Compatibility of subsystem states

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In memoriam Asher Peres

Abstract

We examine the possible states of subsystems of a system of bits or qubits. In the classical case (bits), this means the possible marginal distributions of a probability distribution on a finite number of binary variables; we give necessary and sufficient conditions for a set of probability distributions on all proper subsets of the variables to be the marginals of a single distribution on the full set. In the quantum case (qubits), we consider mixed states of subsets of a set of qubits; in the case of three qubits, we find quantum Bell inequalities — necessary conditions for a set of two-qubit states to be the reduced states of a mixed state of three qubits. We conjecture that these conditions are also sufficient.

1 Introduction

What can we believe about some parts of a system without contradicting what we believe about other parts? If the system is described by a set of numbers, and our beliefs are the probabilities that these numbers take given values, then a part of the system is described by a subset of the numbers and our beliefs about it will be given by marginal probabilities derived from the probability distribution of the full set of numbers. The marginal distributions of different parts are constrained by the fact that they all come from a
single set of probabilities on the full system. Bell’s inequalities are an example of such constraints. The conclusion of the EPR argument is that a single quantum system like an electron has a set of numbers giving the results of all possible measurements, even though these cannot be measured simultaneously. Wigner [24] presented Bell’s theorem by considering the probabilities for subsets of electron observables which could be measured simultaneously (either directly, or by measuring the electron’s partner in a singlet state), and showing that these subset probabilities, if they derived from a single probability distribution on the full set, would be constrained by inequalities which were not satisfied by the predictions of quantum mechanics.

Other forms of Bell inequalities can also be understood in this way, as compatibility conditions on the marginal distributions of subsets. Asher Peres [18] has considered this problem in complete generality, bringing out its formidable computational complexity. In this paper we solve the special case in which one is given joint probability distributions for all proper subsets of a set of binary variables, finding necessary and sufficient conditions for these distributions to be the marginals of a single distribution on the full set.

The motivation for this study is to investigate our initial question for quantum systems. In this case our knowledge of the system is represented by a mixed state, or density matrix, and our knowledge of a part of the system is given by the reduced state, obtained by tracing the full density matrix over the rest of the system. What are the constraints on these reduced states? Our answer to the classical problem yields a possible answer to the quantum question, as the conditions on marginal probability distributions have immediate analogues for quantum states of a finite set of qubits. They can be translated into conditions on the density matrices of proper subsets of the qubits, which we prove, in the case of a system of three qubits, to be necessary for the density matrices to be the reductions of a (mixed) state of the full set of qubits. We conjecture that these quantum Bell-Wigner inequalities are also sufficient conditions. For more than three qubits the corresponding conditions are not even necessary; this gives rise to new separability criteria (the generalised reduction criteria) [23].

A still more general problem in classical probability, which was introduced by George Boole [1], is to ask when a set of real numbers $p_{ijk...}$ can be simultaneous probabilities $P(E_i \& E_j \& E_k \& ...)\) for some events $E_i$. This problem has been investigated by Pitowsky [20, 19], who has shown [21] that the problem of deciding whether the relevant conditions are satisfied is NP-complete. The relation to the problem considered here (and by Peres) is that we assume that the full sample space is a Cartesian product of finite sets and that our events $E_i$ are slices of this product.

Work on this problem appears to have concentrated on a (discrete or
continuous) infinity of real-valued variables, i.e. a stochastic process, in which case there are no conditions other than the obvious ones (see (2.1) below); the Kolmogorov-Daniell theorem [15] asserts essentially that if these are satisfied for all finite subsets of the variables, then there is a stochastic process of which they are the finite-time marginals. The focus then is on the range of possible processes having these marginals. This problem for bipartite quantum states has been studied by Parthasarathy [17] and Rudolph [22].

The situation in the quantum problem for pure states is, in a sense, inverse to this. It is not at all easy to construct an overall pure state which has given marginals: there are other conditions to be satisfied in addition to the obvious ones [11, 10, 2, 9], and there is usually only one state with these marginals (this is the generic situation if one is given the reduced states of subsets containing more than half of the total number of qubits [13, 8]). This can be interpreted [16] as meaning that irreducible $n$-way correlation is exceptional in pure $n$-qubit states.

However, it is not surprising that the quantum pure-state problem should be different from the general classical problem, since the classical pure-state problem is also very different. Classically, a pure probability distribution consists of certainty; its marginals are also pure, the only conditions to be satisfied by them are the obvious compatibility conditions (2.1), and the marginals of singleton subsets uniquely determine the overall distribution. The quantum analogue of the non-trivial classical problem is to ask when a set of subsystem states is compatible with a mixed overall state. For identical particles, this problem has been much studied [6], but the case of distinguishable particles has only recently received attention. One approach to it is outlined in [13]; in this paper we suggest another line of attack.

The paper is organised as follows. In section 2 we consider the classical problem and present necessary and sufficient conditions for compatibility of probability distributions on proper subsets of a finite set of binary variables. In section 3 we describe the quantum problem, prove necessary conditions for compatibility of reduced states of two-qubit subsystems of a system of three qubits, and show that the corresponding conditions are not necessarily satisfied for a system of more than three qubits. In an appendix we review other work on the quantum marginal problem.
classical marginals

The general classical problem is as follows. Let \( S = \{X_1, \ldots, X_n\} \) be a set of random variables, with \( X_i \) taking values in a finite set \( V_i \). Let \( A, B, \ldots \) be a set of subsets of \( \{1, \ldots, n\} \), and let \( S_A, S_B, \ldots \subset S \) be the corresponding sets of variables: \( S_A = \{X_i : i \in A\} \). Suppose we are given joint probability distributions \( P_A, P_B, \ldots \) for these sets of variables. What are the conditions for these to be the marginal distributions of a single probability distribution \( P(x_1, \ldots, x_n) \)? This means that if, for example, \( A = \{1, \ldots, r\} \), then

\[
P_A(x_1, \ldots, x_r) = \sum_{x_{r+1}, \ldots, x_n} P(x_1 \ldots, x_n)
\]

which we write as

\[
P_A = \Sigma_{S \setminus A}(P).
\]

There are some obvious necessary conditions:

\[
\Sigma_B(P_{A \cup B}) = \Sigma_C(P_{A \cup C}) \quad \text{if} \quad A \cap B = A \cap C = \emptyset.
\] (2.1)

In particular, \( P_A \) is determined by \( P_S \) if \( A \subset S \). We may therefore assume that in our given set of subsets, none is contained in another. We will say that the subset distributions are \textit{equimarginal} if they satisfy the conditions (2.1). We ask what further conditions must be satisfied.

The simplest non-trivial case — which we discuss separately, for ease of reading, even though it is contained in the general case which follows — is where \( S \) is a set of three binary variables and \( A, B, C \) are the three two-element subsets, so that we are considering three marginal two-variable distributions \( P_{12}(x, y), P_{13}(x, z) \) and \( P_{23}(y, z) \) where \( x, y, z \in \{0, 1\} \). Wigner [24] pointed out that these must satisfy

\[
P_{12}(x, y) \leq P_{13}(x, z) + P_{23}(y, \bar{z})
\] (2.2)

where \( \bar{z} = 1 - z \) (but these inequalities are not satisfied by the predictions of quantum mechanics for the measurements of the spin components of an electron in three directions, where joint measurements in two different directions are performed by measuring two electrons in a singlet state). Pitowsky [20] showed that the inequalities (2.2), and the inequalities related to them by permuting (1,2,3), are sufficient for \( P_{12}(x, y), P_{13}(x, z) \) and \( P_{23}(y, z) \) to be the marginals of a single three-variable distribution \( P(x, y, z) \).

To put these inequalities in a form which has a quantum analogue, we regard \( P_{12}(x, y) \) as a function of three variables \( x, y, z \) which is constant in
and similarly for \( P_{13}(x, z) \) and \( P_{23}(y, z) \). Then the functions \( P_{12}, P_{13}, P_{23} \) are equimarginal if they satisfy three equations like

\[
P_{12}(x, y, z) + P_{12}(x, \overline{y}, z) = P_{13}(x, y, z) + P_{13}(x, y, \overline{z}) = P_1(x, y, z)
\]

where \( P_1 \) is constant in \( y \) and \( z \).

Now the observation of Wigner and Pitowsky can be expressed in terms of three-variable functions as

Theorem 2.1. Three equimarginal two-variable functions of three binary variables, \( P_{12}, P_{13} \) and \( P_{23} \), are the two-variable marginals of a three-variable probability distribution if and only if

\[
0 \leq \Delta(x, y, z) \leq 1 \quad \text{for all } x, y, z \in \{0, 1\}
\]

where \( \Delta = 1 - P_1 - P_2 - P_3 + P_{12} + P_{13} + P_{23} \).

Proof. For \( x \in \{0, 1\} \), define \( \sigma(x) = (-1)^x \), and write

\[
\sigma_1(x, y, z) = \sigma(x), \quad \sigma_2(x, y, z) = \sigma(y), \quad \sigma_3(x, y, z) = \sigma(z).
\]

Then any probability distribution \( P \) on \( \{0, 1\}^3 \) can be written

\[
P = \frac{1}{8} + a\sigma_1 + b\sigma_2 + c\sigma_3 + d\sigma_1\sigma_2 + e\sigma_1\sigma_3 + f\sigma_2\sigma_3 + g\sigma_1\sigma_2\sigma_3
\]

for some real constants \( a, \ldots, g \). The marginals of \( P \) are given by

\[
P_{12} = \frac{1}{4} + 2a\sigma_1 + 2b\sigma_2 + 2d\sigma_1\sigma_2, \quad P_{13} = \frac{1}{4} + 2a\sigma_1 + 2c\sigma_3 + 2e\sigma_1\sigma_3, \quad P_{23} = \frac{1}{4} + 2b\sigma_2 + 2c\sigma_3 + 2f\sigma_2\sigma_3
\]

and

\[
P_1 = \frac{1}{2} + 4a\sigma_1, \quad P_2 = \frac{1}{2} + 4b\sigma_2, \quad P_3 = \frac{1}{2} + 4c\sigma_3.
\]

Hence

\[
\Delta = \frac{1}{4} + 2(d\sigma_1\sigma_2 + e\sigma_1\sigma_3 + f\sigma_2\sigma_3),
\]

i.e.

\[
\Delta(x, y, z) = P(x, y, z) + P(\overline{x}, \overline{y}, \overline{z}).
\]

It follows that the inequality (2.3) is a necessary condition for the existence of the probability distribution \( P(x, y, z) \).

To prove that it is sufficient, note that the equimarginal condition forces the \( P_{ij} \) to be of the form (2.6). We have to prove that there is a value of \( g \) such that \( P \) defined by (2.5) is a positive function. Let

\[
Q = \frac{1}{8} + a\sigma_1 + b\sigma_2 + c\sigma_3 + d\sigma_1\sigma_2 + e\sigma_1\sigma_3 + f\sigma_2\sigma_3;
\]
then the conditions on $g$ are

$$-Q(x, y, z) \leq g \leq 1 - Q(x, y, z) \quad \text{if } \sigma(x)\sigma(y)\sigma(z) = 1,$$  \hfill (2.9)

and

$$-1 + Q(x, y, z) \leq g \leq Q(x, y, z) \quad \text{if } \sigma(x)\sigma(y)\sigma(z) = -1. \quad (2.10)$$

But

$$Q = \frac{1}{4}(P_{12} + P_{13} + P_{23} + \Delta) - \frac{1}{8}. \quad (2.11)$$

Hence the condition $0 \leq \Delta \leq 1$, together with $0 \leq P_{ij} \leq 1$, gives

$$-\frac{1}{8} \leq Q(x, y, z) \leq \frac{7}{8}. \quad (2.12)$$

It follows that every lower bound is less than every upper bound in (2.9) for different values of $(x, y, z)$; the same is true of (2.10); and every lower bound in (2.10) is less than every upper bound in (2.9).

Now suppose that $\sigma(x)\sigma(y)\sigma(z) = 1$ and $\sigma(x')\sigma(y')\sigma(z') = -1$. Then in the equations

$$\sigma(x) = \pm \sigma(x'), \quad \sigma(y) = \pm \sigma(y'), \quad \sigma(z) = \pm \sigma(z')$$

either one or three of the signs are negative. If all three are negative, then

$$Q(x, y, z) + Q(x', y', z') = \frac{1}{4} + 2(d\sigma(x) + e\sigma(x)\sigma(z) + f\sigma(y)\sigma(z)) = \Delta(x, y, z).$$

If just one sign is negative, say the first, then

$$Q(x, y, z) + Q(x', y', z') = \frac{1}{4} + 2(b\sigma(y) + c\sigma(z) + f\sigma(y)\sigma(z)) = P_{23}(y, z).$$

In both cases we have

$$Q(x, y, z) + Q(x', y', z') \geq 0 \quad (2.11)$$

so that every lower bound in (2.9) is less than every upper bound in (2.10). Thus there is a $g$ satisfying all of these inequalities and giving the required probability distribution $P(x, y, z)$. \hfill \Box

A classical probabilist would (probably) find it more natural to prove necessity from the inclusion-exclusion principle, which gives $1 - \Delta(x, y, z)$ as the probability that $X_1 = x$ or $X_2 = y$ or $X_3 = z$. We have given our
rather clumsier proof because it connects both with the proof of sufficiency and with the quantum problem.

We now move on to the general case of \( n \) binary variables \( x_1, \ldots, x_n \). Let \( N = \{1, \ldots, n\} \); for subsets of \( N \), we write \( A \subset B \) to mean that \( A \) is a proper subset of \( B \), writing \( A \subseteq B \) when we want to allow \( A = B \); and \( |A| \) denotes the number of elements of \( A \).

We consider probability distributions \( P_A \) for subsets \( A \subset N \), regarding \( P_A \) as a function of \( (x_1, \ldots, x_n) \) which is constant in \( x_i \) for \( i \notin A \). If \( P(x_1, \ldots, x_n) \) is a probability distribution on all \( n \) variables, its marginal distributions \( P_A \) can be written in terms of operators \( M_i \) on functions of \( n \) binary variables defined by

\[
M_i f(x_1, \ldots, x_n) = f(x_1, \ldots, x_n) + f(x_1, \ldots, \overline{x_i}, \ldots, x_n).
\]

Then

\[
P_A = M_{i_1} \ldots M_{i_r} P \quad \text{where} \quad N \setminus A = \{i_1, \ldots, i_r\}.
\]

The distribution \( P(x_1, \ldots, x_n) \) can be expanded as

\[
P = \sum_{A \subseteq N} c_A \sigma_A \tag{2.12}
\]

where the \( c_A \) are real coefficients, with \( c_{\emptyset} = 2^{-n} \), and

\[
\sigma_A(x_1, \ldots, x_n) = \prod_{i \in A} \sigma(x_i), \quad \sigma_{\emptyset} = 1.
\]

Then the corresponding expansion of the marginal \( P_A \) is

\[
P_A = 2^{n-|A|} \sum_{B \subseteq A} c_B \sigma_B. \tag{2.13}
\]

This equation can be inverted to give \( c_A \sigma_A \) in terms of the marginals \( P_A \):

\[
c_A \sigma_A = \sum_{B \subseteq A} \frac{(-1)^{|A| - |B|}}{2^{n-|B|}} P_B. \tag{2.14}
\]

We can now state the generalisation of Theorem 2.1 to any number of variables:

**Theorem 2.2.** Let \( P_A \ (A \subset N) \) be an equimarginal set of probability distributions on subsets of the variables \( x_1, \ldots, x_n \). These are the marginals of a

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single distribution $P(x_1, \ldots, x_n)$ if and only if for each subset $A \subseteq N$ with an odd number of elements,

$$0 \leq \sum_{A \cup B = N} (-1)^{|A \cap B|} P_B(x) \leq 1 \quad (2.15)$$

for all $x \in \{0, 1\}^n$.

**Proof.** To prove that the condition is necessary, suppose the distribution $P$ exists and let $A$ be a subset of $N$ with an odd number of elements. Let $x = (x_1, \ldots, x_n)$ and let $x'$ be the sequence which differs from $x$ just in places belonging to $A$:

$$x'_i = \begin{cases} x_i & \text{if } i \in A \\ x_i & \text{if } i /\in A. \end{cases}$$

Then

$$0 \leq P(x) + P(x') \leq 1.$$ 

Expanding $P$ as in (2.12), we have

$$P(x) + P(x') = 2 \sum_{|A \cap B| \text{ even}} c_B \sigma_B(x).$$

Using (2.14), we can express this in terms of the probability distributions $P_B$; the result is the sum in (2.15). This can be verified by using (2.13) to expand (2.15):

$$\sum_{N \setminus A \subseteq B \subset N} (-1)^{|A \cap B|} P_B = \sum_{N \setminus A \subseteq B \subset N} (-1)^{|A \cap B|} 2^{n-|B|} \sum_{D \subseteq B} c_D \sigma_D \quad (2.16)$$

in which the coefficient of $c_D \sigma_D$ is

$$\sum_{B \supseteq D} (-1)^{|A \cap B|} 2^{n-|B|} = \sum_{m=|A \cap D|}^{|A|-1} (-1)^m 2^{|A|-m} \left( \frac{|A| - |A \cap D|}{m - |A \cap D|} \right)$$

( writing $m = |A \cap B|$)

$$= (-1)^{|A \cap D|} 2^{|A \setminus D|} \left\{ \left( 1 - \frac{1}{2} \right)^{|A \setminus D|} - \left( -\frac{1}{2} \right)^{|A \setminus D|} \right\}$$

$$= (-1)^{|A \cap D|} \left\{ 1 - (-1)^{|A \setminus D|} \right\},$$

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so the right-hand side of (2.16) is
\[ 2 \sum_{|A \setminus D| \text{ odd}} c_D \sigma_D = 2 \sum_{|A \cap D| \text{ even}} c_D \sigma_D \]
since |A| is odd. Thus if the distribution \( P \) exists, the inequality (2.15) must be satisfied for each subset \( A \) with an odd number of elements.

To show that these inequalities are sufficient for the existence of the distribution \( P \), we first note, as in Theorem 2.1, that the equimarginality of the distributions \( P_A \) gives us coefficients \( c_B \) such that
\[ P_A = \sum_{B \subseteq A} c_B \sigma_B. \]

We have to prove that the stated conditions are sufficient to ensure that there is a coefficient \( c_N \) such that
\[ P = \sum_{A \subseteq N} c_A \sigma_A + c_N \sigma_N \]
satisfies \( 0 \leq P(x) \leq 1 \) for all \( x \in \{0, 1\}^n \). Writing
\[ Q(x) = \sum_{A \subseteq N} c_A \sigma_A(x), \]
we therefore need to be able to satisfy the inequalities
\[ -Q(x) \leq c_N \leq 1 - Q(x) \quad \text{whenever } \sigma_N(x) = 1 \quad (2.17) \]
and
\[ -1 + Q(x') \leq c_N \leq Q(x') \quad \text{whenever } \sigma_N(x') = -1. \quad (2.18) \]
Using (2.14), we can express \( Q(x) \) in terms of the distributions \( P_A(x) \) as
\[ Q = \sum_{A \subseteq N} \sum_{B \subseteq A} \frac{(-1)^{|A| - |B|}}{2^{n-|B|}} P_B \]
\[ = \sum_{B \subseteq N} P_B \frac{2^{|B|}}{2^{n-|B|}} \sum_{B' \subseteq A \subseteq N} (-1)^{|A| - |B|} \]
\[ = \sum_{B \subseteq N} P_B \frac{2^{|B|}}{2^{n-|B|}} \sum_{m=|B|}^{n-1} (-1)^{n-|B|} \left( \binom{n-|B|}{m-|B|} \right) \]
\[ = \sum_{B \subseteq N} \frac{(-1)^{n-|B|-1}}{2^{n-|B|}} P_B. \quad (2.19) \]
We will now show that the inequalities (2.15) imply

$$-\frac{1}{2^n} \leq Q \leq 1 - \frac{1}{2^n} \quad (2.20)$$

Indeed, summing these inequalities over all subsets $A$ with an odd number of elements (of which there are $2^{n-1}$) gives

$$0 \leq \sum_{B \subset N} d_B P_B(x) \leq 2^{n-1}$$

where

$$d_B = \sum_{A \cup B = N \atop |A| \text{ odd}} (-1)^{|A \cap B|}$$

$$= \sum_{r=0}^{|B|} \sum_{s \text{ odd}} (-1)^r \binom{|B|}{r} \left( \text{number of } s\text{-element subsets } A \text{ with } |A \cap B| = r \right)$$

and $A \cup B = N$

$$= \sum_{r=0}^{|B|} (-1)^r \binom{|B|}{r} \left( \text{number of } s\text{-element subsets } A \text{ with } |A \cap B| = r \text{ and } A \cup B = N \right)$$

$$= \begin{cases} 1 & \text{if } B = \emptyset \text{ and } n \text{ is odd} \\ 0 & \text{if } B = \emptyset \text{ and } n \text{ is even} \\ (-1)^{n-|B|+1}2^{|B|-1} & \text{otherwise} \end{cases}$$

since the sum of every other binomial coefficient in the $m$th row of Pascal’s triangle is $2^{m-1}$ if $m \geq 1$. Hence

$$0 \leq \frac{1}{2} + \sum_{B \subset N} (-1)^{n-|B|+1}2^{|B|-1} P_B \leq 2^{n-1}$$

which, together with (2.19), gives (2.20).

It follows from (2.20) that if the inequalities (2.15) are satisfied, then every lower bound is less than every upper bound in (2.17), and therefore it is possible to satisfy all of these inequalities with a single choice of $c_N$; and the same is true of (2.18).
To be able to satisfy both sets of inequalities simultaneously, we need
\[ 0 \leq Q(x) + Q(x') \leq 2 \text{ whenever } \sigma(x) = 1 \text{ and } \sigma(x') = -1. \]

If \( \sigma(x) = 1 \) and \( \sigma(x') = -1 \), \( x \) and \( x' \) must differ in an odd number of places.

Let \( A \) be the set of indices \( i \) such that \( x_i \neq x'_i \); then \( \sigma_B(x) = -\sigma_B(x') \) if and only if \( |A \cap B| \) is odd, so
\[ Q(x) + Q(x') = 2 \sum_{|A \cap B| \text{ even}} c_B \sigma_B(x), \]
which, as we have already shown, is equal to the sum in (2.15). Hence if (2.15) is satisfied, then \( Q(x) + Q(x') \geq 0 \), so no lower bound in (2.17) is greater than any upper bound in (2.18); and \( Q(x) + Q(x') \leq 2 \), so no lower bound in (2.18) is greater than any upper bound in (2.17). It follows that it is possible to find a suitable coefficient \( c_N \), i.e. the conditions are sufficient for the existence of a distribution \( P \).

The proof of this theorem suggests an alternative set of necessary and sufficient conditions. Define the “bit flip” operator \( \kappa_i \) on functions of \( n \) binary variables \( x_i \in \{0, 1\} \) by
\[ (\kappa_i f)(x_1, \ldots, x_n) = f(x_1, \ldots, x_{i-1}, \overline{x_i}, x_{i+1}, \ldots, x_n). \quad (2.21) \]
and for any subset \( A = \{i_1, \ldots, i_r\} \), let \( \kappa_A = \kappa_{i_1} \cdots \kappa_{i_r} \). Then

**Theorem 2.3.** Let \( P_A (A \subset N) \) be an equimarginal set of probability distributions on subsets of the variables \( x_1, \ldots, x_n \). These are the marginals of a single distribution \( P(x_1, \ldots, x_n) \) if and only if, for all \( x \in \{0, 1\}^n \),
\[ -\frac{1}{2^n} \leq Q(x) \leq 1 - \frac{1}{2^n} \quad (2.22) \]
and, for each odd subset \( A \subset \{1, \ldots, n\} \),
\[ 0 \leq Q(x) + \kappa_A Q(x) \leq 2 \quad (2.23) \]
where
\[ Q = \sum_{A \subset N} \frac{(-1)^{n-|A|-1}}{2^n-|A|} P_A. \]

**Proof.** If the distribution \( P(x_1, \ldots, x_n) \) exists, then we can expand it in terms of the functions \( \sigma_A \) for subsets \( A \subset N \) as in (2.12), and we have \( Q(x) = \)
\( P(x) - c_N \sigma_N(x) \), as in (2.19). The inequalities (2.17) and (2.18) follow, giving
\[
0 \leq Q(x) + Q(x') \leq 2 \quad \text{whenever} \quad \sigma(x) = 1 \text{ and } \sigma(x') = -1.
\]
This is equivalent to (2.23). Moreover, if \( P \) exists then Theorem 2.2 holds and the inequalities (2.22) follow, as was shown in the proof of Theorem 2.2.

Conversely, the stated inequalities on \( Q \) guarantee that every left-hand side is less than every right-hand side in both (2.17) and (2.18), and therefore there exists a coefficient \( c_N \) such that \( P = Q + c_N \sigma_N \) is a probability distribution. As in Theorem 2.2, the equimarginal distributions \( P_A \) can be expanded as
\[
P_A(x) = \sum_{B \subseteq A} c_B \sigma_B(x)
\]
and then, by (2.19),
\[
Q(x) = \sum_{B \subset N} c_B \sigma_B(x) \quad \text{where} \quad P_A(x) = \sum_{B \subseteq A} c_B \sigma_B(x)
\]
Hence the marginal distribution of \( P = Q + c_N \sigma_N \) over the subset \( A \) is
\[
\Sigma_{N \setminus A}(P) = \Sigma_{N \setminus A}(Q) = \sum_{B \subseteq A} c_B \sigma_B = P_A,
\]
as required. \( \square \)

3 Quantum reduced states

The general quantum problem concerns subsystems of a multipartite system, with state space \( \mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n \) where \( \mathcal{H}_1, \ldots, \mathcal{H}_n \) are the state spaces of the individual parts of the system. For each subset \( A \subset N = \{1, \ldots, n\} \), we denote the state space of the corresponding subsystem by \( \mathcal{H}_A = \bigotimes_{i \in A} \mathcal{H}_i \). Then the problem is: Given a set of subsets \( A, B, \ldots \) and states \( \rho_A, \rho_B, \ldots \) (density matrices on \( \mathcal{H}_A, \mathcal{H}_B, \ldots \)), does there exist a state \( \rho \) on \( \mathcal{H} \) whose reduction to \( \mathcal{H}_A \) is \( \rho_A \), i.e.
\[
\rho_A = \text{tr}_A(\rho) ? \quad (3.1)
\]
(Here \( \tilde{A} \) is the complement of \( A \) in \( \{1, \ldots, n\} \), and \( \text{tr}_A \) denotes the trace over \( \mathcal{H}_A \) in the decomposition \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_{\tilde{A}} \).) The obvious compatibility conditions, corresponding to the classical conditions (2.1), are
\[
\text{tr}_B(\rho_{A \cup B}) = \text{tr}_C(\rho_{A \cup C}) \quad \text{if} \quad A \cap B = A \cap C = \emptyset. \quad (3.2)
\]
As in the classical case, we will call a set of states equimarginal if they satisfy these conditions, and we can assume that none of the subsets $A, B, \ldots$ is a subset of any other.

There is a further question in the quantum case: as well as asking whether there is any overall state with the given subsystem states as reduced states, one can ask whether there is a pure state with this property. This problem has a simplest case for which the classical and mixed problems are trivial: if the given marginals are those of all one-element subsets, then one can always construct the classical probability distribution

$$f(x_1, \ldots, x_n) = f_1(x_1) \cdots f_n(x_n)$$

with one-variable marginals $f_1, \ldots f_n$, and one can always construct the quantum multipartite mixed state

$$\rho = \rho_1 \otimes \cdots \otimes \rho_n$$

with one-party reduced states $\rho_1, \ldots, \rho_n$ (though not for fermions: see the appendix). But it is not always possible to find a pure state with these reductions. For a set of qubits, necessary and sufficient conditions were found in [11]:

**Theorem 3.1.** Let $\rho_1, \ldots, \rho_n$ be a set of one-qubit density matrices, and let $\lambda_i$ be the smaller eigenvalue of $\rho_i$. Then there is an $n$-qubit pure state $|\Psi\rangle$ with one-qubit reduced states $\rho_1, \ldots, \rho_n$ if and only if $\lambda_1, \ldots, \lambda_n$ satisfy the polygon inequalities

$$\lambda_i \leq \sum_{j \neq i} \lambda_j. \quad (3.3)$$

This result has been extended and generalised by a number of authors. Details are given in the appendix.

Now let us consider the conditions for the existence of a mixed state with given reduced states. The simplest case, as for the classical problem, is a system of three qubits for which we are given two-qubit reduced states $\rho_{12}, \rho_{13}, \rho_{23}$. The form in which we have given the classical necessary and sufficient conditions can be immediately translated into quantum conditions by replacing probability distributions by density matrices, and inequalities between functions (holding for all values of the variables) by inequalities between expectation values of operators, holding for all states — that is, positivity conditions on operators. We can prove that this results in necessary conditions for the quantum problem, and we conjecture that they are also sufficient.
We will regard the reduced density matrix of a subsystem as an operator on the full system by supposing that it acts as the identity on the remaining factors of the full tensor product state space. That is, for three qubits, we identify $\rho_{12}$ with $\rho_{12} \otimes 1$, $\rho_2$ with $1 \otimes \rho_2 \otimes 1$, etc. Then we have

**Theorem 3.2. Quantum Bell-Wigner inequalities** Suppose $\rho_{12}, \rho_{13}, \rho_{23}$ are the two-qubit reductions of a three-qubit mixed state. Then

$$0 \leq \langle \Psi | \Delta | \Psi \rangle \leq 1$$

for all normalised pure three-qubit states $|\Psi\rangle$, where

$$\Delta = 1 - \rho_1 - \rho_2 - \rho_3 + \rho_{12} + \rho_{13} + \rho_{23}.$$

*Proof.* This can be proved in a similar way to the classical version, Theorem 2.1, with the help of the antiunitary “universal NOT” operator $\tau$ defined for one qubit by

$$\tau (a|0\rangle + b|1\rangle) = a^*|1\rangle - b^*|0\rangle.$$ 

This operator satisfies $\tau^2 = -1$ and anticommutes with all three Pauli operators $\sigma_i$ ($i = 1, 2, 3$). It is antiunitary, i.e.

$$\tau |\phi\rangle = |\overline{\phi}\rangle, \tau |\psi\rangle = |\overline{\psi}\rangle \implies \langle \phi | \overline{\psi}\rangle = \langle \overline{\phi} | \overline{\psi}\rangle = \langle \phi | \psi\rangle^*.$$  \hspace{1cm} (3.4)

We extend this to three-qubit states and define

$$\tau \left( \sum_{\alpha \beta \gamma} c_{\alpha \beta \gamma} |\alpha\rangle |\beta\rangle |\gamma\rangle \right) = (-1)^{\alpha+\beta+\gamma} c_{\alpha \beta \gamma}^* |\overline{\alpha}\rangle |\overline{\beta}\rangle |\overline{\gamma}\rangle$$  \hspace{1cm} (3.5)

where $\alpha, \beta, \gamma \in \{0, 1\}$ and $\overline{\alpha} = 1 - \alpha$, etc. This three-qubit operator is also antiunitary and squares to $-1$, which implies the “universal NOT” property that it takes every pure state to an orthogonal state. It anticommutes with the single-qubit Pauli operators $\sigma_i \otimes 1 \otimes 1, 1 \otimes \sigma_j \otimes 1$ and $1 \otimes 1 \otimes \sigma_k$.

Any three-qubit mixed state can be written as

$$\rho = \frac{1}{8} 1 + a_i \sigma_i \otimes 1 \otimes 1 + b_j 1 \otimes \sigma_j \otimes 1 + c_k 1 \otimes 1 \otimes \sigma_k + d_{ij} \sigma_i \otimes \sigma_j \otimes 1 + e_{ik} \sigma_i \otimes 1 \otimes \sigma_k + f_{jk} 1 \otimes \sigma_j \otimes \sigma_k + g_{ijk} \sigma_i \otimes \sigma_j \otimes \sigma_k.$$  \hspace{1cm} (3.6)

(using the summation convention for repeated indices), with real coefficients $a_i, \ldots, g_{ijk}$. The reduced states of $\rho$ are

$$\rho_{12} = \frac{1}{4} 1 + 2a_i \sigma_i \otimes 1 + 2b_j 1 \otimes \sigma_j + 2d_{ij} \sigma_i \otimes \sigma_j,$$

$$\rho_{13} = \frac{1}{4} 1 + 2a_i \sigma_i \otimes 1 + 2c_k 1 \otimes \sigma_k + 2e_{ik} \sigma_i \otimes \sigma_k,$$

$$\rho_{23} = \frac{1}{4} 1 + 2b_j 1 \otimes \sigma_j + 2c_k 1 \otimes \sigma_k + 2f_{jk} \sigma_j \otimes \sigma_k.$$  \hspace{1cm} (3.7)
\[ \rho_1 = \frac{1}{2} \mathbf{1} + 4a_i \sigma_i, \quad \rho_2 = \frac{1}{2} \mathbf{1} + 4b_j \sigma_j, \quad \rho_3 = \frac{1}{2} \mathbf{1} + 4c_k \sigma_k. \]

Hence
\[ \Delta = \frac{1}{4} \mathbf{1} + 2\left( d_{ij} \sigma_i \otimes \sigma_j \otimes \mathbf{1} + e_{ik} \sigma_i \otimes \mathbf{1} \otimes \sigma_3 + f_{jk} \mathbf{1} \otimes \sigma_j \otimes \sigma_k \right) = \rho + \tau^{-1} \rho \tau \]

since \( \tau \) anticommutes with single-qubit Pauli operators. Thus
\[ \langle \Psi | \Delta | \Psi \rangle = \langle \Psi | \rho | \Psi \rangle + \langle \Psi | \rho \tau | \Psi \rangle \]

\[ \geq 0 \quad \text{since } \rho \text{ is a positive operator.} \]

Since \( |\Psi\rangle \) is orthogonal to \( |\Psi\rangle \), (3.8) also gives
\[ \langle \Psi | \Delta | \Psi \rangle \leq \text{tr} \rho = 1, \]

establishing the theorem. \( \square \)

We conjecture that the condition \( 0 \leq \Delta \leq 1 \) is also sufficient for the existence of a three-qubit state with marginals \( \rho_{12}, \rho_{13}, \rho_{23} \).

In the general multipartite case, the classical compatibility conditions of Theorem 2.2 also have quantum analogues, namely
\[ 0 \leq \sum_{A \cup B = N} (-1)^{|A \cap B|} \langle \Psi | \rho_B | \Psi \rangle \leq 1 \]

(3.9)

where \( A \subseteq N \) is a subset with an odd number of elements. However, for \( n > 3 \) these are not even necessary conditions for compatibility (except for the case \( A = N, n \) odd [23]). The proof given above for \( n = 3 \) fails because the universal-NOT operator \( \tau \) is antilinear, not linear (which has the consequence that \( \tau \otimes \mathbf{1} \) does not commute with \( \mathbf{1} \otimes \sigma_i \)). We illustrate this failure with a counter-example for \( n = 4 \). In this case (3.9) becomes
\[ 0 \leq \langle \Psi | \Delta_i | \Psi \rangle \leq 1, \quad i = 1, 2, 3, 4 \]

(3.10)

where
\[ \Delta_1 = \rho_1 - \rho_{12} - \rho_{13} - \rho_{14} + \rho_{123} + \rho_{124} + \rho_{134} \]

and \( \Delta_2, \Delta_3, \Delta_4 \) are defined similarly. But consider
\[ \rho = |\Psi\rangle \langle \Psi | \quad \text{where } |\Psi\rangle = \frac{1}{\sqrt{2}}( |0000\rangle + |1100\rangle ) \]

We find that for this state
\[ \Delta_1 = \frac{1}{2} (\mathbf{1} \otimes \mathbf{1} - 2P_+ \otimes P_1 \otimes P_1 + P_+ \otimes P_0 \otimes P_0 \otimes P_0) \]
where \( P_+ \) is the two-qubit projector onto the maximally entangled state \( \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \), and \( P_0 \) and \( P_1 \) are the one-qubit projectors onto \( |0\rangle \) and \( |1\rangle \). Thus \( \Delta_1 \) has a negative eigenvalue \(-\frac{1}{2}\) with eigenvector \( \frac{1}{\sqrt{2}}(|0011\rangle + |1111\rangle) \).

Since the classical inequalities are satisfied by all classical states, it is not surprising to find that the quantum analogues like (3.10) are satisfied by separable states [23]. Thus they constitute a set of separability criteria. These multipartite versions of the reduction criterion [12, 3] have been investigated by Hall [23].

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### Appendix: Beyond Qubits

Tripartite systems made up of state spaces with dimensions \( d_i \) not all equal to 2 have been studied by Higuchi \((d_1 = d_2 = d_3)\) and Bravyi \((d_1 = d_2 = 2, d_3 = 4)\), who have found necessary conditions for a set of one-party mixed states to be the reductions of a pure tripartite state. Their results are as follows:

**Theorem A.1.** (Higuchi [10]) Three \( 3 \times 3 \) hermitian matrices \( \rho_a \) \((a = 1, 2, 3)\) with eigenvalues \( \lambda_1^{(a)} \leq \lambda_2^{(a)} \leq \lambda_3^{(a)} = 1 - \lambda_1^{(a)} - \lambda_2^{(a)} \) are the reduced one-qutrit states of a pure three-qutrit state if and only if

\[
\begin{align*}
\alpha_a &\leq \alpha_b + \alpha_c, \\
\beta_a &\leq \beta_b + \beta_c, \\
\gamma_a &\leq \alpha_b + \beta_c, \\
\delta_a &\leq \delta_b + \delta_c, \\
\epsilon_a &\leq \delta_b + \epsilon_c, \\
\zeta_a &\leq \delta_b + \zeta_c,
\end{align*}
\]

and \( \{a, b, c\} = \{1, 2, 3\} \) in any order.

**Theorem A.2.** (Bravyi [2]) Let \( \rho_1 \) and \( \rho_2 \) be two \( 2 \times 2 \) density matrices with eigenvalues \( \lambda_a \leq \mu_a = 1 - \lambda_a \) \((a = 1, 2)\), and let \( \rho_3 \) be a \( 4 \times 4 \) density matrix

where

\[
\begin{align*}
\alpha_a &= \lambda_1^{(a)} + \lambda_2^{(a)}, \\
\beta_a &= \lambda_1^{(a)} + \lambda_3^{(a)}, \\
\gamma_a &= \lambda_2^{(a)} + \lambda_3^{(a)}, \\
\delta_a &= \lambda_1^{(a)} + 2\lambda_2^{(a)}, \\
\epsilon_a &= 2\lambda_1^{(a)} + \lambda_2^{(a)}, \\
\zeta_a &= 2\lambda_2^{(a)} + \lambda_3^{(a)}, \\
\eta_a &= 2\lambda_3^{(a)} + \lambda_2^{(a)}
\end{align*}
\]

and \( \{a, b, c\} = \{1, 2, 3\} \) in any order.

**Theorem A.2.** (Bravyi [2]) Let \( \rho_1 \) and \( \rho_2 \) be two \( 2 \times 2 \) density matrices with eigenvalues \( \lambda_a \leq \mu_a = 1 - \lambda_a \) \((a = 1, 2)\), and let \( \rho_3 \) be a \( 4 \times 4 \) density matrix

where

\[
\begin{align*}
\alpha_a &= \lambda_1^{(a)} + \lambda_2^{(a)}, \\
\beta_a &= \lambda_1^{(a)} + \lambda_3^{(a)}, \\
\gamma_a &= \lambda_2^{(a)} + \lambda_3^{(a)}, \\
\delta_a &= \lambda_1^{(a)} + 2\lambda_2^{(a)}, \\
\epsilon_a &= 2\lambda_1^{(a)} + \lambda_2^{(a)}, \\
\zeta_a &= 2\lambda_2^{(a)} + \lambda_3^{(a)}, \\
\eta_a &= 2\lambda_3^{(a)} + \lambda_2^{(a)}
\end{align*}
\]

and \( \{a, b, c\} = \{1, 2, 3\} \) in any order.
with eigenvalues $\lambda_3 \leq \mu_3 \leq \nu_3 \leq \xi_3 = 1 - \nu_1 - \nu_2 - \nu_3$. Then $\rho_1, \rho_2$ and $\rho_3$ are the reduced states of a pure state in $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^4$ if and only if

$$
\begin{align*}
\lambda_a &\geq \lambda_3 + \mu_3 \quad (a = 1, 2), \\
\lambda_1 + \lambda_2 &\geq 2\lambda_3 + \mu_3 + \nu_3, \\
\text{and} \quad |\lambda_1 - \lambda_2| &\leq \min\{\nu_3 - \lambda_3, \xi_3 - \mu_3\}.
\end{align*}
$$

The general version of this inequality has been found by Han, Zhang and Guo [9], who, however, only proved that it is necessary:

**Theorem A.3.** (Han, Zhang and Guo [9]) Let $\rho_1, \ldots, \rho_n$ be the reduced one-particle density matrices of a pure state of a system of $n$ particles each with an $m$-dimensional state space. Let $\lambda_i^{(a)} (i = 1, \ldots, n)$ be the eigenvalues of $\rho_a$, with $\lambda_1^{(a)} \leq \cdots \leq \lambda_n^{(a)}$. Then for each pair $(a, b)$ of distinct particles and for each $p = 1, 2, \ldots m - 1$,

$$
\sum_{i=1}^{p} \lambda_i^{(a)} \leq \sum_{i=1}^{p} \lambda_i^{(b)} + \sum_{c=1 \atop c \neq a, b}^{n} \sum_{i=1}^{m-1} \lambda_i^{(c)}.
$$

These results can now be seen as special cases of a very general theorem due to Klyachko [14]. A pure state is a special case of a mixed state with a given spectrum $(1, 0, \ldots, 0)$. One can consider a mixed state with any given spectrum and then, given a set of one-particle states, ask whether there is a mixed many-particle state with that spectrum which yields the given one-particle states. Klyachko has shown how to obtain sets of linear inequalities which give necessary and sufficient conditions on the one-particle spectra. For systems larger than four qubits, there are thousands of inequalities. Klyachko’s methods belong to symplectic geometry, and are similar to the methods he used to solve the long-standing problem of Horn, who asked “What are the possible spectra of a sum of hermitian matrices with given spectra?” Daftuar and Hayden have used these methods to find the possible spectra of a single reduced state $\rho_A$ obtained from a bipartite state $\rho_{AB}$; their paper [7] contains a very readable introduction to the relevant ideas from algebraic topology and symplectic geometry. There is a surprising connection to the representation theory of the symmetric group, which was also found by Christandl and Mitchison [4]; roughly speaking, their result is that if the spectra of $\rho_{AB}, \rho_A$ and $\rho_B$ approximate the ratios of row lengths of Young diagrams $\lambda, \mu, \nu$, each with $N$ boxes, then the representation of the symmetric group $S_N$ labelled by $\lambda$ must occur in the tensor product of the representations labelled by $\mu$ and $\nu$. 

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Finally, we note that for fermions there is a non-trivial compatibility problem for the one-particle reduced states of a mixed state. The solution is as follows:

**Theorem A.4.** (Coleman [5]) An \( m \times m \) density matrix \( \rho \) is the reduced one-party state of a system of \( n \) fermions if and only if each of its eigenvalues \( \lambda \) satisfies \( 0 \leq \lambda \leq 1/n \).

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