Fig.\(\text{4}\) and compare this collection with other objects that can be associated with this Q-FG.

### III. Contributions

To better understand classicable variables’ marginals, we define the set $\mathcal{M}(N_4)$, which is the set of the marginals created by the classicable variables in the two-qubit system $N_4$, as shown in Fig.\(\text{4}\). One of our paper’s main topics is to fully characterize $\mathcal{M}(N_4)$. For comparison, we introduce $\mathcal{LM}(\mathcal{K})$ (the local marginal polytope of the S-FG chain $N_3$ in Fig.\(\text{1}\)), $\mathcal{M}(N_1)$ (the set of realizable marginals of $N_1$), $\mathcal{M}(N_2)$ (the set of realizable marginals of the Markov chain $N_2$ in Fig.\(\text{2}\)), and $\mathcal{M}(N_3)$ (the set of realizable marginals of $N_3$ in Fig.\(\text{3}\)). We have the following results.

- We prove the Venn diagram in Fig.\(\text{6}\) by showing that each part in the diagram is non-empty. We can see that $\mathcal{M}(N_3)$ and $\mathcal{M}(N_4)$ are strict subsets of $\mathcal{LM}(\mathcal{K})$; both $\mathcal{M}(N_1)$ and $\mathcal{M}(N_2)$ have marginals that are not in $\mathcal{LM}(\mathcal{K})$.

\(^5\)For a discussion of the latter in terms of SQMFs, see \([8]\).

\(^6\)Local marginal polytopes are of relevance, for example, when characterizing locally operating message-passing iterative algorithms like the sum-product algorithm \([16]\).
quantities of interest in quantum information processing. In particular, given that factor graphs have been proven very useful in classical information processing, but can also be used for doing quantum information processing, they allow one to understand and appreciate the similarities and the differences between classical and quantum information processing.

The rest of this paper is structured as follows. Section IV reviews some basics of S-FGs. In particular, Section IV.A proves the PCC-based CHSH inequality by the classicable variables in maximum quantum violation of the PCC-based CHSH inequality. Many details are left out due to space constraints; a more detailed discussion is given in [20].

A. Basic Notations and Definitions

The sets $\mathbb{R}$, $\mathbb{R}_{\geq 0}$, $\mathbb{R}_{> 0}$, and $\mathbb{C}$ denote the field of real numbers, the set of nonnegative real numbers, the set of positive real numbers, and the field of complex numbers, respectively. An overline denotes complex conjugation. For any statement $S$, by the Iverson’s convention, the function $[S]$ is defined to be $[S] := 1$ if $S$ is true and $[S] := 0$ otherwise.

IV. STANDARD NORMAL FACTOR GRAPHS (S-NFGs)

In this section, we review some basic concepts and properties of an S-NFG. The word “normal” refers to the fact that variables are arguments of only one or two local functions. We use an example to introduce the fundamental concepts of an S-NFG first.

Example 4. [17] Consider the multivariate function

$$g_{N_4}(x_1, \ldots, x_4) := f_{1,2}(x_1, x_2) \cdot f_{1,4}(x_1, x_4) \cdot f_{3,2}(x_3, x_2) \cdot f_{3,4}(x_3, x_4),$$

where $g_{N_4}$, the so-called global function, is defined to be the product of the so-called local functions $f_{1,2}$, $f_{1,4}$, $f_{3,2}$ and $f_{3,4}$. We can visualize the factorization of $g$ with the help of the S-FG $N_1$ in Fig. 7. Note that the S-FG $N_4$ consists of four function nodes $f_{1,2}$, $f_{1,4}$, $f_{3,2}$ and $f_{3,4}$.

For an S-NFG, a half edge is an edge incident on one function node only and a full edge is an edge incident on two function nodes.

**Definition 5.** The S-NFG $N(\mathcal{F}(N), \mathcal{E}(N), \mathcal{X}(N))$ consists of:

1. The graph $(\mathcal{F}(N), \mathcal{E}(N))$ with vertex set $\mathcal{F}(N)$ and edge set $\mathcal{E}(N)$, where $\mathcal{E}(N)$ consists of all full edges and half edges in $N$. With some slight abuse of notation, an $f \in \mathcal{F}(N)$ will denote a function node and the corresponding local function.

2. The alphabet $\mathcal{X}(N)$ := $\prod_{e \in \mathcal{E}(N)} \mathcal{X}_e$, where $\mathcal{X}_e$ is the alphabet associated with the edge $e \in \mathcal{E}(N)$.

**Definition 6.** Given $N(\mathcal{F}(N), \mathcal{E}(N), \mathcal{X}(N))$, we make the following definitions:

1. For every function node $f \in \mathcal{F}(N)$, the set $\partial f$ is the set of edges incident on $f$.

2. An assignment $x := (x_e)_{e \in \mathcal{E}(N)} \in \mathcal{X}(N)$ is called a configuration of the S-NFG.
3) The local function \( f \) associated with function node \( f \in \mathcal{F}(N) \) denotes an arbitrary mapping \( f : \prod_{e \in \partial f} x_e \rightarrow \mathbb{R}_{\geq 0} \).

4) The global function is \( g_N(x) := \prod_{f \in \mathcal{F}(N)} f(x_{\partial f}) \).

5) The partition function is \( Z(N) := \sum_x g_N(x) \), where \( \sum_x \) denotes \( \sum_{x \in X(N)} \).

6) The PMF induced on \( N \) is \( p_N(x) := g_N(x)/Z(N) \).

7) Let \( \mathcal{I} \) be a subset of \( \mathcal{E}(N) \) and let \( \mathcal{I}^c := \mathcal{E}(N) \setminus \mathcal{I} \) be its complement. The marginal \( p_{N}\mathcal{I}(x_{\mathcal{I}}) \) is defined to be \( p_{N}\mathcal{I}(x_{\mathcal{I}}) := \sum_{x_{\mathcal{I}^c}} p_N(x) \).

**Definition 7.** Considering \( N \in \{N_1, N_2, N_3\} \), we make the following definitions:

1) The alphabet \( x_e \) is \( x_e := \{0, 1\} \) for all \( e \in \mathcal{E}(N) \).

2) The set \( K \) is \( K := \{(1, 2), (1, 4), (2, 3), (3, 4)\} \).

3) For \( \{i, j\} \in K \), the marginal \( \pi_{i,j} \) is defined to be a \( |x_e| \)-by-\( |x_e| \) matrix with the entry \( \pi_{i,j}(x_i, x_j) \) and the marginal \( \pi_{i} \) is defined to be a \( |x_e| \)-by-\( |x_e| \) diagonal matrix with \( \pi_{i}(x_i) \) being the \( i \)-th diagonal term.

4) The collection of matrices \( \beta \) is defined to be \( \beta := (\beta_{i,j})_{\{i,j\} \in K} \). In particular, the matrix \( \beta_{i,j} \) is defined to be a \( |x_e| \)-by-\( |x_e| \) matrix with entry \( \beta_{i,j}(x_i, x_j) \in \mathbb{R}_{\geq 0} \) and the matrix \( \beta \) is defined to be a \( |x_e| \)-by-\( |x_e| \) diagonal matrix with \( \beta_{i}(x_i) \in \mathbb{R}_{\geq 0} \) being the \( i \)-th diagonal term.

5) The set of realizable marginals of \( N \) is defined to be

\[ \mathcal{M}(N) := \left\{ \beta \mid \text{there exists an } \mathcal{F}(N) \text{ such that } \beta_{i,j} = \pi_{i,j}, \beta_{i} = \pi_{i}, \{i,j\} \in K \right\} . \]

6) The set \( \mathcal{LM}(K) \) is defined to be

\[ \mathcal{LM}(K) := \left\{ \beta \mid \begin{array}{l}
0 \leq \beta_{i,j}(x_i, x_j) \leq 1, \forall x_i, x_j, i, j \\
\sum_{x_j} \beta_{i,j}(x_i, x_j) = \beta_i(x_i), \forall x_i, i \\
\sum_{x_i} \beta_{i,j}(x_i, x_j) = \beta_j(x_j), \forall x_j, j \\
\sum_{x_i} \beta_i(x_i) = 1, \forall i
\end{array} \right\} . \]

The set \( \mathcal{LM}(K) \) is essentially the local marginal polytope of the S-NFG \( N_1 \) in Fig. 7. The definition of the local marginal polytope for an S-NFG is given in [13 Section 4.1.1].

7) For each \( \beta \in \mathcal{LM}(K) \) and \( \{i,j\} \in K \), each marginal \( \beta_{i,j} \) can be used to represent the PMF for two random variables \( Y_1, Y_2 \in \mathcal{X}_e \) by setting the probability \( \Pr(Y_1 = x_1, Y_2 = x_2) = \beta_{i,j}(x_1, x_2) \), \( x_i, x_j \in \mathcal{X}_e \). The functions \( \text{Cov}(Y_1, Y_2), \text{Var}(Y_1), \text{Var}(Y_2) \) are defined to be the covariance of \( Y_1 \) and \( Y_2 \), and the variances of \( Y_1 \) and \( Y_2 \), respectively. When \( \text{Var}(Y_1), \text{Var}(Y_2) > 0 \), the PCC of \( Y_1 \) and \( Y_2 \) is defined to be \( \text{Corr}(\beta_{i,j}) := \text{Cov}(Y_1, Y_2)/\sqrt{\text{Var}(Y_1) \cdot \text{Var}(Y_2)} \).

When there is no ambiguity, we use short-hands \( \langle i,j \rangle \), \( \langle \cdot \rangle \), \( \{i,j\} \), \( \langle \cdot \rangle_{\{i,j\} \in K} \), \( \langle \cdot \rangle_{\{i \in E(N_1) \}} \), \( \sum_{x \in \mathcal{X}_e} \), and \( \{\cdot\}_{x \in \mathcal{X}_e} \) respectively.

Because \( \mathcal{LM}(K) \) is a convex set by definition, Carathéodory’s theorem [27 Proposition B.6] states that each element in \( \mathcal{LM}(K) \) can be written as a convex combination of the vertices in \( \mathcal{LM}(K) \). The full list of the vertices in \( \mathcal{LM}(K) \) is given in [20 Appendix A].

**Proposition 8.** For \( \{i,j\} \in K \) and \( 0 < \beta_i(0), \beta_j(0) < 1 \), the PCC \( \text{Corr}(\beta_{i,j}) \) satisfies

\[ \text{Corr}(\beta_{i,j}) = \frac{\det(\beta_{i,j})}{\sqrt{\det(\beta_i) \cdot \det(\beta_j)}}. \]

The requirement \( 0 < \beta_i(0), \beta_j(0) < 1 \) ensures that \( \det(\beta_i), \det(\beta_j) > 0 \), and thus \( \text{Corr}(\beta_{i,j}) \) is well-defined.

**Proof.** See the proof of [20 Corollary 9]. ■

**Definition 9.** Suppose that \( \beta \in \mathcal{LM}(K) \) and \( 0 < \beta_i(0) < 1, i \in \mathcal{E}(N_1) \), we define

\[ \text{CorrCHSH}(\beta) := \text{Corr}(\beta_{1,2}) + \text{Corr}(\beta_{1,4}) + \text{Corr}(\beta_{3,2}) - \text{Corr}(\beta_{3,4}). \]

**A. Properties for \( N_3 \)**

In this subsection, we prove inequalities with respect to \( \text{CorrCHSH}(\beta) \) for \( \beta \in \mathcal{LM}(N_3) \). These inequalities genuinely are (nonlinear) Bell inequalities [22] in the usual sense. By definition, it holds that

\[ \mathcal{M}(N_1) \subseteq \mathcal{M}(N_3), \quad \mathcal{M}(N_2) \subseteq \mathcal{M}(N_3), \]

so any inequality that holds for all \( \beta \in \mathcal{M}(N_3) \) also holds for all \( \beta \in \mathcal{M}(N_1) \cup \mathcal{M}(N_2) \).

**Theorem 10.** For any \( \beta \in \mathcal{M}(N_3) \) such that \( 0 < \beta_i(0) < 1 \) for all \( i \in \mathcal{E}(N_1) \), we have

\[ |\text{CorrCHSH}(\beta)| < 2\sqrt{2}. \]

**Proof.** We prove it by contradiction. On the one hand, the set \( \mathcal{M}(N_3) \) consists of marginals for binary random variables only. On the other hand, to have \( \text{CorrCHSH}(\beta) = 2\sqrt{2} \) for some \( \beta \in \mathcal{M}(N_3) \), the PMF realizing \( \beta \) needs to be the joint PMF for random variables with alphabet size greater than two. For details, see the proof in [20 Appendix C]. ■

The main idea in the proof of Theorem 10 can be used to verify whether a proposed bound for a function with binary random variables is achievable. It is different from the idea in the proof of the upcoming Theorem 11.

**Theorem 11.** For any \( \beta \in \mathcal{LM}(N_3) \) such that \( 0 < \beta_i(0) < 1 \) for all \( i \in \mathcal{E}(N_1) \), we have \( |\text{CorrCHSH}(\beta)| \leq 5/2 \).

**Proof.** We give a proof sketch here. For details, see the proof in [20 Appendix E].

- Consider a subset of \( \mathcal{LM}(K) \) such that in this subset, \( 0 < \beta_i(0) < 1 \) for \( i \in \mathcal{E}(N_1) \), and the elements in \( \beta \) satisfy the original linear CHSH inequality. Denote this set as \( \mathcal{LM}_{\text{CHSH}}(K) \). We have \( \mathcal{M}(N_3) \subseteq \mathcal{LM}_{\text{CHSH}}(K) \).
- Find a \( \beta^* \in \mathcal{LM}(N_3) \) such that \( \text{CorrCHSH}(\beta^*) = 5/2 \).
- We formulate an optimization problem where \( \text{CorrCHSH}(\beta) \) is maximized over \( \beta \in \mathcal{LM}_{\text{CHSH}}(K) \) such that \( \beta \) has a similar structure as \( \beta^* \), e.g., having the same number of zero entries in \( \beta_{i,j} \). Note that this optimization problem has linear constraints only, which helps determine the optimal solution. We prove \( \text{CorrCHSH}(\beta) \leq 5/2 \) in this case.
The matrices $\tilde{q}$ with $\tilde{q}$ on the jointly classicable variables $x$ can be proven directly by Definition 1.

Theorem 11 proves the conjecture stated in 19. The key idea of the proof is that we consider $L_{\mathcal{M}_{\text{CHSH}}}(K)$ for $\beta \in M(N_1)$ instead of $\beta$. Suppose that we want to prove CorrCHSH($\beta$) $\leq 5/2$ for $\beta \in M(N_1)$ directly. Because $M(N_1)$ is a convex set, for any $\beta \in M(N_1)$, the marginal $\beta_{i,j}$ can be written as a convex combination of some joint PMF for $x_1, \ldots, x_4$, i.e., $\{p_{i,j}(x)\}_{x}$, which makes the expression of CorrCHSH($\beta$) non-trivial. By considering a superset of $M(N_1)$, i.e., $L_{\mathcal{M}_{\text{CHSH}}}(K)$, we can simplify CorrCHSH($\beta$). We suspect that this idea can be generalized in the proof of non-linear Bell inequalities.

**B. Markov Chain in Fig. 2**

In this subsection, we consider the Markov chain $N_2$ in Fig. 2.

**Theorem 12.** For the Markov chain $N_2$ in Fig. 2 we have

$$\text{Corr}(\beta_{3,4}) = \text{Corr}(\beta_{3,2}) \cdot \text{Corr}(\beta_{1,2}) \cdot \text{Corr}(\beta_{1,4}).$$

**Proof.** See [20, Corollary 19].

**Corollary 13.** For the Markov chain $N_2$ in Fig. 2 it holds that $|\text{Corr}(\beta_{3,4})| \leq |\text{Corr}(\beta_{1,2})| \leq 1$.

**Proof.** It can be proven using Theorem 12 and $|\text{Corr}(\beta_{i,j})| \leq 1$ for $\{i, j\} \in K$.

We prove another variation of the PCC-based CHSH inequality for $N_2$.

**Corollary 14.** For the Markov chain $N_2$ in Fig. 2 we have

$$|\text{Corr}(\beta_{1,2}) + \text{Corr}(\beta_{2,4}) + \text{Corr}(\beta_{1,3}) - \text{Corr}(\beta_{3,4})| \leq 2.$$

**Proof.** See the proof of [20, Proposition 20].

**V. Quantum-Probability Normal Factor Graphs (Q-NFGs)**

This section considers a quantum system represented by the Q-NFG $N_2$ in Fig. 3. Such Q-NFGs have been discussed thoroughly in 17, 18. Note that in Fig. 4 and Fig. 5 the row index of a matrix is marked by a black dot. The details of $N_4$ are shown in [20, Definition 21].

**Proposition 15.** For any $\{i, j\} \in K$, the variables $\tilde{x}_i$ and $\tilde{x}_j$ are jointly classicable, which implies that the marginals $q_{i,j}(\tilde{x}_i, \tilde{x}_j)$ and $q_i(\tilde{x}_i)$ are non-negative real numbers for any $\tilde{x}_i, \tilde{x}_j \in \mathbb{R}^2$.

**Proof.** It can be proven directly by Definition 1.

Then we define the set of realizable marginals of $N_4$ based on the jointly classicable variables $\tilde{x}_i$ and $\tilde{x}_j$ for all $\{i, j\} \in K$.

**Definition 16.** With $\tilde{0} := (0, 0)$, $\tilde{1} := (1, 1)$, and $\{i, j\} \in K$, the matrices $q_{i,j}$ and $q_{i}$ induced by $q_{i,j}$ are defined to be

$$q_{i,j} := \begin{pmatrix} q_{i,j}(\tilde{0}, \tilde{0}) & q_{i,j}(\tilde{0}, \tilde{1}) \\ q_{i,j}(\tilde{1}, \tilde{0}) & q_{i,j}(\tilde{1}, \tilde{1}) \end{pmatrix}, \quad q_{i} := \begin{pmatrix} q_i(\tilde{0}) & 0 \\ 0 & q_i(\tilde{1}) \end{pmatrix}.$$
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