Factorization of Quantum Density Matrices According to Bayesian and Markov Networks

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Abstract

We show that any quantum density matrix can be represented by a Bayesian network (a directed acyclic graph), and also by a Markov network (an undirected graph). We show that any Bayesian or Markov net that represents a density matrix, is logically equivalent to a set of conditional independencies (symmetries) satisfied by the density matrix. We show that the d-separation theorems of classical Bayesian and Markov networks generalize in a simple and natural way to quantum physics. The quantum d-separation theorems are shown to be closely connected to quantum entanglement. We show that the graphical rules for d-separation can be used to detect pairs of nodes (or of node sets) in a graph that are unentangled. CMI entanglement (a.k.a. squashed entanglement), a measure of entanglement originally discovered by analyzing Bayesian networks, is an important part of the theory of this paper.
1 Introduction

A Bayesian network is a directed graph; that is, a set of nodes with arrows connecting some pairs of these nodes. Each node is assigned a transition matrix. For a classical Bayesian net, each transition matrix is real, and the product the transition matrices for all the nodes gives a joint probability distribution for the states of all the nodes. For a quantum Bayesian net, each transition matrix is complex, and the product of the transition matrices gives a joint probability amplitude instead.

A Markov network is an undirected graph; that is, a set of nodes with undirected links connecting some pairs of these nodes. Each super-clique (maximal fully-connected subgraph) of the graph is assigned an affinity. For a classical Markov net, each affinity is real, and their product gives a joint probability distribution for the states of all the nodes. For a quantum Markov net, each affinity is complex, and their product gives a joint probability amplitude instead.

Bayesian and Markov networks will be defined more precisely later on in this paper.

The literature on classical Bayesian nets is vast. Some textbooks that were invaluable in writing this paper are Refs.[1],[2]. Classical Bayesian nets were invented by geneticist Sewall Wright[3] in the early 1930’s. The theory of Bayesian nets was extended substantially by Judea Pearl[4][5][6] and collaborators in the late 1980’s. They gave us the theory that culminates in the d-separation rules. See Scheines[7] for a more complete review of the history of d-separation. Nowadays, classical Bayesian nets are used widely in Data mining, AI, etc.

There exist only a small number of papers on quantum Bayesian nets. The first paper[8] on the subject appears to be mine. Since then, I have written several papers applying quantum Bayesian nets to quantum information theory[9] and quantum computing[10]. I have also written a Mac application called Quantum Fog[11] (freeware but patented) that implements the ideas behind quantum Bayesian networks. Laskey has also written some papers[12] about quantum Bayesian nets.

It’s known that any probability distribution can be represented by a Bayesian net, and also by a Markov net. It’s known that any Bayesian or Markov net that represents a probability distribution, is logically equivalent to a set of conditional independencies satisfied by the probability distribution.

In this paper, we show that the last paragraph is true if we replace probability distribution by density matrix.

We also show that the d-separation theorems of classical Bayesian and Markov networks generalize in a simple and natural way to quantum physics. The quantum d-separation theorems are shown to be closely connected to quantum entanglement. We show that the graphical rules for d-separation can be used to detect pairs of nodes (or of node sets) in a graph that are unentangled. CMI entanglement (a.k.a. squashed entanglement)[13], a measure of entanglement originally discovered by analyzing Bayesian networks, is an important part of the theory of this paper.
This paper is fairly self-contained; readers previously acquainted with quantum physics but not with classical Bayesian nets should have no trouble following this paper. Results about classical Bayesian nets are derived in parallel with those about their quantum brethren. The paper has pretensions of being pedagogical.

2 Notation and Other Preliminaries

In this section, we define some notation, and review various prerequisite ideas that will be used in the rest of the paper.

2.1 General Notation

As usual, \(\mathbb{Z}, \mathbb{R}, \mathbb{C}\) will denote the integers, real numbers, and complex numbers, respectively. Let \(\text{Bool} = \{0,1\}\), \(0 = \text{false}\) and \(1 = \text{true}\). For \(a, b \in \mathbb{Z}\) such that \(a \leq b\), let \(\mathbb{Z}_{a,b} = \{a, a+1, \ldots, b\}\).

For any set \(J\), let \(|J|\) denote the number of elements in \(J\).

For any set \(J\), its power-set is defined as \(\{J' : J' \subset J\}\). This set includes the empty set \(\emptyset\) and the full set \(J\). The power-set of \(J\) is often denoted by \(2^J\) because \(|2^J| = 2^{|J|}|\).

Let \(\delta^x_y = \delta(x, y)\) denote the Kronecker delta function; it equals 1 if \(x = y\) and 0 if \(x \neq y\).

For any matrix \(M \in \mathbb{C}^{p \times q}\), \(M^*\) will denote its complex conjugate, \(M^T\) its transpose, and \(M^\dagger = M^*^T\) its Hermitian conjugate. Let \(\text{diag}(x_1, x_2, \ldots, x_r)\) denote a diagonal matrix with diagonal entries \(x_1, x_2, \ldots, x_r\).

For any \(z \in \mathbb{C}\), \(\text{phase}(z)\) will denote its phase. If \(r, \theta \in \mathbb{R}\), \(\text{phase}(re^{i\theta}) = \theta + 2\pi \mathbb{Z}\).

For any expression \(f(x)\), we will sometimes abbreviate

\[
\sum_x f(x) = \frac{f(x)}{\sum_x \text{numerator}}. \tag{1}
\]

The abbreviation with the word “numerator” is especially helpful when \(f(x)\) is a long expression, and we want to write it only once instead of twice.

For \(f_1, f_1 \in \mathbb{C}\), let

\[
\begin{bmatrix} f_1 \\ f_2 \end{bmatrix}^\times = f_1 \times f_2. \tag{2}
\]

This notation saves horizontal space: it allows us to indicate the product of two numbers with the numbers written in a column instead of a row.

Given expressions A,B,X,Y, we will often say things like “A (ditto, X) is B (ditto, Y)”; by this, we will mean that “A is B” and “X is Y”.

3
2.2 Classical Probability Theory
and Quantum Physics Preliminaries

Random variables will be denoted by underlined letters; e.g., \( \underline{a} \). The set of values (states) that \( \underline{a} \) can assume will be denoted by \( St_{\underline{a}} \). Let \( N_{\underline{a}} = |St_{\underline{a}}| \). The probability that \( \underline{a} = a \) will be denoted by \( P(\underline{a} = a) \) or \( P_{\underline{a}}(a) \), or simply by \( P(a) \) if the latter will not lead to confusion in the context it is being used. We will use \( pd(St_{\underline{a}}) \) to denote the set of all probability distributions with domain \( St_{\underline{a}} \).

In this paper, we consider networks with \( N \) nodes. Each node is labelled by a random variable \( \underline{x}_j \), where \( j \in Z_{1,N} \). For any \( J \subset Z_{1,N} \), the ordered set of random variables \( \underline{x}_j \) for \( j \in J \) (ordered so that the integer indices \( j \) increase from left to right) will be denoted by \( (\underline{x})_J \) or \( \underline{x}_J \). For example, \( (\underline{x})_{\{2,4\}} = (x_2,x_4) \) or \( x_{2,4} \). We will often call the values that \( \underline{x} \) can assume \( \underline{x}_J \) or \( x_J \). For example, \( (\underline{x})_{\{2,4\}} = x_{2,4} = (x_2,x_4) \). We will often abbreviate \( \underline{x} \) or \( x \) for \( \underline{x}_{Z_{1,N}} \) or \( x_{Z_{1,N}} \) by just \( \underline{x} \) or \( x \). We will often call the values that \( \underline{x} \) can assume \( x \).

In this paper, we will often divide by probabilities without specifying that they should be non-zero. Most of the time, this cavalier attitude will not get us into trouble. That’s because one can always replace all vanishing probabilities by a positive infinitesimal \( \epsilon \). Our results can then be expressed as a power series in \( \epsilon \). As long as our inferences depend only on terms that are zeroth order in \( \epsilon \), our inferences will be well-defined and unique as \( \epsilon \) tends to 0. There are, however, situations when dividing by a probability can be fatal. Such situations ultimately boil down to trying to infer something from terms that are first order in \( \epsilon \); for example, when we erroneously conclude that \( A\epsilon = 0 \) implies \( A = 0 \). In the future, we will divide by probabilities without assuming that they should be non-zero, except in those cases when doing so is being used to infer something that becomes false when \( \epsilon \to 0 \).

In quantum physics, \( \underline{a} \) has a fixed, orthonormal basis \( \{|a\} : a \in St_{\underline{a}} \} \) associated with it. The vector space spanned by this basis will be denoted by \( \mathcal{H}_{\underline{a}} \). In quantum physics, instead of probabilities \( P(\underline{a} = a) \), we use “probability amplitudes” (or just “amplitudes” for short) \( A(\underline{a} = a) \) (also denoted by \( A_{\underline{a}}(a) \) or \( A(a) \)). Whereas \( P \geq 0 \) and \( \sum_a P(a) = 1 \), \( \sum_a |A(a)|^2 = 1 \). Besides probability amplitudes, we also use density matrices. A density matrix \( \rho_{\underline{a}} \) is a Hermitian, non-negative, unit trace operator acting on \( \mathcal{H}_{\underline{a}} \). We will use \( \text{dm}(\mathcal{H}_{\underline{a}}) \) to denote the set of all density matrices acting on \( \mathcal{H}_{\underline{a}} \).

If \( \rho_{\underline{a}} \in \text{dm}(\mathcal{H}_{\underline{a}}) \), \( \rho_{\underline{a}} \in \text{dm}(\mathcal{H}_{\underline{a}}) \), and \( \rho_{\underline{a}} = \text{tr}_{\underline{a}}(\rho_{\underline{a}}) \), we will say that \( \rho_{\underline{a}} \) is a partial trace of \( \rho_{\underline{2}} \), and \( \rho_{\underline{2}} \) is a traced dm-extension of \( \rho_{\underline{2}} \). Given a density matrix \( \rho_{\underline{a}} = x_{\underline{a}} \), its partial traces will be denoted by omitting its subscripts for the random variables that have been traced over. For example,

\[^1\text{We will use random variables in both classical and quantum physics. Normally, random variables are defined only in classical physics, where they are defined to be functions from an outcome space to a range of values. For technical simplicity, here we define a random variable \( \underline{a} \) in both classical and quantum physics, to be merely the label of a node in a graph, or an n-tuple \( \underline{x}_{\mathcal{K}} \) of such labels.}\]
\[ \rho_{x_2} = tr_{x_1,x_3} \rho_{x_1,x_2,x_3}. \]

We will sometimes abbreviate \(|a\rangle\langle a|\) by \(\text{proj}(|a\rangle)\). This abbreviation is especially convenient when the label \(a\) is a long expression, for then we only have to write \(a\) once instead of twice.

### 2.3 Graph Theory Preliminaries

Next, we review some basic definitions from Graph Theory.

A **graph** \(G\) is pair \((V,E)\), where \(V\) is a set of **nodes** (vertices), and \(E\) is a set of **connections** (edges) between some pairs of these nodes. (No self-connections allowed). A **subgraph** \(G' = (V',E')\) of a graph \(G = (V,E)\) is a graph such that \(V' \subset V\), and \(E'\) is defined as the subset of \(E\) that survives after we erase from \(E\) all edges that mention a node in \(V - V'\).

We will abbreviate **Directed Acyclic Graph** by DAG. A DAG is a graph with arrows as its edges, and without any cycles. A **cycle** is a finite sequence of arrows that one can follow, in the direction of the arrows, and come back to where one started. The set of all possible DAGs with node labels \(x\) will be denoted by \(\text{DAG}(x)\).

We will abbreviate **Undirected Graph** by UG. An UG is a graph with (undirected) links as its edges. The set of all possible UGs with node labels \(x\) will be denoted by \(\text{UG}(x)\).

One can also define hybrid graphs that contain both arrows and undirected links\(^2\), but we won’t consider them in this paper.

Consider a DAG whose nodes are labelled by \(x\). Any node \(x_j\) has parent nodes (those with arrows pointing from them to \(x_j\)) and **children nodes** (those with arrows pointing from \(x_j\) to them). \(\text{pa}(j), \text{ch}(j) \subset Z_{1,N}\) are defined as the sets of integer indices of the **parent and children nodes** of \(x_j\). For example, in Fig.1(a), \(\text{pa}(4) = \{2, 3\}\) and \(\text{ch}(1) = \{2, 3\}\). \(\text{an}(j), \text{de}(j) \subset Z_{1,N}\) are defined as the sets of integer indices of the **ancestor and descendant nodes** of \(x_j\). That is, \(\text{an}(j) = \text{pa}(j) \cup \text{pa}^2(j) \cup \text{pa}^3(j) \cup \ldots\). By this we mean that \(\text{an}(j)\) is obtained by taking the union of the integer indices of the parents of \(x_j\), and of the parents of the parents of \(x_j\), and so on. Likewise, \(\text{de}(j) = \text{ch}(j) \cup \text{ch}^2(j) \cup \text{ch}^3(j) \cup \ldots\). The set of integer indices of the **non-descendants** of \(x_j\) will be denoted by \(\text{de}(j) = Z_{1,N} - \text{de}(j) - \{j\}\). The set of integer indices of the **non-ancestors** of \(x_j\) will be denoted by \(\text{an}(j) = Z_{1,N} - \text{an}(j) - \{j\}\). Let \(\overline{s}(j) = s(j) \cup \{j\}\) for \(s \in \{\text{pa}, \text{ch}, \text{an}, \text{de}, \text{~de}, \text{~an}\}\). In other words, we will use an overline over a set \(s(j)\) that does not include \(j\) to denote the “closure” set obtained by adding \(j\) to \(s(j)\).

Next consider an UG whose nodes are labelled by \(x\). Any node \(x_j\) has **neighbor nodes** (those with links between \(x_j\) and them). \(\text{ne}(j)\) is defined as the set of integer indices of the neighbor nodes of \(x_j\). For example, in Fig.1(b), \(\text{ne}(2) = \{1, 4\}\). We will also use \(\overline{\text{ne}}(j) = \text{ne}(j) \cup \{j\}\).
For either a DAG or an UG, a path from node $x$ to node $y$ is a finite sequence of nodes, starting with $x$ and ending with $y$, such that adjacent nodes in the sequence are connected. Note that for a DAG, the arrows in a path need not all be oriented in the same sense. If they are, we call the path a directed path.

In a DAG, a path from $x$ to $y$ can have 3 (mutually exclusive and exhaustive) types of nodes. A serial node $a$ equals one of the endpoints ($x$ and $y$), or else, it is connected to its path neighbors in this manner:

\[ \rightarrow (a) \rightarrow \] (3)

or this

\[ \leftarrow (a) \leftarrow \] (4)

manner. A divergence node $a$ is connected to its path neighbors in this manner:

\[ \leftarrow (a) \rightarrow \] (5)

manner. A convergence (a.k.a. collider) node $a$ is connected to its path neighbors in this manner:

\[ \rightarrow (a) \leftarrow \] (6)

A DAG (ditto, an UG) is fully connected if it is impossible to add any more legal arrows (ditto, links) to it. A fully connected subgraph (of either a DAG or an UG) is called a clique. A clique for which there is no larger clique that contains it, is called a super-clique. For any graph $G$, we define super-cliques ($G$) (a subset of $2^{Z_1,N}$) to be the set of the super-cliques of $G$. For example, super-cliques ($G$) for both graphs in Fig.1 is \{\{1, 2\}, \{1, 3\}, \{2, 4\}, \{3, 4\}\}.

![Figure 1](image-url)

Figure 1: (a) An example of a Bayesian net. (b) An example of a Markov net.

A classical Bayesian network is a DAG with labelled nodes (let $(x_j)_{Z_1,N}$ be the labels), together with a transition matrix $P(x_j|x_{pa(j)})$ associated with each node $x_j$ of the graph. The quantities $P(x_j|x_{pa(j)})$ are probabilities; they are non-negative and satisfy $\sum_j P(x_j|x_{pa(j)}) = 1$. The probability of the whole net is defined as the product of the probabilities of the nodes.
A quantum Bayesian network is a DAG with labelled nodes (let \((x)_{j=1,\ldots,N}\) be the labels), together with a transition matrix \(A(x_j|x_{pa(j)})\) associated with each node \(x_j\) of the graph. The quantities \(A(x_j|x_{pa(j)})\) are probability amplitudes; they satisfy \(\sum_j |A|^2(x_j|x_{pa(j)}) = 1\). The probability amplitude of the whole net is defined as the product of the amplitudes of the nodes. For example, for the quantum Bayesian net of Fig.1(a), one has

\[
A(x_1, x_2, x_3, x_4) = A(x_4|x_2, x_3)A(x_3|x_1)A(x_2|x_1)A(x_1),
\]

where \(x_j \in St_{x_j}\) for \(j = 1, 2, 3, 4\).

A classical (ditto, quantum) Markov network is an UG with labelled nodes (let \((x)_{j=1,\ldots,N}\) be the labels), together with an affinity \(\phi(x_K)\) (ditto, \(\alpha(x_K)\)) associated with each super-clique \(K\) of the graph. The probability (ditto, probability amplitude) of the whole net is defined as the normalized product of the affinities of the super-cliques of \(G\). For example, for the quantum Markov net of Fig.1(b), one has

\[
A(x_1, x_2, x_3, x_4) = \frac{\alpha(x_4, x_3)\alpha(x_4, x_2)\alpha(x_3, x_1)\alpha(x_2, x_1)}{\sqrt{\sum_{x_1,x_2,x_3,x_4} |\text{numerator}|^2}},
\]

where \(x_j \in St_{x_j}\) for \(j = 1, 2, 3, 4\).

We will sometimes use \(\tilde{G}\) to denote a Bayesian (ditto, Markov) network associated with a DAG (ditto, UG) \(G\).

### 2.4 Information Theory Preliminaries

Next, we review some basic definitions from Information Theory\[14\].

First consider classical physics. For any \(P \in pd(St_{x})\), the entropy (a measure of the variance of \(P\)) is defined by

\[
H(x) = -\sum_x P(x) \ln P(x).
\]

Sometimes the entropy is denoted instead by \(H(P_x)\). CMI (usually pronounced “see-me”) stands for “Conditional Mutual Information”. For \(P \in pd(St_{x,y,e})\), the CMI (a measure of conditional information transmission) is defined by

\[
H(x : y|e) = \sum_{x,y,e} P(x,y,e) \ln \frac{P(x,y|e)}{P(x|e)P(y|e)}.
\]

In general, \(H(x : y|e) \geq 0\). When \(N_e = 1\), CMI degenerates into the mutual
information \( H(x : y) \). Note that

\[
H(x : y|e) = \sum_{x,y,e} P(x, y, e) \ln \frac{P(x, y, e)P(e)}{P(x, e)P(y, e)} \tag{11a}
\]

\[
= H(x, e) + H(y, e) - H(x, y, e) - H(e) \,. \tag{11b}
\]

Classical CMI satisfies the chain rule

\[
H(x : y_1, y_2|e) = H(x : y_1|y_2, e) + H(x : y_2|e) \,. \tag{12}
\]

Now consider quantum physics. For \( \rho_x \in dm(\mathcal{H}_x) \), the entropy is defined by

\[
S(x) = -\text{tr}_x(\rho_x \ln \rho_x) \,. \tag{13}
\]

Sometimes the entropy is denoted instead by \( S(\rho_x) \) or by \( S_\rho(x) \), where \( \rho \) is a traced dm-extension of \( \rho_x \). For \( \rho_{xye} \in dm(\mathcal{H}_{xye}) \), the CMI is defined by analogy to Eq.(11b):

\[
S(x : y|e) = S(\rho_{xe}) + S(\rho_{ye}) - S(\rho_{xye}) - S(\rho_e) \,. \tag{14}
\]

In general, \( S(x : y|e) \geq 0 \) (this is known as the Strong Subadditivity of quantum entropy). Sometimes the CMI is denoted instead by \( S_\rho(x : y|e) \), where \( \rho \) is a traced dm-extension of \( \rho_{xye} \). When \( N_e = 1 \), CMI degenerates into the mutual information \( S(x : y) \). Just like classical CMI, quantum CMI satisfies the chain rule

\[
S(x : y_1, y_2|e) = S(x : y_1|y_2, e) + S(x : y_2|e) \,. \tag{15}
\]

Given \( \rho_{xye} \in dm(\mathcal{H}_{xye}) \), the CMI entanglement (an information theoretic measure of quantum entanglement) is defined as

\[
E^{CMI}(x : y) = \frac{1}{2} \inf_{\rho_{xye} \in K} (S(\rho_{xye}(x : y|e))) \,. \tag{16}
\]

where the infimum (a generalized minimum) is taken over the set \( K \) of all density matrices \( \rho_{xye} \in dm(\mathcal{H}_{xye}) \) such that \( \text{tr}_e \rho_{xye} = \rho_{xy} \). Sometimes, the CMI entanglement is denoted instead by \( E^{CMI}(\rho_{xy}) \), or by \( E^{CMI}_\rho(x : y) \), where \( \rho \) is a traced dm-extension of \( \rho_{xye} \). CMI entanglement is also known by the less scientific name of “squashed entanglement”. For more information about CMI entanglement, see Ref.[13].

If we apply the definition of CMI entanglement to the right hand side of Eq.(15), we get

\[
S(x : y_1, y_2|e) \geq 2E^{CMI}(x : y_1) + 2E^{CMI}(x : y_2) \,. \tag{17}
\]

Now we are free to apply the definition of CMI entanglement to the left hand side of the previous equation to get:
\[ E^{CMI}(x : y_1, y_2) \geq E^{CMI}(x : y_1) + E^{CMI}(x : y_2). \] (18)

Eq. (18) can be called super-additivity of the right side argument of \( E^{CMI} \). Since entanglement is symmetric (i.e., \( E(x : y) = E(y : x) \)), there is also super-additivity of the left side argument \( E^{CMI} \). Eq. (18) can also be called the synergism of entanglement, because the whole has more entanglement than the sum of its parts. If the inequality in Eq. (18) were in the opposite direction, we could call it sub-additivity or anti-synergism.

3 Meta Density Matrix and Purification of a Density Matrix

In this section, we define meta density matrices, and purifications of density matrices. We show that any density matrix has a purification.

A pure density matrix \( \mu \in dm(\mathcal{H}_z) \) of the form \( \mu = \text{proj}(\sum_x A(x)|x\rangle\langle x|) \) will be called a meta density matrix. If \( A(x) \) is the full joint amplitude associated with a Bayesian or Markov network \( \tilde{G} \), we will call \( \mu \) the meta density matrix of the network \( \tilde{G} \).

Suppose \( J \subset Z_{1,N} \) and \( J^c = Z_{1,N} - J \). Given a density matrix \( \rho \in dm(\mathcal{H}_{z,J}) \), we will call any pure density matrix \( \mu \in dm(\mathcal{H}_{z,J}) \) such that \( \text{tr}_{z,J^c}(\mu) = \rho \), a traced purification of \( \rho \). More generally, if \( \rho = \Omega(\mu) \) where the operator \( \Omega \) is not a trace operator, we will call \( \mu \) a generalized purification of \( \rho \).

Crucial to this paper is the well known fact that any density matrix has a traced purification. Next, we will present a proof of this fact. Our proof is a nice showcase of Bayesian net ideas and of our notation.

Consider any \( \rho \in dm(\mathcal{H}_{z,J}) \). Let
\[
\rho = \sum_{x,x'} \rho(x,x')|x\rangle\langle x'|.
\] (19)

Let \( M \) be the matrix with entries \( \rho(x,x') \), where \( x \in St_{z,J} \) labels its rows and \( x' \in St_{z,J} \) its columns. \( M \) is a Hermitian matrix so it can be diagonalized. Let \( M = UDU^\dagger \), where \( U \) is a unitary matrix, and \( D \) is a real, diagonal matrix. Set \( U_{x,j} = A(x|j) \) and \( D_{j,j} = |A|^2(j) \), where \( N_{z,J} = N_{z,J} \). Then
\[
\rho(x,x') = \sum_j A(x|j)|A|^2(j)A^\ast(x'|j).
\] (20)

If we define
\[
\mu = \sum_{x,j} A(x|j)A(j)|x,j\rangle,
\] (21)
then
\[ \rho = \text{tr}_j \text{proj}(\mu) . \]  

(22)

A Bayesian net representation of the previous equation is

\[ \rho = (x) \leftarrow \text{tr}(j) . \]  

(23)

The tr over the \( j \) is intended to indicated that node \( j \) should be traced over. Note that the eigenvectors of \( \rho \) become the transition amplitudes of node \( x \), whereas the square root of the eigenvalues of \( \rho \) become the amplitudes of node \( j \).

4 Measurements of the Meta Density Matrix

We’ve shown that any density matrix \( \rho \) has a traced purification \( \mu \). Thus, without loss of generality, we need only consider meta density matrices \( \mu \) and those density matrices obtained by applying measurement operators to \( \mu \). In this section, we describe a “complete” set of measurement operators that can be applied to a meta density matrix to obtain all measurable probabilities codified within it.

First, consider classical physics. In particular, consider \( N \) random variables \( x_1, \ldots, x_N \) described by a probability distribution \( P(x) \). Suppose

\[ Z_{1,N} = Z_{\text{vis}} \cup Z_{\text{sum}} , \]  

(24)

where \( Z_{\text{vis}} \) and \( Z_{\text{sum}} \) are disjoint sets. Here “vis” stands for “visible” and “sum” for “summed”. The probability that \( x_{Z_{\text{vis}}} = x_{Z_{\text{vis}}} \) is defined as

\[ P(x_{Z_{\text{vis}}}) = \sum_{x_{Z_{\text{sum}}}} P(x) . \]  

(25)

\( Z_{\text{vis}} \) can also be split into two parts. Let

\[ Z_{\text{vis}} = Z_{\text{post}} \cup Z_{\text{pre}} , \]  

(26)

where \( Z_{\text{post}} \) and \( Z_{\text{pre}} \) are disjoint sets. The conditional probability that \( x_{Z_{\text{post}}} = x_{Z_{\text{post}}} \) given \( x_{Z_{\text{pre}}} = x_{Z_{\text{pre}}} \) is defined as

\[ P(x_{Z_{\text{post}}} \mid x_{Z_{\text{pre}}}) = \frac{P(x_{Z_{\text{post}}, x_{Z_{\text{pre}}}})}{P(x_{Z_{\text{pre}}})} . \]  

(27)

The conditional expected value (a.k.a. conditional expectation) of any complex valued function \( f(\cdot) \) of the random variable \( x_{Z_{\text{vis}}} \) is defined as:

\[ E[f(x_{Z_{\text{vis}}}) \mid x_{Z_{\text{pre}}} = x_{Z_{\text{pre}}} ] = \sum_{x_{Z_{\text{post}}}} f(x_{Z_{\text{vis}}}) P(x_{Z_{\text{post}}} \mid x_{Z_{\text{pre}}}) . \]  

(28)

Visible (either pre or post viewed) and hidden nodes will be indicated on a Bayesian network by the node decorations show in Fig. 2
Figure 2: Various node decorations, used with both classical and quantum Bayesian networks, to indicate visible and hidden nodes. In a probability $P(a|e) = \sum_h P(a, h|e)$, $h$ is hidden, $a, e$ are visible, $e$ is pre-viewed and $a$ is post-viewed.

Next, consider quantum physics. In particular, consider $N$ random variables $x$ described by a pure state

$$|\phi_{\text{meta}}\rangle = \sum_x A(x.)|x.\rangle,$$

or, equivalently, by the meta density matrix

$$\mu = |\phi_{\text{meta}}\rangle \langle \phi_{\text{meta}}| = \text{proj}(|\phi_{\text{meta}}\rangle) .$$

Our next goal is to generalize the classical physics definitions Eqs. (24) to (28) to quantum physics. Let

$$Z_{1,N} = Z_{\text{vis}} \cup Z_{\text{sum}}, \quad Z_{\text{sum}} = Z_{\text{Asum}} \cup Z_{\text{Psum}},$$

where $Z_{\text{vis}}$, $Z_{\text{Asum}}$ and $Z_{\text{Psum}}$ are disjoint sets. Here “Asum” stands for “amplitude summed” and “Psum” stands for “probability summed”. The probability that $x_{Z_{\text{vis}}} = x_{Z_{\text{vis}}}$ is defined as

$$P(x_{Z_{\text{vis}}})_{x_{Z_{\text{Psum}}}} = \frac{\sum_{x_{Z_{\text{Psum}}}} |\sum_{x_{Z_{\text{Asum}}}} A(x.)|^2}{\sum_{x_{Z_{\text{vis}}}} \text{numerator}} .$$

Note that, contrary to the classical physics case, this probability depends on which random variables are summed coherently (A summed) and which are summed incoherently (P summed). We’ve indicated this dependence by the subscript $\backslash_{x_{Z_{\text{Psum}}}}$. The backslash in this notation is intended to evoke a mental picture of the diagonal of a matrix, because the variables that are P summed are “diagonalized” (why we say these variables are diagonalized will become clear to the reader later on, once he sees Eq. (47b)). As in the classical physics case, let
\[ Z_{\text{vis}} = Z_{\text{post}} \cup Z_{\text{pre}}, \quad (33) \]

where \( Z_{\text{post}} \) and \( Z_{\text{pre}} \) are disjoint sets. The conditional probability that \( x_{\text{post}} = x_{\text{post}} \) given \( x_{\text{pre}} = x_{\text{pre}} \) is defined, in analogy to the classical physics case, by

\[
P(x_{\text{post}} | x_{\text{pre}})_{\sum} \frac{P(x_{\text{post}}, x_{\text{pre}})_{\sum}}{P(x_{\text{pre}})_{\sum}}. \quad (34)\]

Consider a Hermitian operator \( \Omega_{x_{\text{vis}}} \) acting on \( \mathcal{H}_{x_{\text{vis}}} \). Suppose \( \{ | x_{\text{vis}} \rangle : \forall x_{\text{vis}} \} \) are the eigenstates of \( \Omega_{x_{\text{vis}}} \), so that

\[
\Omega_{x_{\text{vis}}} = \sum_{x_{\text{vis}}} \lambda_{x_{\text{vis}}} | x_{\text{vis}} \rangle \langle x_{\text{vis}} |. \quad (35)\]

In analogy to the classical physics case, one defines the conditional expected value of \( \Omega_{x_{\text{vis}}} \) by

\[
E[\Omega_{x_{\text{vis}}}|x_{\text{post}} = x_{\text{pre}}]_{\sum} = \sum_{x_{\text{post}}} \lambda_{x_{\text{vis}}} P(x_{\text{post}} | x_{\text{pre}})_{\sum}. \quad (36)\]

At this point, we have achieved our goal of generalizing the classical physics definitions Eqs. (24) to (28) to quantum physics. In doing so, we’ve introduced the probability \( P(x_{\text{post}} | x_{\text{pre}})_{\sum} \). The rest of this section will be devoted to explaining how this probability can be measured.

To measure \( P(x_{\text{post}} | x_{\text{pre}})_{\sum} \) instead of \( P(x_{\text{vis}})_{\sum} \), one restricts the range of the random variable \( x_{\text{pre}} \) to the single value \( x_{\text{pre}} \). Of course, one must also divide ("normalize") the restricted meta density matrix by a constant so that its trace remains 1. Next, we show how to measure \( P(x_{\text{vis}})_{\sum} \).

Note that \( P(x_{\text{vis}})_{\sum} \) given by Eq. (32) can be expressed as the expected value, in the meta density matrix \( \mu \), of a projection operator \( \pi^{(a)} \pi^{(b)} \pi^{(c)} \):

\[
P(x_{\text{vis}})_{\sum} = \frac{\text{tr}_x (\pi^{(a)} \pi^{(b)} \pi^{(c)} \mu)}{\text{numerator}}. \quad (37)\]

The projection operator \( \pi^{(a)} \pi^{(b)} \pi^{(c)} \) consists of a product of 3 mutually commuting projection operators defined by

\[
\pi^{(a)} = \text{proj}(|x_{\text{vis}}\rangle) , \quad (38)\]

\[
\pi^{(b)} = \text{proj}(|AV x_{\text{Asum}}\rangle) , \quad (39)\]

and
\[ \pi^{(c)} = \sum_{x \not\in \mathcal{P}_{\text{sum}}} \text{proj}(|x_{\mathcal{P}_{\text{sum}}}) \, . \] (40)

In \( \pi^{(b)} \), we use the “average” state vector \(|AV_x\rangle\), for \( J \subset Z_{1,N} \). This vector is defined as

\[ |AV_x\rangle = \frac{\sum_{x \in J} |x\rangle}{\sqrt{|J|}} . \] (41)

The fact that \( P(x_{\text{vis}} \setminus \mathcal{P}_{\text{sum}}) \) can be expressed as an expected value of a projection operator suggests one way of measuring it.

![Diagram](image)

Figure 3: Various node decorations used with quantum Bayesian networks to indicate operators acting on the meta density matrix associated with the network.

Suppose \( \Omega_{x,y} \) is an operator acting on \( \mathcal{H}_{x,y} \). It is convenient at this point to define the following super-operators acting on \( \Omega_{x,y} \):

\[ e_{x=x}(\Omega_{x,y}) = \langle x|\Omega_{x,y}|x\rangle , \text{ (entry)} \] (42)

\[ e_{\Sigma_x}(\Omega_{x,y}) = \sum_{x,x'} \langle x|\Omega_{x,y}|x'\rangle , \text{ (entry sum)} \] (43)

\[ \text{tr}_{x} (\Omega_{x,y}) = \sum_{x} \langle x|\Omega_{x,y}|x\rangle , \text{ (trace)} \] (44)

\[ \text{diag}_{x} (\Omega_{x,y}) = \sum_{x} |x\rangle\langle x| \langle x|\Omega_{x,y}|x\rangle . \text{ (diagonal matrix)} \] (45)
We’ve shown in parenthesis on the right hand side what we call these operators. Note that \( \text{diag} \mathbf{x}_\omega \mathbf{y} \) diagonalizes \( \Omega_{\mathbf{x}_\omega \mathbf{y}} \) partially. \( \text{diag} \mathbf{x}_\omega \mathbf{y} \) diagonalizes it fully. 

\[ e^\Sigma \text{diag} \mathbf{x} = \text{tr} \mathbf{x} \quad (46) \]

Fig. 3 gives node decorations that will be used to indicate these operators when acting on a Bayesian network.

In Eq. (37), we obtained \( P(x_{\text{vis}})|x_{\text{sum}} \) as an expected value of a projection operator. Alternatively, \( P(x_{\text{vis}})|x_{\text{sum}} \) can be obtained by successive applications of the operators \( e() \), \( e\Sigma() \), \( \text{tr}() \), and \( \text{diag}() \) to \( \mu \):

\[
P(x_{\text{vis}})|x_{\text{sum}} = \frac{e^\Sigma_{x_{\text{vis}} - x_{\text{vis}}} e \Sigma_{x_{\text{sum}} - x_{\text{sum}}} \text{tr}_{x_{\text{sum}}} \mu}{\sum_{x_{\text{vis}}} \text{numerator}} \quad (47a)
\]

\[
P(x_{\text{vis}})|x_{\text{sum}} = \frac{e^\Sigma_{x_{\text{vis}} - x_{\text{vis}}} e \Sigma_{x_{\text{sum}} - x_{\text{sum}}} \text{diag}_{x_{\text{sum}}} \mu}{\sum_{x_{\text{vis}}} \text{numerator}} \quad (47b)
\]

Eq. (47b) follows from Eq. (46). Here, the operators \( e() \), \( e\Sigma() \), \( \text{tr}() \), and \( \text{diag}() \) can be interpreted as measurements (or lack thereof) of the density matrix they act upon.

In Eqs. (47), \( \text{tr}_{x_{\text{sum}}} \) means observe (=measure) the random variable \( x_{\text{sum}} \), and then forget the outcome. \( e^\Sigma_{x_{\text{vis}} - x_{\text{vis}}} \) means measure of the random variable \( x_{\text{vis}} \) once. \( e \Sigma_{x_{\text{sum}} - x_{\text{sum}}} \) means do no observe the random variable \( x_{\text{sum}} \). It remains for us to interpret \( \text{diag}_{x_{\text{sum}}} \) as a measurement.

For any density matrix \( \rho_{x_{\text{sum}}} \in \mathcal{M}(\mathcal{H}_{x_{\text{sum}}}) \), the operator \( \text{diag}_{x} \) is what is called a von Neumann measurement. It can be implemented physically in two steps: (1) measure the random variable \( x \); if the outcome is \( x \), emit \( |x\rangle\langle x| \), and (2) repeat the measurement many times, without discriminating on any of the outcomes (mathematically, this corresponds to summing over the outcomes \( x \) of the measurements).

A second way of implementing \( \text{diag}_{x} \) is as follows. The Bayesian net

\[
(x) \leftarrow (y) \quad (48)
\]

\footnote{Previously, we defined \( \text{diag}(\cdot) \) to be a function that takes a vector \( \mathbf{x} \) and returns a diagonal matrix with \( \mathbf{x} \) along its diagonal. Here we are defining a different \( \text{diag}(\cdot) \) function. Both of these functions return a diagonal matrix, but they have different domains. We will use the symbol \( \text{diag}(\cdot) \) for both of these functions. Which function we mean will be clear from the context.}

\footnote{The software program Quantum Fog can calculate \( P(z_{\text{post}}|z_{\text{pre}}) \) \( z_{\text{sum}} \) numerically. Conditioning on \( z_{\text{pre}} \) is already implemented in the current version, 2.0, of Quantum Fog; it corresponds to allowing only one “active” state for each of the nodes \( x_j \) for \( j \in z_{\text{pre}} \). On the other hand, only a special case of the distinction between P-summed and A-summed is implemented in version 2.0. In version 2.0, \( z_{\text{sum}} \) is always assumed to equal the set of external nodes minus the set of visible ones. More general sets \( z_{\text{sum}} \) will be implemented in future versions of Quantum Fog.}
with transition matrix $A(x|y)A(y)$ can be replaced by a Bayesian net

$$(x') \leftarrow (x) \leftarrow (y)$$

with transition matrix $A(x'|x)A(x|y)A(y)$, where $A(x|x') = e^{i\theta_x}\delta(x', x)$ $\forall x, x' \in St_x$. Assume that the variables $\{\theta_x : \forall x\}$ are i.i.d. (independent, identically distributed) classical random variables, and each is uniformly distributed over $[0, 2\pi]$. Let an overline denote an average over these variables. An effect of adding the node $x'$ to the network is that we must replace

$$\rho_{z,y} = \sum_{x,y,x',y'} \rho_{xy,x'y}|xy\rangle \langle x'y'|$$

by

$$\rho_{z',y} = \sum_{x,y,x',y'} \rho_{xy,x'y}e^{i\theta_x}|xy\rangle \langle x'y'|e^{-i\theta_x}. $$

Clearly,

$$\bar{\rho}_{z',y} = \text{diag}_z \rho_{z,y}, $$

and

$$\text{tr}_z[\Omega \rho_{z',y}] = \text{tr}_z[\Omega \bar{\rho}_{z',y}] = \text{tr}_z[\Omega \text{diag}_z \rho_{z,y}], $$

for any operator $\Omega$ acting on $H_{z,y}$. Thus, the operator $\text{diag}_z$ can be implemented physically merely by taking many measurements for which $\theta_x$ varies randomly.

A third way of implementing $\text{diag}_z$ is by adding an additional node that is traced over. For example, suppose $\rho_z \in dm(H_z)$ can be expressed in the form

$$\rho_z = \text{diag}_z(\mu) \quad \mu = \text{proj}(\sum_x A(x|\{x\})). $$

We can introduce a node $j$ such that $St_j = St_z$ and $A(j) = A(z = j)$. Then

$$\rho_z = \text{tr}_z(\bar{\rho}), \quad \bar{\mu} = \text{proj}(\sum_{x,j} \delta_j^z A(j|x,j)). $$

$\mu$ is a generalized purification of $\rho_z$ whereas $\bar{\mu}$ is a traced one. By expressing $\rho_z$ in terms of $\bar{\mu}$ instead of $\mu$, we get rid of the $\text{diag}_z$ operator at the expense of adding an additional node $j$ that we trace over. A Bayesian network representation of the essence of Eqs.(54) and (55) is:

---

4 Of course, for an arbitrary polynomial function $f$, one has $\bar{f}(\rho_{z',y}) \neq f(\rho_{z',y})$, but this is not a show stopper, since the density matrix only enters linearly in the formula for the expected value of any observable.
\[
\text{diag} (x) = (x) \leftarrow (j) . \quad (56)
\]

As a more general example of this method of implementing \(\text{diag} (x)\), suppose \(\rho_{y,x} \in dm(\mathcal{H}_{y,x})\) can be expressed in the form

\[
\rho_{y,x} = \text{diag}_x (\mu), \quad \mu = \text{proj}\left(\sum_{y,x} A(y|x)A(x|y,x)\right). \quad (57)
\]

Once again, introduce a node \(j\) such that \(St_j = St_x\) and \(A(j) = A(x = j)\). Then

\[
\rho_{y,x} = \text{tr}_j (\tilde{\mu}), \quad \tilde{\mu} = \text{proj}\left(\sum_{y,x,j} A(y|x)\delta^x_j A(j|y,x,j)\right), \quad (58)
\]

A Bayesian network representation of the essence of Eqs. (57) and (58) is:

\[
\text{diag} (y) \leftarrow (x) = (y) \leftarrow (x) \leftarrow (j) . \quad (59)
\]

The Schmidt Decomposition is very popular in the Quantum Information Theory literature. As an illustration of the use of the entry-sum operator \(\Sigma\), let us consider the Schmidt Decomposition from the point of view of Bayesian networks. The Schmidt Decomposition is the statement that given a pure state \(\mu_1 \in dm(\mathcal{H}_{x,y})\) of the form

\[
\mu_1 = \text{proj}\left(\sum_{x,y} A(x,y)|x,y\rangle\langle x,y|\right), \quad (60)
\]

the coefficients \(A(x,y)\) can be expressed in the form

\[
A(x,y) = \sum_j A(x|j)A(y|j)A(j) , \quad (61)
\]

where \(A(j) \geq 0 \forall j, \sum_j |A(j)|^2 = 1, \sum_x |A(x|j)|^2 = 1 \forall j, \sum_y |A(y|j)|^2 = 1 \forall j\).

The fact that any \(A(x,y)\) can be expressed in the form given by Eq. (61) is a re-statement of the Singular Value Decomposition Theorem. This is why. Let \(M\) be the matrix with entries \(A(x,y)\), where \(x \in St_x\) labels its rows and \(y \in St_y\) its columns. According to the Singular Value Decomposition theorem, \(M\) can be expressed in the form \(M = UDV^\dagger\), where \(U\) and \(V\) are unitary matrices and \(D\) is a non-negative, diagonal matrix. If we let \(U_{x,j} = A(x|j), D_{j,j} = A(j), V^*_{y,j} = A(y|j)\), then Eq. (61) follows.

To obtain a Bayesian net picture of the Schmidt Decomposition, note that if we define \(\mu_2 \in dm(\mathcal{H}_{x,y,j})\) by

\[
\mu_2 = \text{proj}\left(\sum_{x,y,j} A(x|j)A(y|j)A(j|x,y,j)\right), \quad (62)
\]
then

$$e_{\Sigma_j}(\mu_2) = \text{proj}(\sum_{x,y,j} A(x|j)A(y|j)A(j)|x,y))$$

$$= \mu_1.$$ 

(63a)

$$(63b)$$

$$x \rightarrow y = e_{\Sigma}^j$$

Figure 4: Bayesian net representation of the Schmidt Decomposition, as given by Eq.(63). Eq.(63) is illustrated by Fig.4.

Eq.(63b) gives an example of the use of the entry-sum operator $e_{\Sigma}$. Note that this operator takes a pure state of tensor rank $n \geq 2$ into a pure state of tensor rank $n-1$. Indeed,

$$e_{\Sigma_a} \text{proj}(\sum_{x,a} A(x,a)|x,a)) = \text{proj}(\sum_{x,a} A(x,a)|x)) .$$

(64)

e_{\Sigma} also takes a pure state of tensor rank $n = 1$ into a non-negative number. Indeed, for $|\psi\rangle \in \mathcal{H}_a$,

$$e_{\Sigma_a}|\psi\rangle\langle\psi| = \left| \sum_a \langle a|\psi| \right|^2 .$$

(65)

Note that when $N_a = 1$, the entry-sum operator $e_{\Sigma_a}$ equals the entry operator $e_{a=1}$. Thus, $e_{a=1}$ can be viewed as a special case of $e_{\Sigma_a}$. It’s clear that $e_{a=1}$ inherits from $e_{\Sigma_a}$ the property that: it takes a pure state of tensor rank $n \geq 2$ into a pure state of tensor rank $n-1$, and it takes a pure state of tensor rank $n = 1$ into a non-negative number.

Suppose $\mu \in dm(\mathcal{H}_{\omega_{z_{1,n}}})$ is a pure density matrix, and $\rho$ is a density matrix, and $\rho = (\prod_{j \in J} \omega_{z_j})\mu$, where $J \subset Z_{1,N}$ and $\omega_{z_j} \in \{e_{z_j-x_j}, e_{z_j}, \text{tr}_{z_j}, \text{diag}_{z_j}\}$. We’ve shown that $e_{z_j-x_j}$ and $e_{z_j}$ both take a pure density matrix to another pure density matrix, so one can easily find a pure density matrix $\mu' \in dm(\mathcal{H}_{\omega_{z_{1,n'}}})$ such that $\rho = (\prod_{j \in J'} \omega_{z_j})\mu'$, where $J' \subset Z_{1,N'}$ and $\omega_{z_j} \in \{\text{tr}_{z_j}, \text{diag}_{z_j}\}$. We’ve shown that each operator $\text{diag}_{z_j}$ can be traded for an extra node that is traced over. Thus, one can easily find a pure density matrix $\mu'' \in dm(\mathcal{H}_{\omega_{z_{1,n''}}})$ such that $\rho = (\prod_{j \in J''} \text{tr}_{z_j})\mu''$, where $J'' \subset Z_{1,N''}$. To summarize, given a generalized (i.e, made with entry, entry-sum,
trace and diag operators) purification of $\rho$, one can easily find a traced purification of $\rho$. A generalized purification of $\rho$ might be convenient for certain purposes, but not for others. Luckily, it can be easily replaced by a traced one.

5 Conditional Amplitudes

In this section, we define conditional amplitudes. These are a natural generalization of conditional probabilities.

Consider a meta density matrix $\mu = \proj(\sum_x A(x.)|x.)$ Its complex amplitude $A(x.)$ can be parameterized as

$$A(x.) = e^{i\theta(x.)} P^{\frac{1}{2}}(x.) ,$$

where the $\theta(x.)$ are real and $P \in \text{pd}(St_{x.})$. Choose an arbitrary state of $(x.)$, and call it the reference state $(x.o)$. It is convenient to constrain $\theta(x.)$ by assuming that it vanishes at the reference state:

$$\theta(x.o) = 0 .$$

For $J \subset Z_{1,N}$ and $J^c = Z_{1,N} - J$, we define

$$\theta(x.J) = \theta(x.J, x_.^o) ,$$

$$P(x.J) = \sum_{x.J^c} P(x.) ,$$

and

$$A(x.J) = e^{i\theta(x.J)} P^{\frac{1}{2}}(x.J) .$$

For disjoint sets $J_1, J_2 \subset Z_{1,N}$, we define

$$\theta(x.J_1|x.J_2) = \theta(x.J_1, x_.^o) - \theta(x.J_2) ,$$

$$P(x.J_1|x.J_2) = \frac{P(x.J_1, x_.^o)}{P(x.J_2)} ,$$

and

$$A(x.J_1|x.J_2) = \frac{A(x.J_1, x_.^o)}{A(x.J_2)} .$$

Note that

$$\theta(x_.^o|x.J_2) = 0 ,$$
\[ \text{phase}(\langle x. | \mu | y. \rangle) = \theta(x.) - \theta(y.) , \]  

and

\[ \theta(x.) = \text{phase}(\langle x. | \mu | x.^o \rangle) . \]  

\[ \text{phase}(\langle x. | \mu | y. \rangle) = \theta(x.) - \theta(y.) , \]  

6 Probabilistic Conditional Independence

This section, divided into 3 subsections, explores the notion of conditional independence in both classical and quantum physics.

Henceforth, by an independency, we will mean a triplet \((x. \perp x. K \mid x. E)\), where \(J, K, E \subseteq \mathbb{Z}_{1,N}\) are disjoint. (If \(J\) and \(K\) are disjoint but overlap with \(E\), replace \((x. J \perp x. K \mid x. E)\) by \((x. J-E \perp x. K-E \mid x. E)\)). If the sets \(J\) and \(K\) both contain more than one element, we will call it a global independency. If \(|J| + |K| + |E| = N\), we will say that \((x. J \perp x. K \mid x. E)\) is an all-encompassing independency. We will use the word I-set as an abbreviation for “independencies set”; that is, a set whose members are independencies. It is convenient to introduce a symbol for the set of all possible independencies:

\[ \mathcal{I}(x.) = \{ I : I = (x. J \perp x. K \mid x. E) ; J, K, E \subset \mathbb{Z}_{1,N} \text{ are disjoint} \} . \]  

6.1 Types of Probabilistic Conditional Independence

In this section, we define classical conditional independence and three quantum analogues of it, type-A, type-CMI, and type-CMI’.

Consider first classical physics and probability. Let \(J, K, E \subset \mathbb{Z}_{1,N}\) be disjoint sets. We say \(x. J\) and \(x. K\) are conditionally independent given \(x. E\) iff

\[ P(x. J, x. K \mid x. E) = P(x. J \mid x. E)P(x. K \mid x. E) \ \forall x. J, x. K, x. E . \]  

Eq.(74) is clearly equivalent to requiring that

\[ P(x. J \mid x. K, x. E) = P(x. J \mid x. E) , \]  

or

\[ P(x. K \mid x. J, x. E) = P(x. K \mid x. E) . \]  

We define the function \(\tau^P : \mathcal{I}(x.) \to \text{Bool}\) by the statement: \(\tau^P(x. J \perp x. K \mid x. E)\) is true iff Eq.(74) is true. Think of \(\tau^P\) as a “truth function” that decides whether its argument is false=0 or true=1.

In classical physics, conditional independence and vanishing CMI are equivalent. Indeed,
**Theorem 1**

\[ H(x : y) = 0 \text{ iff } P(x, y) = P(x)P(y) \ \forall x, y, \ \ (77) \]

and

\[ H(x : y|e) = 0 \text{ iff } P(x, y|e) = P(x|e)P(y|e) \ \forall x, y, e. \ \ (78) \]

**proof:** The proof can be found in Ref. [14].

**QED**

Now consider quantum physics. Our goal is to find the quantum counterpart of Eq. (74) and Theorem 1. Consider a meta density matrix

\[ \mu = \text{proj}\left( \sum_A A(x.) |x.\rangle \right). \]

Let \( J, K, E \subset Z_{1,N} \) be disjoint sets. We say \( x_J \) and \( x_K \) are **type-A conditionally independent** given \( x_E \) iff

\[ A(x_J, x_K|x_E) = A(x_J|x_E)A(x_K|x_E) \ \forall x_J, x_K, x_E. \ \ (79) \]

We say \( x_J \) and \( x_K \) are **type-CMI conditionally independent** given \( x_E \) iff

\[ S_\mu(x_J : x_K|x_E) = 0. \ \ (80) \]

(Note that we trace over all random variables \( x_n \) such that \( n \notin J \cup K \cup E \)). We say \( x_J \) and \( x_K \) are **type-CMI’ conditionally independent** given \( x_E \) iff

\[ S_{\text{diag}_{\mu}}(x_J : x_K|x_E) = 0. \ \ (81) \]

We define the function \( \tau^A : I(x.) \to \text{Bool} \) by the statement: \( \tau^A(x_J \perp x_K|x_E) \) is true iff Eq. (79) is true. Likewise, \( \tau^{\text{CMI}}(x_J \perp x_K|x_E) \) iff Eq. (80). Likewise, \( \tau^{\text{CMI’}}(x_J \perp x_K|x_E) \) iff Eq. (81).

In classical physics, type-A and type-CMI conditional independence are equivalent, but in quantum physics, neither one implies the other. We will give counterexamples of this later. But first, we will give easy-to-check necessary and sufficient conditions for a vanishing quantum CMI.

**Theorem 2** For \( \rho_{xy} \in \text{dm}(H_{xy}) \),

\[ S_{\rho_{xy}}(x : y) = 0 \text{ iff } \rho_{xy} = \rho_x \rho_y, \ \ (82) \]

where \( \rho_x \) and \( \rho_y \) are partial traces of \( \rho_{xy} \). For \( \rho_{xye} \in \text{dm}(H_{xy|e}) \),

\[ S_{\rho_{xye}}(x : y|e) = 0 \text{ iff } \rho_{xye} = \sum_e |e\rangle \langle e|w(e)\rho^{(e)}_x \rho^{(e)}_y, \ \ (83) \]

where \( w(\cdot) \in \text{pd}(\text{St}_{\rho_y}) \), and, for all \( e \), \( \rho^{(e)}_x \in \text{dm}(H_x) \), \( \rho^{(e)}_y \in \text{dm}(H_y) \).

**proof:** Eq. (83) implies Eq. (82). Proving \( \Rightarrow \) for Eq. (83) is a simple calculation. It was pointed out in Ref. [15]. Proving \( \Rightarrow \) for Eq. (83) is much more technical. A weak version of it was proven in Ref. [15]. The strong version presented here was first proven in Ref. [16].

**QED**
Theorem 3 Consider a meta density matrix $\mu = \text{proj}(\sum_x A(x)\langle x \rangle)$.
Suppose $K_1, K_2, E \subset Z_{\overline{1,N}}$ are disjoint sets, $U = K_1 \cup K_2 \cup E$, and $U^c = Z_{\overline{1,N}} - U$. Let 
$I = (\underline{x}_{K_1} \perp \underline{x}_{K_2} | \underline{x}_E)$. 
\(\tau^{CMI'}(I) \iff \forall (x_E, x_{K_1}, x_{K_2}, x_{K_1'}, x_{K_2'})\)

\[
\sum_{x_{U^c}} \left[ A(x_{K_1}, x_{K_2}, x_{U^c}, x_E) \right]^\times = w(x_E)\rho_1^{(x_E)}(x_{K_1}, x_{K_1'})\rho_2^{(x_E)}(x_{K_2}, x_{K_2'}) , \quad (84)
\]

where $w(\cdot) \in \text{pd}(St_{\underline{x}_E})$, and where, for $j \in \{1,2\}$, $\forall x_E$, $\rho_j^{(x_E)} \in \text{dm}(H_{\underline{x}_{K_j}})$.

proof:
Define $\rho$ by

\[
\rho = \text{diag}_{\underline{x}_E} \text{tr}_{\underline{x}_{U^c}} \mu 
\]

(85a)

\[
= \sum_{x_E} |x_E\rangle\langle x_E| \sum_{x_{K_1}x_{K_2}} \sum_{x_{U^c}} \left[ A(x_{K_1}, x_{K_2}, x_{U^c}, x_E) \right]^\times \left[ A^*(x_{K_1'}, x_{K_2'}, x_{U^c}, x_E) \right] |x_{K_1}, x_{K_2}\rangle \langle x_{K_1'}, x_{K_2'}|.
\]

(85b)

\(\tau^{CMI'}(I)\) is equivalent to $S_{\rho}(\underline{x}_{K_1} : \underline{x}_{K_2} | \underline{x}_E) = 0$.

Recall that for any $\rho_{sol} \in \text{dm}(H_{\underline{x}_E})$,

\[
S_{\rho_{sol}}(\underline{x}_{K_1} : \underline{x}_{K_2} | \underline{x}_E) = 0 \iff \rho_{sol} = \sum_{x_E} |x_E\rangle\langle x_E| w(x_E)\rho_{K_1}^{(x_E)}\rho_{K_2}^{(x_E)} . \quad (86)
\]

($\Rightarrow$) By setting $\rho$ equal to $\rho_{sol}$, we prove Eq.(84).

($\Leftarrow$) By plugging Eq.(84) into Eq.(85b), we show that $\rho$ satisfies the right hand side of Eq.(86), so it satisfies the left hand side of the same equation.

QED

We are finally ready to prove that for type-A and type-CMI conditional independence, neither one of these implies the other.

Theorem 4 Suppose $K_1, K_2, E \subset Z_{\overline{1,N}}$ are disjoint sets, and $I = (\underline{x}_{K_1} \perp \underline{x}_{K_2} | \underline{x}_E)$. 
\(\tau^{CMI}(I) \not\Rightarrow \tau^A(I)\) and \(\tau^{CMI}(I) \not\Leftarrow \tau^A(I)\). Also, \(\tau^{CMI'}(I) \not\Rightarrow \tau^A(I)\) and \(\tau^{CMI'}(I) \not\Leftarrow \tau^A(I)\). Also, \(\tau^{CMI}(I) \Rightarrow \tau^{CMI'}(I)\).

proof: Let $U = K_1 \cup K_2 \cup E$, and $U^c = Z_{\overline{1,N}} - U$. For our counterexamples, we will assume $x_{K_1} \rightarrow x_1$, $x_{K_2} \rightarrow x_2$, $x_{U^c} \rightarrow a$, where $x_1, x_2, a$ are Boolean variables. We will take $N_{\underline{x}_E} = 1$, and indications of any dependence on $x_E$ will be suppressed.
We will take $(0, 0, 0)$ to be our reference state (i.e., the state $(x_1^0, x_2^0, a^0)$ for which $\theta(x_1^0, x_2^0, a^0) = 0$). We will abbreviate $\theta(x_1, x_2, a)$ by $\theta_{x_1, x_2, a}$.

$\tau^{CMI}(I) \Rightarrow \tau^{CMI'}(I)$ is obvious. Since we will assume $N_{\theta} = 1$, our example of $\tau^{CMI'}(I) \not\Rightarrow \tau^A(I)$ will also prove $\tau^{CMI}(I) \not\Rightarrow \tau^A(I)$. Likewise, our example of $\tau^{CMI'}(I) \not\Leftrightarrow \tau^A(I)$ will also prove $\tau^{CMI}(I) \not\Leftrightarrow \tau^A(I)$.

(proof of $\tau^{CMI'} \not\Rightarrow \tau^A$) Assume

$$\begin{align*}
A(x_1, x_2, a) &= \delta^{1,1}_{x_1, x_2} e^{i\theta_{x_1, x_2, a}} \\
\theta_{x_1, x_2, a} &= \xi \delta^{1,1}_{x_1, x_2, a}, \text{ where } \xi \in \mathbb{R} - 2\pi \mathbb{Z}.
\end{align*}$$

This $A(x_1, x_2, a)$ satisfies

$$\sum_a \left[ A(x_1, x_2, a) \right]^{\times} = \delta^{1,1}_{x_1, x_1} \delta^{1,1}_{x_2, x_2}.$$  

Therefore, $\tau^{CMI'}(I)$ is true. This $A(x_1, x_2, a)$ also satisfies

$$\begin{align*}
A(x_1, x_2) &= \delta^{1,1}_{x_1, x_2} = \delta^{1,1}_{x_1, x_2} e^{i\xi} = \delta^{1,1}_{x_1, x_2} e^{i\theta_{010}} = \delta^{1,1}_{x_1, x_2} e^{i\theta_{000}} = \delta^{1,1}_{x_2, x_2} = \delta^{1,1}_{x_2, x_2} e^{i\theta_{0010}} = \delta^{1,1}_{x_2, x_2} e^{i\theta_{0001}} = \delta^{1,1}_{x_2, x_2} e^{i\theta_{0100}} = \delta^{1,1}_{x_2, x_2}.
\end{align*}$$

Hence

$$A(x_1, x_2) \neq A(x_1) A(x_2),$$

which means $\tau^A(I)$ is false.

(proof of $\tau^{CMI'} \not\Leftrightarrow \tau^A$) Assume

$$\begin{align*}
A(x_1, x_2, a) &= \frac{e^{i\theta_{x_1, x_2, a}}}{\sqrt{8}} \\
\theta_{x_1, x_2, a} &= \xi \delta^{1,1}_{x_1, x_2, a}, \text{ where } \xi \in \mathbb{R} - 2\pi \mathbb{Z}.
\end{align*}$$

This $A(x_1, x_2, a)$ satisfies

$$\begin{align*}
A(x_1, x_2) &= \frac{e^{i\theta_{x_1, x_2}}}{\sqrt{4}} = \frac{1}{\sqrt{4}} \\
A(x_1) &= \frac{e^{i\theta_{x_1}}}{\sqrt{2}} = \frac{1}{\sqrt{2}} \\
A(x_2) &= \frac{e^{i\theta_{x_2}}}{\sqrt{2}} = \frac{1}{\sqrt{2}}
\end{align*}$$

Therefore,

$$A(x_1, x_2) = A(x_1) A(x_2),$$

which means $\tau^A(I)$ is true. This $A(x_1, x_2, a)$ also satisfies

$$\sum_a \left[ A(x_1, x_2, a) \right]^{\times} = \frac{1 + e^{i\xi[\delta^{1,1}_{x_1, x_2} - \delta^{1,1}_{x_1', x_2'}}}}{8}.$$
Let’s show that assuming $\tau^{CMI'}(I)$ leads to a contradiction. Theorem 3 implies (i) and Eq. (94) implies (ii) in the following:

$$\text{phase}[\rho_1(0,0)\rho_2(1,0)] \overset{(i)}{=} \text{phase}(\sum_a \left[ A(0,1,a) A^*(0,0,a) \right]^\times) \overset{(ii)}{=} 0,$$

and

$$\text{phase}[\rho_1(1,1)\rho_2(1,0)] \overset{(i)}{=} \text{phase}(\sum_a \left[ A(1,1,a) A^*(1,0,a) \right]^\times) \overset{(ii)}{=} \text{phase}(1 + e^{i\xi}).$$

Since $\rho_1(0,0)$ and $\rho_1(1,1)$ are supposed to be real, the right hand sides of the two previous equations are supposed to be equal. They aren’t—a contradiction.

QED

There is, however, one subset of $I(x)$ over which $\tau^A$ and $\tau^{CMI'}$ agree.

**Theorem 5** Suppose $K_1, K_2, E \subset Z_{1, N}$ are disjoint sets, and $I = (x_{K_1} \perp x_{K_2} | x_E)$. If $|K_1| + |K_2| + |E| = N$, then $\tau^A(I) = \tau^{CMI'}(I)$.

**proof:** According to Theorem 3, $\tau^{CMI'}(I)$ is equivalent to:

$$\left[ \begin{array}{c} A(x_{K_1}, x_{K_2}, x_E) \\ A^*(x_{K_1}, x'_{K_2}, x_E) \end{array} \right]^\times = w(x_E) \rho_1^{(x_E)}(x_{K_1}, x'_{K_1}) \rho_2^{(x_E)}(x_{K_2}, x'_{K_2}),$$

where $w(\cdot)$ is a probability distribution, and for $j = 1, 2$, $\forall x_E$, $\rho_j^{(x_E)}$ are density matrices. $\tau^A(I)$, on the other hand, is equivalent to

$$A(x_{K_1}, x_{K_2}, x_E) = A(x_{K_1} | x_E) A(x_{K_2} | x_E) A(x_E).$$

Clearly, $\tau^A(I)$ implies $\tau^{CMI'}(I)$. To show that $\tau^{CMI'}(I)$ implies $\tau^A(I)$, define $\theta(x) = \text{phase}(A(x))$, $|A|(x_E) = \sqrt{w(x_E)}$, and, for $j = 1, 2$, $|A|(x_{K_j} | x_E) = \sqrt{\rho_j^{(x_E)}(x_{K_j}, x_{K_j})}$.

QED

### 6.2 Reduction and Combination Rules for Independencies

Consider the following reduction and combination rules for independencies:

(a) **(Decomposition/2 → 1)**

$$\tau^n(x \perp y_1, y_2 | \epsilon) \Rightarrow \tau^n(x \perp y_1 | y_2, \epsilon)$$

(b) **(Weak Union/2 → 1')**

$$\tau^n(x \perp y_1, y_2 | \epsilon) \Rightarrow \tau^n(x \perp y_1 | y_2, \epsilon)$$
(c) **(Contraction/1′, 1 → 2)**
\[ \tau^n(x \perp y_1|y_2, e) \text{ and } \tau^n(x \perp y_2|e) \Rightarrow \tau^n(x \perp y_1, y_2|e) \]

(d) **(Intersection/1′, 1′ → 2)**
\[ P \neq 0 \text{ and } \tau^n(x \perp y_1|y_2, e) \text{ and } \tau^n(x \perp y_2|y_1, e) \Rightarrow \tau^n(x \perp y_1, y_2|e) \]

The function \( \tau^n : \mathcal{I}(x) \to \text{Bool} \) remains to be specified. \( x, y_1, y_2, e \) stand for mutually exclusive n-tuples of the form \( x_K \) for some \( K \in \mathbb{Z}_{1,N} \). Rules (a) and (b) perform a “reduction” whereas (c) and (d) perform a “combination”.

An independency \( I = (\cdot \perp \cdot|\cdot) \) has 3 slots. In the above rule statements, we’ve denoted all random variables in the second slot (slot-2) by the letter \( y \) with a subscript.

The above rule statements start with the rule name, in parenthesis. Within the parenthesis, to the left of the slash is the name given by Judea Pearl in Ref.\[5\]. To the right of the slash is a new name, first given in this paper. In the new rule names, the symbol \( \Rightarrow \) stands for implication, and there is one number, indicating the number of \( y \)’s in slot-2, for each independency. For example, in rule 1, 1′ → 2, there are: one \( y \) in slot-2 of the first independency, one \( y \) in slot-2 of the second independency, two \( y \)’s in slot-2 of the third independency. The prime in 1′ indicates that, besides there being one \( y \) in slot-2, there also is one \( y \) in slot-3.

Note that in rule (d) above, we specify that \( P \neq 0 \). That’s because, as we shall see, this rule arises from one of those unusual cases, mentioned earlier, in which dividing by a probability causes trouble. Later on, we will state and prove theorems whose proof assumes rule (d). The fact that such theorems assume rule (d) will show up in that they inherit \( P \neq 0 \) as one of their premises.

Next we will show that the reduction and combination rules are obeyed by \( \tau^A \) and \( \tau^{CMI} \).

**Theorem 6** The above reduction and combination rules are true in classical physics with \( \eta = P \).

**proof:** The classical CMI satisfies
\[
\overline{H(x : y_1, y_2|e)} = \overline{H(x : y_1|y_2, e)} + \overline{H(x : y_2|e)} .
\]
\[ (99) \]
Permuting \( y_1 \) and \( y_2 \) in the previous equation yields
\[
\overline{H(x : y_2, y_1|e)} = \overline{H(x : y_2|y_1, e)} + \overline{H(x : y_1|e)} .
\]
\[ (100) \]
Recall that the CMI is non-negative.

- proof of (a)(2 → 1):\( h_1 = 0 \Rightarrow h_3 = 0 \).
- proof of (b)(2 → 1′):\( h_1 = 0 \Rightarrow h_2 = 0 \).
• proof of (c)(1′, 1 → 2): \( h_2 = h_3 = 0 \Rightarrow h_1 = 0 \).

• proof of (d)(1′, 1′ → 2): We want to show that \( h_2 = h_5 = 0 \Rightarrow h_1 = 0 \). Why would this be? \( h_2 = 0 \) and \( h_5 = 0 \) imply, respectively,

\[
P(x, y_1, y_2, e) = P(x|y_2, e)P(y_1|y_2, e)P(y_2, e), \tag{101a}
\]

and

\[
P(x, y_1, y_2, e) = P(x|y_1, e)P(y_2|y_1, e)P(y_1, e). \tag{101b}
\]

We can equate the right hand sides of the two previous equations, and then divide both sides of the resulting equation by \( P(y_1, y_2, e) \) (here we use \( P \neq 0 \)). This yields (i) below. Since we can vary \( y_1 \) and \( y_2 \) independently in equation (i) below, equation (ii) follows.

\[
P(x|y_1, e) \overset{(i)}{=} P(x|y_2, e) \overset{(ii)}{=} P(x|e). \tag{102}
\]

Combining Eqs. (101a) and (102) then yields,

\[
P(x, y_1, y_2, e) = P(x|e)P(y_1, y_2, e), \tag{103}
\]

which, in turn, yields

\[
P(x, y_1, y_2|e) = P(x|e)P(y_1, y_2|e). \tag{104}
\]

QED

**Theorem 7** The above reduction and combination rules are true in quantum physics with \( \eta = A \).

proof:

• proof of (a)(2 → 1): The premise is that

\[
A(x, y_1, y_2|e) = A(x|e)A(y_1, y_2|e). \tag{105}
\]

Eq. (105) implies

\[
P(x, y_1, y_2|e) = P(x|e)P(y_1, y_2|e). \tag{106}
\]

Summing both sides of the previous equation over \( y_1 \) yields

\[
P(x, y_2|e) = P(x|e)P(y_2|e). \tag{107}
\]
Eq. (105) also implies

$$\theta(x, y_1, y_2 | e) = \theta(x | e) \theta(y_1, y_2 | e) .$$ \hfill (108)

If, in the previous equation, we set $y_1$ to its reference state $y_1^o$, we get

$$\theta(x, y_2 | e) = \theta(x | e) \theta(y_2 | e) .$$ \hfill (109)

Combining Eqs. (107) and (109) yields

$$A(x, y_2 | e) = A(x | e) A(y_2 | e) .$$ \hfill (110)

- Proof of (b)(2 → 1'): One has

$$A(x|y_1, y_2, e) \overset{(i)}{=} A(x|e) \overset{(ii)}{=} A(x|y_2, e) .$$ \hfill (111)

(i) follows from the premise $\tau^A(x \perp y_1, y_2 | e)$. Plugging the premise into rule (a)(2 → 1) gives (ii).

- Proof of (c)(1', 1 → 2): One has

$$A(x|y_1, y_2, e) \overset{(i)}{=} A(x|y_2, e) \overset{(ii)}{=} A(x|e) .$$ \hfill (112)

(i) follows from the part $\tau^A(x \perp y_1, y_2 | e)$ of the premise. (ii) follows from the other part $\tau^A(x \perp y_2 | e)$ of the premise.

- Proof of (d)(1', 1' → 2): The premise is that

$$A(x|y_1, y_2, e) = A(x|y_2, e) ,$$ \hfill (113)

and

$$A(x|y_1, y_2, e) = A(x|y_1, e) .$$ \hfill (114)

Thus, if $A(x, y_1, y_2, e) \neq 0$,

$$A(x|y_2, e) = A(x|y_1, e) = A(x|e) .$$ \hfill (115)

Combining Eqs. (113) and (115) now yields

$$A(x|y_1, y_2, e) = A(x|e) .$$ \hfill (116)

QED

Exercise for reader: Find out whether $\tau_{sepG}^C, \tau_{CMI}^C$ and $\tau_{CMI'}^C$ satisfy the reduction and combination rules.
6.3 Probabilistic I-sets

In this section, we define certain probabilistic I-sets; that is, I-sets whose members are defined in terms of a probability distribution (or a meta density matrix).

First consider classical physics. For any $P \in pd(\text{St}_x)$, define

$$I(P) = \{ I : I = (x_J \perp x_K | x_E); J, K, E \subset Z_{1,N} \text{ are disjoint}; \tau^P(I) \}.$$  \quad (117)

Next consider quantum physics. For any meta density matrix $\mu \in dm(\mathcal{H}_x)$ of the form $\mu = \text{proj}(\sum_x A(x)|x.)$, let

$$I(A) = \{ I : I = (x_J \perp x_K | x_E); J, K, E \subset Z_{1,N} \text{ are disjoint}; \tau^A(I) \}.$$  \quad (118)

For $\eta = P, A$, when we say that an I-set $I$ is satisfied by $\eta$, we will mean that $\tau^\eta(I)$ for all $I \in I$ (or, equivalently, $I \subset I(\eta)$).

7 Bayesian Networks

In this section, we show that any probability distribution can be represented by a fully connected DAG. We also show that any quantum density matrix can be represented by a fully connected DAG. In classical and quantum physics, omitting certain arrows from this fully connected graph indicates certain probabilistic independencies.

7.1 Chain Rule and Factorization According to a Graph

In this section, we define a chain rule and factorization according to a DAG, both for classical and quantum physics.

First consider classical physics. Let $P \in dm(\mathcal{H}_x)$. For $N = 3$, the $P$ chain rule is

$$P(x_3, x_2, x_1) = \underbrace{P(x_3|x_2, x_1)}_{7} \underbrace{P(x_2|x_1)}_{4} \underbrace{P(x_1)}_{1}.$$  \quad (119)

We have indicated under each conditional probability the number of degrees of freedom that it holds, assuming that $x_1, x_2, x_3 \in \text{Bool}$. For arbitrary $N$, the $P$ chain rule is

$$P(x.) = \prod_{j=1}^{N} P(x_j|x_{Z_{1,j-1}}).$$  \quad (120)

Now consider quantum physics. Suppose $\mu \in dm(\mathcal{H}_x)$ is a meta density matrix of the form $\mu = \text{proj}(\sum_x A(x)|x.)$. In analogy to Eq. (119), we would like the $A$ chain rule for $N = 3$ to be
\[ A(x_3, x_2, x_1) = A(x_3|x_2, x_1)A(x_2|x_1)A(x_1) . \]  

(121)

The \( P \) chain rule Eq.(119) was stated without proof, because the equation is well known, and very easy to prove. On the other hand, the \( A \) chain rule Eq.(121) is new, so we prove it next.

From various definitions in Section 5, we get

\[ \theta(x_3|x_2, x_1) = \theta(x_3, x_2, x_1) - \theta(x_3, x_2, x_1) , \]  

(122a)

\[ \theta(x_2|x_1) = \theta(x_3, x_2, x_1) - \theta(x_3, x_2, x_1) , \]  

(122b)

and

\[ \theta(x_1) = \theta(x_3, x_2, x_1) - \theta(x_3, x_2, x_1) . \]  

(122c)

Summing Eqs.(122) (more precisely, equating the sum of the left hand sides of Eqs.(122) to the sum of the right hand sides) yields

\[ \theta(x_3|x_2, x_1) + \theta(x_2|x_1) + \theta(x_1) = \theta(x_3, x_2, x_1) . \]  

(123)

The previous equation, and the \( P \) chain rule, together imply:

\[ e^{i\theta(x_3, x_2, x_1)} P^1_7(x_3, x_2, x_1) = e^{i\theta(x_2|x_2, x_1)} P^1_4(x_3|x_2, x_1) e^{i\theta(x_2|x_1)} P^1_4(x_2|x_1) e^{i\theta(x_1)} P^1_2(x_1) . \]  

(124)

We have indicated under each quantity the number of degrees of freedom it holds, assuming \( x_1, x_2, x_3 \in \text{Bool} \). The previous equation is equivalent to Eq.(121), which we set out to prove. For arbitrary \( N \), Eq.(123) generalizes to

\[ \theta(x) = \sum_{j=1}^{N} \theta(x_j|x_{Z_{1,j}}) . \]  

(125)

The previous equation, and Eq.(120) (the \( P \) chain rule), together imply the \( A \) chain rule:

\[ A(x) = \prod_{j=1}^{N} A(x_j|x_{Z_{1,j}}) . \]  

(126)

Note that the conditional amplitudes \( A(x_j|x_{Z_{1,j}}) \) used above have **constrained phases (CP)**, meaning that their phases are subject to the constraint that \( A(x_j|x_{Z_{1,j}}) \) be real for all \( x_{Z_{1,j}} \). Let \( M \) be the matrix with entries \( A(x_j|x_{Z_{1,j}}) \), with the rows of \( M \) labelled by the states of \( x_j \) and the columns labelled by the states of \( x_{Z_{1,j}} \). CP means that \( M \) must have one row (the one with \( x_j = x_j^0 \)) consisting
entirely of real numbers. On the other hand, Quantum Fog allows conditional amplitudes \( A(x_j|x_{Z_1,j-1}) \) with **free phases** (FP), meaning that the phases of \( A(x_j|x_{Z_1,j-1}) \) are arbitrary. Clearly, it is often convenient, not just in Quantum Fog, to allow FP amplitudes. Luckily, one can always replace an FP amplitude \( A(x_j|x_{Z_1,j-1}) \) by a product of CP amplitudes. This is how. To simplify our notation, let \( x_j \to a \) and \( x_{Z_1,j-1} \to b \). Replace an FP amplitude \( A(b|a) \) by a product of three CP amplitudes \( A(b|a''), A(a''|a') \) and \( A(a'|a) \):

\[
A(b|a) = \sum_{a',a''} A(b|a'')A(a''|a')A(a'|a) , \tag{127}
\]

where \( a', a'' \in St_a \). \( A(b|a) \) can be interpreted as the transition matrix of node \( b \) in a subgraph

\[
(b) \leftarrow (a) . \tag{128}
\]

This subgraph is being replaced by a Markov-chain graph

\[
(b) \leftarrow (a'') \leftarrow (a') \leftarrow (a) . \tag{129}
\]

Define the following matrices:

\[
[A(b|a)] = F , \quad [A(b|a'')] = C_1 , \quad [A(a''|a')] = C_2 , \quad [A(a'|a)] = C_3 . \tag{130}
\]

Eq.(127), expressed in matrix form, is

\[
F = C_1C_2C_3 . \tag{131}
\]

Suppose the first row of \( F \) is \( [x_1 e^{i\phi_1}, x_2 e^{i\phi_2}, \ldots, x_N e^{i\phi_N}] \), where \( x_j, \phi_j \in \mathbb{R} \). Let

\[
C_1 = F \text{diag}(e^{-i\phi_1}, e^{-i\phi_2}, \ldots, e^{-i\phi_N}) , \quad C_2 = \text{diag}(1, e^{i\phi_2}, e^{i\phi_3}, \ldots, e^{i\phi_N}) , \quad C_3 = \text{diag}(e^{i\phi_1}, 1, 1, \ldots, 1) . \tag{132}
\]

The matrices \( C_1, C_2, C_3 \) all have at least one row that consisting entirely of reals, so these matrices specify CP amplitudes. (If global phases are allowed, only 2 C’s are necessary).

We end this section by defining graphic factorization. In classical physics, we say \( P \in pd(St_x) \) **factors according to** \( G \in DAG(x) \) iff

\[
P(x.) = \prod_{j=1}^{N} P(x_j|x_{pa(j)}) . \tag{133}
\]

In quantum physics, for a meta density matrix \( \mu \in dm(H_x) \) of the form \( \mu = \text{proj}(\sum_x A(x.)|x.>) \), we say \( A \) **factors according to** \( G \in DAG(x) \) iff
\[ A(x.) = \prod_{j=1}^{N} A(x_j|x_{pa(j)}) . \] (134)

By virtue of the \( P \) (ditto, \( A \)) chain rule, any probability distribution (ditto, probability amplitude) of \( x \) factors according to an \( N \)-node fully-connected DAG. If the probability distribution (ditto, probability amplitude) has higher symmetry, then it may also factor according to another \( N \)-node graph that possess fewer arrows than the fully-connected one.

### 7.2 Graphic I-sets

In Section 6.3, we defined some probabilistic I-sets. The elements of a **probabilistic I-set** are defined in terms of a probability distribution (or a meta density matrix). In this section, we define some graphic I-sets for a DAG. The elements of a **graphic I-set** are defined with respect to a graph.

For \( G \in \text{DAG}(x.) \), we define (loc=local, glo=global)

\[ \mathcal{I}_{\text{loc}}(G) = \{ I : I = (x_j \perp x_{\text{de}(j)}|x_{pa(j)}), j \in Z_{1,N} \} , \] (135)

and

\[ \mathcal{I}_{\text{glo}}(G) = \{ I : I = (x_I \perp x_K|x_E); J, K, E \subset Z_{1,N} \text{ are disjoint; } \tau_{\text{sep} G}(I) \} . \] (136)

The function \( \tau_{\text{sep} G} : \mathcal{I}(x.) \to \text{Bool} \) will be defined later on.

For example, if \( G \) is the graph of Fig.1(a), then

\[ \mathcal{I}_{\text{loc}}(G) = \{ (x_3 \perp x_2|x_1), (x_4 \perp x_1|x_2, x_3) \} . \] (137)

### 7.3 Graphic Factorization iff an I-set is satisfied

In this section, we show that a probability distribution (ditto, probability amplitude) factors according to a DAG iff the probability distribution (ditto, probability amplitude) satisfies a graphic I-set.

As motivation for the main theorem of this section, let \( G \) be the DAG of Fig.1(a). Note that \( \mathcal{I}_{\text{loc}}(G) \subset \mathcal{I}(P) \) iff \( \tau^P(I) \) for all \( I \in \mathcal{I}_{\text{loc}}(G) \). Therefore, for the graph \( G \) of Fig.1(a), \( \mathcal{I}_{\text{loc}}(G) \subset \mathcal{I}(P) \) is equivalent to

\[ \begin{cases} \tau^P(x_3 \perp x_2|x_1) \\ \tau^P(x_4 \perp x_1|x_2, x_3) \end{cases} . \] (138)

Eq.(138) is itself equivalent to

\[ \begin{cases} P(x_3|x_2, x_1) = P(x_3|x_1) \\ P(x_4|x_3, x_2, x_1) = P(x_4|x_3, x_2) \end{cases} . \] (139)
Define $P_{\text{chain}}$ and $P_{\text{graph}}$ as the following two probability distributions of $x$:

\[ P_{\text{chain}}(x.) = P(x_4|x_3, x_2, x_1)P(x_3|x_2, x_1)P(x_2|x_1)P(x_1), \]  

and

\[ P_{\text{graph}}(x.) = P(x_4|x_3, x_2)P(x_3|x_1)P(x_2|x_1)P(x_1). \]  

$P_{\text{chain}}$ comes from the $P$ chain rule and $P_{\text{graph}}$ from the definition of factorization according to the graph of Fig. 1(a). From Eqs. (139), (140) and (141), it is clear that:

If $\tau^P(I)$ for all $I \in \mathcal{I}_{\text{loc}}(G)$, then $P_{\text{chain}} = P_{\text{graph}}$. The converse statement is also true. This is why. $P_{\text{chain}} = P_{\text{graph}}$ implies

\[ P(x_4|x_3, x_2, x_1)P(x_3|x_2, x_1) = P(x_4|x_3, x_2)P(x_3|x_1). \]

Summing both sides over $x_4$ gives $P(x_3|x_2, x_1) = P(x_3|x_1)$. Combining this result with Eq. (142) then gives $P(x_4|x_3, x_2, x_1) = P(x_4|x_3, x_2)$. Thus, Eqs. (139) are obeyed. We have just proven, albeit only for the graph of Fig. 1(a), the following theorem:

**Theorem 8** Suppose $G \in \text{DAG}(x.)$ and $P \in \text{pd}(\text{St}_x)$. $P$ factors according to $G$ iff $\mathcal{I}_{\text{loc}}(G) \subset \mathcal{I}(P)$.

**proof:** The proof is a special case of the proof of the next theorem.

QED

**Theorem 9** Suppose $G \in \text{DAG}(x.)$ and $\mu \in \text{dm}(\mathcal{H}_x)$ is a meta density matrix of the form $\mu = \text{proj}(\sum_x A(x.)|x.)$.

$A$ factors according to $G$ iff $\mathcal{I}_{\text{loc}}(G) \subset \mathcal{I}(A)$.

**proof:** Without loss of generality, we can assume that the nodes are labelled so that $\text{pa}(j) \subset \mathcal{Z}_{1,j-1}$ for all $j$. This means that we can always add arrows to $G$ until we generate a fully connected graph $\overline{G}$ such that $\text{pa}(j) = \mathcal{Z}_{1,j-1}$. We will call $\overline{G}$ a proper fully-connected extension of $G$. What we need to prove can now be rephrased as:

\[ A_{\text{chain}} = A_{\text{graph}} \text{ iff } \tau^A(x_j \perp \underline{x}_{\text{de}(j)}|x_{\text{pa}(j)}) \ \forall j, \]  

where

\[ A_{\text{chain}}(x.) = \prod_{j=1}^{N} A(x_j|x_{\mathcal{Z}_{1,j-1}}), \quad A_{\text{graph}}(x.) = \prod_{j=1}^{N} A(x_j|x_{\text{pa}(j)}). \]  

(\(\Leftrightarrow\)) Define $\mathcal{Z}_{1,j-1}' = \mathcal{Z}_{1,j-1} - \text{pa}(j)$. Since $\tau^A(x_j \perp \underline{x}_{\text{de}(j)}|x_{\text{pa}(j)})$ and $\mathcal{Z}_{1,j-1}' \subset \mathcal{Z}_{1,j-1} \subset \neg\text{de}(j)$, it follows from reduction rule 2 $\rightarrow 1$ that $\tau^A(x_j \perp \underline{x}_{\mathcal{Z}_{1,j-1}'|x_{\text{pa}(j)}}).$ Thus,

\[ A(x_j|x_{\mathcal{Z}_{1,j-1}}) = A(x_j|x_{\mathcal{Z}_{1,j-1}'|x_{\text{pa}(j)}}) \]  

\[ = A(x_j|x_{\text{pa}(j)}). \]  

31
(⇒) $A_{\text{chain}} = A_{\text{graph}}$ implies that

$$\prod_{j=1}^{N} P(x_{j}|x_{Z_{1,j-1}}) = \prod_{j=1}^{N} P(x_{j}|x_{pa(j)}).$$

(146)

- Sum both sides of Eq. (146) over $x_{Z_{2,N}}$. Get $P(x_{1}) = P(x_{1})$.
- Divide both sides of Eq. (146) by $P(x_{1})$, and then sum both sides over $x_{Z_{3,N}}$. Get $P(x_{2}|x_{1}) = P(x_{2}|x_{pa(2)})$.
- Divide both sides of Eq. (146) by $P(x_{2}, x_{1})$, and then sum both sides over $x_{Z_{4,N}}$. Get $P(x_{3}|x_{2}, x_{1}) = P(x_{3}|x_{pa(3)})$.
- Divide both sides of Eq. (146) by $P(x_{3}, x_{2}, x_{1})$, and then sum both sides over $x_{Z_{5,N}}$. Get $P(x_{4}|x_{3}, x_{2}, x_{1}) = P(x_{4}|x_{pa(4)})$.
- And so on.

Thus, by induction,

$$P(x_{j}|x_{Z_{1,j-1}}) = P(x_{j}|x_{pa(j)})$$

(147)

for all $j$.

$A_{\text{chain}} = A_{\text{graph}}$ also implies that

$$\sum_{j=1}^{N} \theta(x_{j}|x_{Z_{1,j-1}}) = \sum_{j=1}^{N} \theta(x_{j}|x_{pa(j)}).$$

(148)

Recall that $\theta(x_{j}^{o}|x_{Z_{1,j-1}}) = 0$.

- Set $x_{Z_{2,N}} \rightarrow x_{Z_{2,N}}^{o}$ in Eq. (148). Get $\theta(x_{1}) = \theta(x_{1})$.
- Set $x_{Z_{3,N}} \rightarrow x_{Z_{3,N}}^{o}$ in Eq. (148) and subtract $\theta(x_{1})$ from both sides. Get $\theta(x_{2}|x_{1}) = \theta(x_{2}|x_{pa(2)})$.
- Set $x_{Z_{4,N}} \rightarrow x_{Z_{4,N}}^{o}$ in Eq. (148) and subtract $\theta(x_{2}, x_{1})$ from both sides. Get $\theta(x_{3}|x_{2}, x_{1}) = \theta(x_{3}|x_{pa(3)})$.
- Set $x_{Z_{5,N}} \rightarrow x_{Z_{5,N}}^{o}$ in Eq. (148) and subtract $\theta(x_{3}, x_{2}, x_{1})$ from both sides. Get $\theta(x_{4}|x_{3}, x_{2}, x_{1}) = \theta(x_{4}|x_{pa(4)})$.
- And so on.
Thus, by induction,

\[ \theta(x_j|x_{Z_{1,j-1}}) = \theta(x_j|x_{pa(j)}) \]  

(149)

for all \( j \). Combining Eq. (147) and (149) yields

\[ A(x_j|x_{Z_{1,j-1}}) = A(x_j|x_{pa(j)}) \]

(150)

for all \( j \). Note that \( \neg de(j) \supset Z_{1,j-1} \). From a proper fully-connected extension of \( G \), it is clear that

\[ A(x_j|x_{\neg de(j)}) = A(x_j|x_{Z_{1,j-1}}) \]

(151)

for all \( j \). Combining the previous two equations yields

\[ A(x_j|x_{\neg de(j)}) = A(x_j|x_{pa(j)}) \]

(152)

for all \( j \). Define \( \neg de'(j) = \neg de(j) - pa(j) \). The previous equation can be written as

\[ A(x_j|x_{\neg de'(j)}, x_{pa(j)}) = A(x_j|x_{pa(j)}) \]

which means that \( \tau^A(x_j \perp \bar{x}_{\neg de'(j)}|x_{pa(j)}) \). Thus, \( \tau^A(x_j \perp \bar{x}_{\neg de(j)}|x_{pa(j)}) \).

QED

7.4 Going Global

In the last section, we showed that a probability distribution \( P \) (or a probability amplitude \( A \)) factors according to a DAG iff it satisfies a certain non-global, graphic I-set. Does a similar result hold if the non-global graphic I-set is replaced by a global graphic one? This section will be devoted to answering this question.
Figure 5: Some simple Bayesian nets and their truth value for $\tau^{\eta}(x \perp y \mid \perp)$, which is the same as their truth value for $\tau^{A}(x \perp y \mid \perp)$. The independency $(x \perp y \mid \perp)$ is conditioned on the grounded nodes. T=true, F=false.

To develop some intuition, we begin by considering Fig.5, which shows some simple Bayesian net examples.

Column 1 of Fig.5 shows four DAGs in which, respectively, node $a$ is:

1. a serial node of a path from $x$ to $y$.
2. (“common cause” graph) a divergence node of a path from $x$ to $y$.
3. (“common effect”, “explaining away” graph) a convergence (a.k.a. collider) node of a path from $x$ to $y$.
4. the descendant of a collider node of a path from $x$ to $y$.
Column 2 of Fig.5 illustrates two special cases of the graphs in column 1: (1) no node is grounded, (2) only node $a$ is grounded. Nodes decorated with a $\Sigma$ are summed over for $\eta = P$ and traced over for $\eta = A$.

In Fig.5 the argument of $\tau^\eta$ is an independency whose third slot is filled with the grounded nodes. In Fig.5, the grounded nodes are always either $a$ or nothing. An independency with no grounded nodes is unconditional. In the classical physics case, column 3 of Fig.5 gives the truth values (T=true, F=false) of $\tau^P(I)$, for the graphs in column 2. In the quantum physics case, column 3 gives the values of $\tau^A(I)$.

Next, we show how we calculated the truth values of $\tau^A(I)$ in Fig.5. Let $A = P_x e^{i\theta}$.

Rows 1 and 2 (graphs in which $a$ is a serial node) satisfy

$$A(x, y, a) = A(y|a)A(a|x)A(x) = A(y|a)A(x|a)A(a),$$

for all $x, y, a$. Eq. (153) implies

$$P(x, y) = \sum_a P(y|a)P(x|a)P(a) \neq P(x)P(y), \quad A(x, y) \neq A(x)A(y).$$

$\tau^P(x \perp y)$ is false so $\tau^A(x \perp y)$ is false too. Eq. (153) implies

$$A(x, y|a) = A(y|a)A(x|a),$$

so $\tau^A(x \perp y|a)$ is true.

Rows 3 and 4 with divergence node $a$ must have the same truth values as rows 1 and 2 with serial node $a$. That’s because the Bayesian nets

$$(x) \rightarrow (a) \rightarrow (y)$$

and

$$(x) \leftarrow (a) \rightarrow (y)$$

are indistinguishable: they both represent the same full joint amplitude. Indeed, $A_1(x, y, a) = A(y|a)A(a|x)A(x)$ for the first and $A_2(x, y, a) = A(y|a)A(x|a)A(a)$ for the second, and $A_1 = A_2$.

Rows 5 and 6 (graphs in which $a$ is a collider node) satisfy

$$A(x, y, a) = A(a|x, y)A(y)A(x),$$

for all $x, y, a$. Therefore, $P(x, y) = P(x)P(y), \theta(x, y) = \theta(x)\theta(y)$. Hence, $\tau^A(x \perp y)$ is true. $\tau^P(x \perp y|a)$ is false so $\tau^A(x \perp y|a)$ is false too.

---

5 Sometimes, some of the arrows of a classical Bayesian can be reversed without changing the full joint probability distribution of the net. General rules have been given in the literature (see Ref.[1]) for deciding which arrows can be reversed with impunity. Similar rules apply for quantum Bayesian nets.
Rows 7 and 8 (graphs in which $a$ is a descendant of a collider node) satisfy
\[ A(x, y, a, b) = \frac{A(a|b)A(b|x, y)A(x)A(y)}{A(b|x)} \]
(159)
for all $x, y, a, b$. Therefore, $P(x, y) = P(x|y)P(y) \theta(x, y) = \theta(x)\theta(y)$. Hence, $\tau^A(x \perp y)$ is true. $\tau^P(x \perp y|a)$ is false so $\tau^A(x \perp y|a)$ is false too.

Note that the calculations of the truth values of $\tau^P(I)$ in Fig.5 are a special case of the just presented calculations of the truth values of $\tau^A(I)$.

The moral of Fig.5 is that grounding a serial node or a divergence node interrupts information transmission between $x$ and $y$. A non-vacuous message has variation in it, and a grounded node in its path prevents transmission of this variation. However, grounding a collider or a descendant of a collider has the opposite effect: it allows information transmission (this is called the “explaining away” phenomenon).

So far, this section has presented merely anecdotal evidence. Next, we will state and prove some general theorems.

Consider any $G \in \text{DAG}(x)$. Suppose $J, K, E \subset Z_{1,N}$ are disjoint sets. Let $I = (x_J \perp x_K | x_E)$. We will abbreviate “dependency separation” by “d-sep” or just “sep”. We define the function $\tau_{\text{sep} G} : I(G) \rightarrow \text{Bool}$ by the statement: $\tau_{\text{sep} G}(I)$ is true iff all paths $\gamma$ in $G$ from a node in $x_J$ to a node in $x_K$ are blocked by $x_E$. We say “$\gamma$ is blocked by $x_E$” iff there exists a node $x_i \in \gamma$ that satisfies one of the following:

1. $x_i$ is a non-collider of $\gamma$ and $i \in E$.
2. $x_i$ is a collider of $\gamma$ and $\overline{\text{de}}(i) \cap E = \emptyset$

**Theorem 10** (Classical d-Separation Theorem) Suppose $G \in \text{DAG}(x)$ and $P \in \text{pd}(\text{St}_X)$. If $P$ factors according to $G$ then $\mathcal{I}_{\text{glo}}(G) \subset \mathcal{I}(P)$.

**proof:** The proof of this theorem can be found in the literature[1][2].

QED

**Theorem 11** (Quantum d-Separation Theorem) Suppose $G \in \text{DAG}(x)$ and $\mu \in \text{dm}(\mathcal{H}_x)$ is a meta density matrix of the form $\mu = \text{proj}(\sum x . A(x) | x .)$. If $A$ factors according to $G$ then $\mathcal{I}_{\text{glo}}(G) \subset \mathcal{I}(A)$.

**proof:** The proof of this theorem is a simple generalization of the proof of Theorem [10]

QED

One can also prove a weak converse of the d-Separation Theorem. The weak converse theorem[1] shows that $\mathcal{I}_{\text{glo}}(G)$ is in some sense the maximal set for which the d-Separation Theorem holds. For this reason, Ref.[1] describes the d-Separation Theorem as a proof of soundness and its weak converse as a proof of completeness.
8 Markov Networks

In this section, we show that any probability distribution can be represented by a fully connected UG. We also show that any quantum density matrix can be represented by a fully connected UG. In classical and quantum physics, omitting certain links from this fully connected graph indicates certain probabilistic independencies.

8.1 Power-set Rule and Factorization According to a Graph

In this section, we define a power-set rule and factorization according to an UG, both for classical and quantum physics. The $P$ power-set rule is well known, but not by that name, which is ours. In some sense, the $P$ (ditto, $A$) power-set rule is to Markov nets what the $P$ (ditto, $A$) chain rule is to Bayesian nets.

**Theorem 12** ($P$ Power-set Rule) Any $P \in \mathrm{pd}(\mathcal{S}_{x_1})$ can be expressed as

$$P(x.) = \prod_{J: J \subset Z_{1,N}} e^{\lambda(x.J)} ,$$  \hspace{1cm} (160)

where $\lambda(x.J)$ is defined by

$$\lambda(x.J) = \sum_{J': J' \subset J} (-1)^{|J-J'|} \ln P(x.J', x^{0}_{(J')c}) .$$  \hspace{1cm} (161)

(Note that if for some point $x.'$, $P(x.'.) = 0$, then $\lambda(x.J) = -\infty$ for some $J$. Instead of permitting such infinities, as we do, some authors restrict this theorem by adding a premise that $P \neq 0$.)

**proof:** The proof is a special case of the proof of the next theorem.

QED

**Theorem 13** ($A$ Power-set Rule) Given a meta density matrix $\mu \in \mathrm{dm}(\mathcal{H}_{x1})$ of the form $\mu = \mathrm{proj}(\sum_{x.} A(x.)|x.\rangle)$, $A$ can be expressed as

$$A(x.) = \prod_{J: J \subset Z_{1,N}} e^{\lambda(x.J)} ,$$  \hspace{1cm} (162)

where $\lambda(x.J)$ is defined by

$$\lambda(x.J) = \sum_{J': J' \subset J} (-1)^{|J-J'|} \ln A(x.J', x^{0}_{(J')c}) .$$  \hspace{1cm} (163)

(Note that if for some point $x.'$, $A(x.'.) = 0$, then $\mathrm{Re}(\lambda(x.J)) = -\infty$ for some $J$. Instead of permitting such infinities, as we do, some authors restrict this theorem by adding a premise that $A \neq 0$.)
proof: Performing a Mobius Inversion (see Appendix A) on Eq.(163), we get
\[
\ln A(x_J, x_{(J^c)}) = \sum_{J', J' \subseteq J} \lambda(x_{J'}) .
\] (164)
Replacing \( J \) by \( Z_{1,N} \) in the previous equation yields:
\[
\ln A(x) = \sum_{J: J \subseteq Z_{1,N}} \lambda(x_J) .
\] (165)
QED

For \( N \) random variables, the \( P \) (ditto, \( A \)) chain rule contains \( N \) factors whereas the \( P \) (ditto, \( A \)) power-set rule contains \( 2^N \). Thus, a power-set rule is not as useful as a chain rule for practical purposes like numerical calculation. It is mainly used to prove other theorems.

We end this section by defining graphic factorization. In classical physics, we say \( P \in pd(St_x) \) factors according to \( G \in UG(x) \) iff \( P \) can be expressed in the form of
\[
P(x) = \prod_{J \in super-cliques(G)} e^{\lambda(x_J)} .
\] (166)
In quantum physics, for a meta density matrix \( \mu \in dm(H_x) \) of the form \( \mu = \text{proj}(\sum_x A(x) | x \rangle \rangle) \), we say \( A \) factors according to \( G \in UG(x) \) iff \( A \) can be expressed in the form of
\[
A(x) = \prod_{J \in super-cliques(G)} e^{\lambda(x_J)} .
\] (167)

When \( G \) is fully connected, Eq.(167) reduces to \( A(x) = e^{\lambda(x)} \), which is always possible. Thus, any probability distribution (ditto, probability amplitude) of \( x \) factors according to an \( N \)-node fully-connected UG. If the probability distribution (ditto, probability amplitude) has higher symmetry, then it may also factor according to another \( N \)-node graph that possess fewer links than the fully-connected one.

8.2 Graphic I-sets

In Section 7.2 we defined some graphic I-sets for a DAG. In this section, we define some graphic I-sets for an UG.

For \( G \in UG(x) \), we define (loc=local, glo=global)
\[
\mathcal{I}_{\text{pair}}(G) = \{ I : I = (x_{j_1} \perp x_{j_2} | x_{Z_{1,N}-(j_1,j_2)}), j_1 \notin ne(j_2); j_1, j_2 \in Z_{1,N} \} ,
\] (168)
\[
\mathcal{I}_{\text{loc}}(G) = \{ I : I = (x_j \perp x_{Z_{1,N}-\overline{ne}(j)} | x_{\overline{ne}(j)}), j \in Z_{1,N} \} ,
\] (169)
\[ \mathcal{I}_{\text{gl}(G)} = \{ I : I = (x_I \perp x_K|x_E) ; J, K, E \subset Z_{1,N} \text{ are disjoint}; \tau_{\text{sep} G}(I) \}. \quad (170) \]

The function \( \tau_{\text{sep} G} : \mathcal{I}(x) \to \text{Bool} \) will be defined later on.

### 8.3 Graphic Factorization iff an I-set is satisfied

In this section, we show that a probability distribution (ditto, probability amplitude) factors according to an UG iff the probability distribution (ditto, probability amplitude) satisfies a graphic I-set.

**Theorem 14** Suppose \( G \in \text{UG}(x) \) and \( P \in \text{pd}(\text{St}(x)) \).

\( P \) factors according to \( G \) \( \iff \) \( \mathcal{I}_{\text{pair}}(G) \subset \mathcal{I}(P) \).

**proof:** The proof is a special case of the proof of the next theorem.

QED

**Theorem 15** Suppose \( G \in \text{UG}(x) \) and \( \mu \in \text{dm}(\mathcal{H}(x)) \) is a meta density matrix of the form \( \mu = \text{proj}(\sum_x A(x)|x>) \).

\( A \) factors according to \( G \) \( \iff \) \( \mathcal{I}_{\text{pair}}(G) \subset \mathcal{I}(A) \).

**proof:** If the number of nodes \( N \) is one then the theorem is satisfied trivially, so assume \( N \geq 2 \). Recall \( A \) factors according to \( G \) iff

\[ A(x) = \prod_{J \in \text{super-cliques}(G)} e^{\lambda(x_J)}. \quad (171) \]

Note that \( \mathcal{I}_{\text{pair}}(G) \subset \mathcal{I}(A) \) iff \( \tau^A(x_{j_1} \perp x_{j_2}|x_{Z_{1,N}-\{j_1,j_2\}}) \) for all \( j_1, j_2 \in Z_{1,N} \) such that \( j_1 \notin \text{ne}(j_2) \).

\[ (\iff) \text{(This direction would require a premise } A \neq 0 \text{ if we weren’t permitting infinite } |\lambda(x_J)|). \]

Consider any \( J \subset Z_{1,N} \). Suppose \( j_1, j_2 \) are any two elements of \( J \) (there may or may not be a link between \( x_{j_1} \) and \( x_{j_2} \) at this point). Let \( J^- \) denote \( J - \{j_1,j_2\} \). Note that for any function \( f_j : 2^J \to \mathbb{C} \)

\[ \sum_{J' : J' \subset J} f_{J'} = \sum_{J' : J' \subset J^-} \left( f_{J'-} + f_{J' \cup \{j_1,j_2\}} + f_{J' \cup \{j_1\}} + f_{J' \cup \{j_2\}} \right) . \quad (172) \]

Now define \( \xi \) by

\[ \xi = (x_{J'-}, x^{o}_{Z_{1,N}-\{j_1,j_2\}-J'}) . \quad (173) \]

Using Eq.(172), Eq.(163) can be re-written as
\[
\lambda(x_j) = \sum_{J' \subseteq J - \{j\}} (-1)^{|J' - J - |} \ln \left[ \frac{A(x_{j_1}, x_{j_2}; \xi)A(x_{j_1}, \xi)}{A(x_{j_1}, x_{j_2}; \xi)A(x_{j_1}, x_{j_2'}, \xi)} \right]. \tag{174}
\]

If \( x_{j_1} \) and \( x_{j_2} \) are not in the same super-clique, then there is no link between them. If \( j_1 \notin ne(j_2) \) so \( \tau^\lambda(x_{j_1}, x_{j_2}; x_{z_1,n-(j_1, j_2)}) \), so

\[
A(x'_{j_1}, x'_{j_2}; \xi) = A(x'_{j_1}; \xi)A(x'_{j_2}; \xi), \tag{175}
\]

for all \( x'_{j_1} \in N_{x_{j_1}} \) and \( x'_{j_2} \in N_{x_{j_2}} \). When Eq.\( (175) \) is true, the right hand side of Eq.\( (174) \) vanishes. In conclusion, if \( j_1, j_2 \in J \) but \( x_{j_1} \) and \( x_{j_2} \) are not in the same super-clique, then \( \lambda(x_j) = 0 \). In general, \( A(x) = \prod_{J \subseteq z_{1,n}} e^{\lambda(x_j)} \). (This would require \( A \neq 0 \) if infinite \( |\lambda(x_j)| \) were not permitted.) But we have shown that \( \lambda(x_j) \) vanishes for any \( J \subseteq z_{1,n} \) which is not a super-clique of \( G \). Thus, Eq.\( (171) \) follows.

\( \Rightarrow \) Let \( j_1, j_2 \in z_{1,n} \) such that \( j_1 \notin ne(j_2) \). Define \( R = z_{1,n} - \{j_1, j_2\}. x_{j_1} \) and \( x_{j_2} \) must belong to different super-cliques of \( G \). This fact and Eq.\( (171) \) together imply that there exist sets \( R_1, R_2 \) (not necessarily disjoint) such that \( R = R_1 \cup R_2 \) and such that \( A(x) \) can be expressed as a product of two terms as follows:

\[
A(x_{j_1}, x_{j_2}, x_R) = \alpha_1(x_{j_1}, x_{R_1})\alpha_2(x_{j_2}, x_{R_2}). \tag{176}
\]

As usual, let \( A(x) = P^\frac{1}{2}(x)e^{\theta(x)} \). The previous equation implies that \( P(x) \) can be expressed as a product of two terms as follows:

\[
P(x_{j_1}, x_{j_2}, x_R) = q_1(x_{j_1}, x_{R_1})q_2(x_{j_2}, x_{R_2}). \tag{177}
\]

Summing both sides of Eq.\( (177) \) over \( x_{j_2} \), over \( x_{j_1} \) and over both, gives, respectively,

\[
P(x_{j_1}, x_R) = q_1(x_{j_1}, x_{R_1})\tilde{q}_2(x_{R_2}), \tag{178}
\]

\[
P(x_{j_2}, x_R) = \tilde{q}_1(x_{R_1})q_2(x_{j_2}, x_{R_2}), \tag{179}
\]

and

\[
P(x_R) = \tilde{q}_1(x_{R_1})\tilde{q}_2(x_{R_2}). \tag{180}
\]

From Eqs.\( (177) \) to \( (180) \), it is clear that

\[
P(x_{j_1}, x_{j_2}, x_R) = P(x_{j_1}, x_R)P(x_{j_2}, x_R). \tag{181}
\]

Eq.\( (176) \) implies that \( \theta(x) \) can be expressed as a sum of two terms as follows:

\[
\theta(x_{j_1}, x_{j_2}, x_R) = \omega_1(x_{j_1}, x_{R_1}) + \omega_2(x_{j_2}, x_{R_2}). \tag{182}
\]
Eq. (182) immediately yields

\[
\theta(x_j, x_{j_2}|x_R) = \theta(x_j, x_j x_R) - \theta(x_j^o, x_{j_2}^o, x_R) \\
= \left\{ \begin{array}{l}
[\omega_1(x_j, x_{R_1}) + \omega_2(x_{j_2}, x_{R_2})] \\
- [\omega_1(x_j^o, x_{R_1}) + \omega_2(x_{j_2}^o, x_{R_2})]
\end{array} \right.,
\]

\[\theta(x_j^o, x_{j_2}^o|x_R) = \omega_1(x_j, x_{R_1}) - \omega_1(x_j^o, x_{R_1}), \quad (183a)\]

\[\theta(x_j^o, x_{j_2}^o|x_R) = \omega_2(x_{j_2}, x_{R_2}) - \omega_2(x_{j_2}^o, x_{R_2}). \quad (183b)\]

and

\[
\theta(x_{j_1}|x_R) = \theta(x_{j_1}, x_{j_2}|x_R) \\
= \omega_1(x_{j_1}, x_{R_1}) - \omega_1(x_{j_1}^o, x_{R_1}), \quad (184a)\]

\[\theta(x_{j_1}, x_{j_2}|x_R) = \theta(x_{j_1}|x_R) + \theta(x_{j_2}|x_R). \quad (184b)\]

Thus,

\[\theta(x_{j_1}, x_{j_2}|x_R) = \theta(x_{j_1}|x_R) + \theta(x_{j_2}|x_R). \quad (185)\]

Combining Eqs. (181) and (186), we get

\[A(x_{j_1}, x_{j_2}|x_R) = A(x_{j_1}|x_R)A(x_{j_2}|x_R). \quad (187)\]

QED

8.4 Going Global

In the last section, we showed that a probability distribution \(P\) (or a probability amplitude \(A\)) factors according to an UG iff it satisfies a certain non-global, graphic I-set. Does a similar result hold if the non-global graphic I-set is replaced by a global graphic one? This section will be devoted to answering this question.

Consider any \(G \in UG(x)\). Suppose \(J, K, E \subset Z_{1,N}\) are disjoint sets. Let \(I = (x_J \perp x_K|x_E)\). We define the function \(\tau_{\text{sep}} G : T(x) \rightarrow \text{Bool}\) by the statement: \(\tau_{\text{sep}} G(I)\) is true iff all paths \(\gamma\) in \(G\) from a node in \(x_J\) to a node in \(x_K\) are blocked by \(x_E\). We say “\(\gamma\) is blocked by \(x_E\)” iff there exists a node \(x_i \in \gamma\) that satisfies \(i \in E\).

**Theorem 16** Suppose \(G \in UG(x)\) and \(P \in pd(St_x)\). For \(\xi \in \{\text{glo, loc, pair}\}\), let \(\Phi_\xi\) denote the statement \(I_\xi(G) \subset \overline{T}(P)\).

\[\Phi_{\text{glo}} \Rightarrow \Phi_{\text{loc}} \Rightarrow \Phi_{\text{pair}}.\]

If \(P \neq 0\), \(\Phi_{\text{glo}} \Leftrightarrow \Phi_{\text{loc}} \Leftrightarrow \Phi_{\text{pair}}.\]
proof: The proof is a special case of the proof of the next theorem.

QED

Theorem 17 Suppose $G \in UG(x)$ and $\mu \in dm(H_\xi)$ is a meta density matrix of the form $\mu = \text{proj}(\sum_x A(x)|x,\xi\rangle).$ For $\xi \in \{\text{glo, loc, pair}\},$ let $\Phi_\xi$ denote the statement $\mathcal{I}_\xi(G) \subset \mathcal{I}(A).$

$\Phi_\text{glo} \Rightarrow \Phi_\text{loc} \Rightarrow \Phi_\text{pair}.$

If $A \neq 0,$ $\Phi_\text{glo} \Leftrightarrow \Phi_\text{loc} \Leftrightarrow \Phi_\text{pair}.$

proof:

proof that $\Phi_\text{glo} \Rightarrow \Phi_\text{loc}:$ Let $I = (x_i \perp x_{Z_{1,N} - \pi e(j)} | x_{ne(j)}) \in \mathcal{I}_\text{loc}(G).$ $\tau^A(I)$ so $\tau^A(I)$.

proof that $\Phi_\text{loc} \Rightarrow \Phi_\text{pair}:$ Suppose $j_1, j_2 \in Z_{1,N}$ and $j_1 \not\in ne(j_2).$ $\tau^A(x_{j_1} \perp x_{Z_{1,N} - \pi e(j_1)} | x_{ne(j_1)})$ and $j_2 \in Z_{1,N} - \pi e(j_1)$ so, using the reduction rule $2 \to 1',$ we get $\tau^A(x_{j_1} \perp x_{j_2} | x_{Z_{1,N} - \{j_1,j_2\}}.$

proof that $(A \neq 0, \Phi_\text{pair}) \Rightarrow \Phi_\text{glo}:$ Suppose $J, K, E \subset Z_{1,N}$ are disjoint sets.

Let $I = (x_J \perp x_K | x_E).$ Note that $\Phi_\text{pair}$ is equivalent to: $\tau^A(x_{j_1} \perp x_{j_2} | x_{Z_{1,N} - \{j_1,j_2\}})$ for $j_1 \not\in ne(j_2).$ What we want to prove is $\Phi_\text{sep},$ which is equivalent to: $\tau_{sep}(I) \Rightarrow \tau^A(I)$. If we can prove the theorem when $|J| + |K| + |E| = N,$ then the other cases will follow. This is why. Suppose $|J| + |K| + |E| < N$ and $r \in Z_{1,N} - J - K - E.$ Assume $\tau_{sep}(I).$ Since $\tau_{sep}(I)$ is true, either $\tau_{sep}(x_J, x_r \perp x_K | x_E)$ or $\tau_{sep}(x_J \perp x_K, x_r | x_E)$ must be true. For if both were false, there would be a path from a node in $x_J$ to a node in $x_K$ that was not blocked by $x_E,$ contradicting $\tau_{sep}(I).$ In general, all the nodes that are not in $x_J, x_K, x_E,$ can be put in either the $J$ side (if they are d-separated from the $K$ side) or the $K$ side (if they are d-separated from the $J$ side). Thus, there exist disjoint sets $J_{fat}$ and $K_{fat}$ such that $J_{fat} \supset J, K_{fat} \supset K,$ $|J_{fat}| + |K_{fat}| + |E| = N,$ and such that $I_{fat} = (x_{J_{fat}} \perp x_{K_{fat}} | x_E)$ satisfies $\tau_{sep}(I_{fat}).$ If we can prove that $\tau_{sep}(I_{fat}) \Rightarrow \tau^A(I_{fat}),$ then, by virtue of the reduction rule $2 \to 1,$ $\tau^A(I)$ will follow.

It now remains for us to prove the theorem for the fat case when $|J| + |K| + |E| = N.$ The proof is by induction in $|J| + |K|.$

When $|J| + |K| = 2,$ $J = \{j\},$ $K = \{k\},$ $I = (x_j \perp x_k | x_e).$ Assume $\tau_{sep}(G).$

It follows that $\tau_{sep}(G).$ Hence, $I \in \mathcal{I}_{\text{pair}}(G).$ Hence, $\tau^A(I).$

Now assume $\tau_{sep}(I) \Rightarrow \tau^A(I)$ when $|J| + |K| \in Z_{2,\alpha}$ and try to prove it for $|J| + |K| = \alpha + 1 > 2.$ Either $|J|$ or $|K|$ is greater than two, so we may assume, without loss of generality, that $|K| > 2.$ Let $k \in K$ and $K' = K - \{k\}.$ Let $I_1 = (x_j \perp x_K, x_{E \cup \{k\}})$, and $I_2 = (x_j \perp x_k, x_{E \cup K}).$ Assume $\tau_{sep}(G).$ It follows that $\tau_{sep}(I_1)$ and $\tau_{sep}(I_2).$ Furthermore, $|J| + |K'| < \alpha + 1$ and $|J| + 1 < \alpha + 1$ so, by the inductive hypothesis, $\tau^A(1)$ and $\tau^A(2)$ together imply $\tau^A(I).$

QED
Theorem 18 (Classical d-Separation Theorem) Suppose \( G \in UG(x) \) and \( P \in pd(St_x) \). If \( P \neq 0 \) and \( P \) factors according to \( G \), then \( \mathcal{I}_{glo}(G) \subset \mathcal{I}(P) \).

**proof:** Follows from Theorems 14 and 16. QED

Theorem 19 (Quantum d-Separation Theorem) Suppose \( G \in UG(x) \) and \( \mu \in dm(\mathcal{H}_x) \) is a meta density matrix of the form \( \mu = \text{proj}(\sum_x A(x)|x.) \). If \( A \neq 0 \) and \( A \) factors according to \( G \), then \( \mathcal{I}_{glo}(G) \subset \mathcal{I}(A) \).

**proof:** Follows from Theorems 15 and 17. QED

### 9 d-Separation and Quantum Entanglement

In this section, we show that the quantum d-separation rules for Bayesian and Markov graphs can be used to detect pairs \((x_J, x_K)\) in a graph that are unentangled.

For \( G \in DAG(x) \), define

\[
\mathcal{D}_{glo}(G) = \{ (x_J, x_K) : J, K \subset Z_{1,N} \text{ are disjoint} ; \tau_{sep G}(x_J \perp x_K | x_{Z_{1,N}-J-K}) \} . \tag{188}
\]

For \( G \in UG(x) \), define \( \mathcal{D}_{glo}(G) \) in the same way. The function \( \tau_{sep G} \) has been defined previously. Its definition is different for DAGs than for UGs.

For a meta-density matrix \( \mu = \text{proj}(\sum_x A(x)|x.) \), define

\[
\mathcal{D}(A) = \{ (x_J, x_K) : J, K \subset Z_{1,N} \text{ are disjoint} ; E^{CMI}_{\mu}(x_J : x_K) = 0 \} . \tag{189}
\]

**Theorem 20** Suppose \( G \in DAG(x) \) (ditto, \( G \in UG(x) \)) and \( \mu \in dm(\mathcal{H}_x) \) is a meta density matrix of the form \( \mu = \text{proj}(\sum_x A(x)|x.) \). If \( A \) factors according to \( G \), then \( \mathcal{D}_{glo}(G) \subset \mathcal{D}(A) \).

**proof:** Assume \( A \) factors according to \( G \in DAG(x) \) (ditto, \( G \in UG(x) \)). Let \( J, K \subset Z_{1,N} \) be disjoint sets. Let \( E = Z_{1,N} - J - K \). Let \( I = (x_J \perp x_K | x_E) \). Assume \( \tau_{sep G}(I) \). The quantum d-separation theorem, namely Theorem 11 (ditto, Theorem 19), tells us that if \( \tau_{sep G}(I) \), then \( \tau^A(I) \). But we know from Theorem 5 that, because \( I \) is all-encompassing, \( \tau^A(I) = \tau^{CMI'}(I) \). It follows that \( S_{\text{diag}_{\mu}}(\mu)(x_J : x_K | x_E) = 0 \).

This and the definition of CMI entanglement imply that \( E^{CMI}_{\mu}(x_J : x_K) = 0 \). QED

Suppose \( J \subset Z_{1,N} \), and we are given a density matrix \( \rho \in dm(\mathcal{H}_x) \) with a generalized purification \( \mu \in dm(\mathcal{H}_x) \). Suppose \( J_1, J_2 \subset J \) are disjoint sets, and we want to decide whether \( E^{CMI}_{\rho}(x_{J_1} : x_{J_2}) \) vanishes. Note that to apply Theorem 20...
we should first replace $\mu$ by a *traced* purification $\tilde{\mu}$ of $\rho$. The reason is that we are interested in $E_{\rho}^{CMI}(\overline{x}_I : \overline{x}_J)$. This quantity is not necessarily equal to $E_{\mu}^{CMI}(\overline{x}_I : \overline{x}_J)$, but it is always equal to $E_{\tilde{\mu}}^{CMI}(\overline{x}_I : \overline{x}_J)$.

In a nutshell, Theorem 20 tells us that, if $J, K \subset Z_{1,N}$ are disjoint sets, and $\tau_{sep}(\overline{x}_I \perp \overline{x}_K | x_{Z_{1,N} - J - K})$, then $E_{\mu}^{CMI}(\overline{x}_I : \overline{x}_K) = 0$. And now, some examples. Let $k = ?$ mean that we can’t conclude anything about the value of $k$. The Bayesian nets

$$(x) \leftarrow (a) \rightarrow (y)$$

(190)

and

$$(x) \rightarrow (a) \rightarrow (y)$$

(191)

both have $E_{\mu}^{CMI}(x : y) = 0$ because $a$ can be grounded and $S_{\mu}(x : y | a) = 0$. On the other hand, the Bayesian net

$$(x) \leftarrow e \Sigma \rightarrow (y)$$

(192)

is equivalent to $\mu = (x) \leftarrow (y)$, for which $S_{\mu}(x : y) = ?$, so $E_{\mu}^{CMI}(x : y) = ?$. The Bayesian net

$$(x) \rightarrow (a) \leftarrow (y)$$

(193)

also has $E_{\mu}^{CMI}(x : y) = ?$, because grounding $a$ allows transmission of information between $x$ and $y$.

A parting observation: Suppose $J, K_1, K_2 \subset Z_{1,N}$ are disjoint sets. Let $D_1 = (\overline{x}_I, \overline{x}_{K_1})$, $D_2 = (\overline{x}_I, \overline{x}_{K_2})$, and $D = (\overline{x}_I, \overline{x}_{K_1 \cup K_2})$. It’s not hard to convince oneself that $[D \in D_{glo}(G)] \Leftrightarrow [D_1, D_2 \in D_{glo}(G)]$. By the synergism of entanglement, $[D \in D(A)] \Rightarrow [D_1, D_2 \in D(A)]$, but the opposite implication does not appear to be true. If we define a perfect graph as one for which $D_{glo}(G) = D(A)$, then it appears that no all graphs are perfect.
A Appendix: Mobius Inversion

In this appendix, we prove the Mobius Inversion Theorem.

Some preliminary observations will facilitate our proof.

For any finite set $J$, consider a table of arbitrary complex numbers, where the rows and columns of the table are both labelled by the elements of $2^J$. Suppose we want to sum over the elements of the table that are below its main diagonal. Fig. 6 illustrates the table for $J = \{a, b, c\}$. The shaded entries of Fig. 6 are the entries we want to sum over. Two simple methods for carrying out such a sum are: (1) sum first over rows and then over columns, (2) sum first over columns and then over rows. Of course, whether we use method (1) or (2), the final value of the sum will not change. This simple observation, that the final value of the sum does not depend on the order of summation, can be stated more formally as

$$
\sum_{J': J' \subset J} \sum_{J'': J'' \subset J'} = \sum_{J': J' \subset J} \sum_{J'': J'' \subset J''}.
$$

(194)

By $\sum_{J': J' \subset J}$ we mean the sum of all subsets $J'$ of $J$, including the empty set $\emptyset$ and $J$. Note that we use $J', J''$ (i.e., $J$ with one or more primes) to denote subsets of $J$.

Another simple observation is that

$$
\sum_{D': D' \subset D} (-1)^{|D'|} = \delta(D, \emptyset).
$$

(195)

For example, suppose $D = \{a, b, c\}$. Fig. 7 lists all the subsets $D'$ of $D$. It associates each distinct $D'$ with a different node of a lattice. (Subsets with the same number of elements are in the same horizontal level. Subsets in lower horizontal levels have more elements. Links connect subsets that differ only by one element.) If we sum $(-1)^{|D'|}$

Figure 6: Table with rows and columns labelled by all the subsets of the set $J = \{a, b, c\}$. We want to sum over the shaded entries of this table.
over all the nodes of the lattice of Fig. 7 we get zero, since the number of even-order subsets equals the number of odd-order subsets. This is true for any set $D$ except for the empty set, which has only a single even-order subset, itself. Eq. (195) yields

$$
\sum_{J: J' \subseteq J} (-1)^{|J' - J''|} = \sum_{\Delta J' \subseteq \Delta J, \Delta J'' \subseteq \Delta J} (-1)^{|\Delta J'|} \delta(J, J'') .
$$

(196a)

(196b)

If $J'' \subset J' \subset J$, then $|J - J'| + |J' - J''| + |J''| = |J|$ so

$$
\sum_{J: J'' \subseteq J' \subseteq J} (-1)^{|J - J'|} = (-1)^{|J| - |J''|} \sum_{J: J'' \subseteq J' \subseteq J} (-1)^{|J' - J''|}
$$

(197a)

$$
= \delta(J, J'').
$$

(197b)

**Theorem 21** For any set $J$, and any functions $f, g : 2^J \to \mathbb{C}$,

$$
g(J) = \sum_{J: J' \subseteq J} (-1)^{|J' - J|} f(J')
$$

(198a)

if and only if

$$
f(J) = \sum_{J: J' \subseteq J} g(J') .
$$

(198b)

**proof:**
\[
(\Rightarrow) \quad \sum_{J':J \subset J} g(J') = \sum_{J':J \subset J} \sum_{J''; J'' \subset J'} (-1)^{|J'-J''|} f(J'') \\
= \sum_{J''; J'' \subset J} \sum_{J':J \subset J} (-1)^{|J'-J''|} f(J'') \\
= f(J) \quad \text{(199a)}
\]

\[
(\Leftarrow) \quad \sum_{J':J \subset J} (-1)^{|J-J'|} f(J') = \sum_{J':J \subset J} (-1)^{|J-J'|} \sum_{J''; J'' \subset J'} g(J'') \\
= \sum_{J''; J'' \subset J} \sum_{J':J \subset J} (-1)^{|J-J'|} g(J'') \\
= g(J) \quad \text{(200a)}
\]

QED

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