Complete separability and Fourier representations of n-qubit states

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Necessary conditions for separability are most easily expressed in the computational basis, while sufficient conditions are most conveniently expressed in the spin basis. We use the Hadamard matrix to define the relationship between these two bases and to emphasize its interpretation as a Fourier transform. We then prove a general sufficient condition for complete separability in terms of the spin coefficients and give necessary and sufficient conditions for the complete separability of a class of generalized Werner densities. As a further application of the theory, we give necessary and sufficient conditions for full separability for a particular set of n-qubit states whose densities all satisfy the Peres condition.

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The study of non-classical correlations has led to a number of surprising results arising from the existence of entangled states of separated subsystems [1–4]. This has led to renewed interest in the study of entanglement itself [5,6] as well as in applications such as quantum information theory and quantum communication [7]. Before one can effectively use entanglement, it is necessary to determine if a given state \( \rho \) actually has entangled subsystems. It is this “separability” problem with which we concern ourselves in this paper.

There exists a useful, general necessary condition for separability [8] and a theoretical necessary and sufficient condition [9], but no operational necessary and sufficient conditions, and as a result attention has tended to focus on classes of densities [10–12]. In this paper, we record a useful variant of the Peres (necessary) condition and prove a new sufficient condition for full separability of mixed states of a system composed of \( n \)-qubits. To do that, we highlight the roles of the computational basis, composed of projections and raising and lowering operators, and the spin basis, composed of the identity and the real Pauli matrices. We derive a change of basis formula which facilitates changing from one basis to another and apply these insights to obtain the general sufficient condition for separability and to obtain both necessary and sufficient conditions for a particular class of states satisfying the Peres condition. In a separate paper we will show how these ideas generalize to higher dimensional states.

A state defined on the Hilbert space \( \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \) is said to be separable if it can be written as

\[
\rho = \sum_a p(a) \rho(a) = \sum_a p(a) \rho_{A_1}(a) \otimes \rho_{A_2}(a),
\]

where \( \rho(a) = \rho_{A_1}(a) \otimes \rho_{A_2}(a) \) with \( \rho_{A_k}(a) \) a state on \( \mathcal{H}_{A_k} \), and the \( p(a) \) are positive numbers that sum to one. Peres showed that a necessary condition for a density matrix of such a bipartite system to be separable is for its partial transpose to be a density matrix [8], where the partial transpose \( \rho^T \) of \( \rho \) is defined by \( \langle a b | \rho^T | a' b' \rangle = \langle a' b | \rho | a b \rangle \). \( \rho^T_{A_2} \) is defined analogously. For \( 2 \otimes 2 \) and \( 2 \otimes 3 \) systems this condition is also sufficient [9]. The Peres condition is basis independent, but to facilitate applications we derive a weaker version which is most usefully expressed in the computational basis. This result is based on the positivity of the subsystem states, the assumed degree of separability and the Cauchy-Schwarz inequality. First, we introduce some notation. Let \( j \) denote an \( n \)-long binary index vector and let \( 0 \) and \( 1 \) stand for the \( n \)-bit numbers consisting of all 0’s and all 1’s, respectively. The binary complement of \( j \) will be denoted by \( j = \overline{1} \oplus j \) where the addition is \( \text{mod} 2 \). We shall write \( j = j^1 j^2 \) to mean that \( j \) is the concatenation of \( j^1 \) and \( j^2 \). Now assume \( \rho \) has the form given in (1). Then

\[
\sqrt{(j|\rho|j)} \sqrt{(k|\rho|k)} = \left[ \sum_a p(a) \rho_{j,j}(a) \right]^{1/2} \left[ \sum_a p(a) \rho_{k,k}(a) \right]^{1/2} \\
\geq \sum_a p(a) \sqrt{\rho_{j,j}(a) \rho_{k,k}(a)} \\
= \sum_a p(a) \sqrt{\rho_{j,j}^{A_1}(a) \rho_{k,k}^{A_1}(a)} \sqrt{\rho_{j,j}^{A_2}(a) \rho_{k,k}^{A_2}(a)}
\]

(2)

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where \( \rho \) is equivalent to (5). In addition to the generalized Werner densities, \( D \) the theorem 1

\[
\text{Let } M_n \text{ be a set of } n \text{ unit vectors, } M_n = \{ \mathbf{m}_1, \cdots, \mathbf{m}_n \} \ \text{and define the usual scalar product of the Pauli matrices with } \mathbf{m}, \sigma_{\mathbf{m}} = \sigma \cdot \mathbf{m}. \text{ Then the density matrix}
\]

\[
\rho^\pm(M_n) = \frac{1}{2^n}(\sigma_0 \otimes \cdots \otimes \sigma_0 \pm \sigma_{\mathbf{m}_1} \otimes \cdots \otimes \sigma_{\mathbf{m}_n})
\]

on \( \mathcal{H}[n] \) is fully separable.
This is easily proved using induction. The densities $P_{\pm}(m) = (\sigma_0 \pm \sigma_m)/2$ on $H_2$ are projections and are trivially separable. Suppose that $\rho^\pm(M_{n-1})$ is fully separable on $H^{[n-1]}$. Then

$$\rho^\pm(M_n) = \frac{1}{2^n}(\sigma_0 \otimes \cdots \otimes \sigma_0 \otimes [P^+(m_n) + P^-(m_n)] \pm \sigma_m \otimes \cdots \otimes \sigma_{m_{n-1}} \otimes [P^+(m_n) - P^-(m_n)]$$

$$= \frac{1}{2}[\rho^\pm(M_{n-1}) \otimes P^+(m_n) + \rho^\mp(M_{n-1}) \otimes P^-(m_n)],$$

(11)

where all the upper signs and all the lower signs go together, is completely separable on $H^{[n]}$, completing the proof. This particular set of separable states has the property that the only non-zero (classical) correlation is among the two sets of 2 operators acting on $H$. The two sets of Pauli matrices.

For the two sets of 2 operators acting on $H$, the factor of $\rho_{ij} = \rho_{j,k} = \sigma_{j,k} \otimes \sigma_{j,k}$. In addition to the unconventional labelling in (12), it is necessary to work with real Pauli matrices, which is why the factor of $i$ appears. It is then easy to check that $S_{j,k} = \sum_r H(j,r) A_{r,k}$, which we record as

$$(S) = H \cdot (A).$$

(13)

The use of the Hadamard matrix allows an easy generalization to tensor product spaces. Define $A^{[n]}_{j,k}$ and $S^{[n]}_{j,k}$ in the usual way: $S^{[n]}_{j,k} = S_{j_1,k_1} \otimes \cdots \otimes S_{j_n,k_n}$ so, for example, $S^{[n]}_{0,0} = I_n$. It then follows easily from $(S) = H \cdot (A)$ that

$$(S^{[n]}) = H^{[n]}(A^{[n]}).$$

(16)

The two sets of 2 operators acting on $H$, the factor of $\rho_{ij} = \rho_{j,k} = \sigma_{j,k} \otimes \sigma_{j,k}$, each form an orthonormal basis of operators on $H_2$ where we use the trace inner product $\langle B, C \rangle = tr(B^\dagger C)$. Therefore, for any $\rho$

$$\rho = \sum_{j,k} a_{j,k} A_{j,k} = \frac{1}{2} \sum_{j,k} s_{j,k} S_{j,k},$$

(14)

where $s_{j,k} = tr(S^{\dagger}_{j,k} \rho)$, $a_{j,k} = tr(A^{\dagger}_{j,k} \rho) = \rho_{j,k\oplus j}$ and it follows that

$$(s) = H \cdot (a).$$

(15)

As a first application we use the spin representation to show the density matrices (7) are fully separable for $j=1/(2^{n-1} + 1)$. Consider $W^{+[n]}(s, \bar{0})$, but the result is independent of which $j$-state we choose. In terms of the adjusted basis,
The first two terms in the brackets are diagonal projections and are therefore fully separable. We write the last two terms in the spin coordinates. The only non-zero spin coefficients are in the last column, and

\[ s_{j,i} = \frac{s}{2} (1 + (-1)^{j \odot 1}) , \]

where we have used \( H^{[n]}_{j,k} = (-1)^{j \odot k} \) with \( j \odot k \) denoting the binary scalar product. Define the set of \( 2^{n-1} \) elements \( \text{Ind} = \{ j : j \odot \overline{1} = \sum r_j r = 0 \mod 2 \} \). It follows from some easy algebra, that adding and subtracting a term proportional to the identity \( I_n = S^{[n]}_{0,0} \) gives

\[ W^{+[n]}(s,0) = \left( \frac{1-s}{2^n} - \frac{s}{2} \right) S^{[n]}_{0,0} + s \frac{1}{2} \left( A^{[n]}_{0,0} + A^{[n]}_{1,1} \right) + s \sum_{j \in \text{Ind}} \frac{1}{2^n} \left( S^{[n]}_{0,0} + S^{[n]}_{j,1} \right) . \]

Notice that \( j \in \text{Ind} \) means that there are an even number of factors of \( S_{1,1} = i \sigma_y \) in \( S^{[n]}_{j,1} \), so that \( S^{[n]}_{j,1} \) is Hermitian. The reason for adding and subtracting the identity is that (10) shows each term in the summation on the right is fully separable. To guarantee that \( W^{+[n]}(s,0) \) is a density matrix, the coefficient of the first term must be non-negative, forcing \( s \leq 1/(2^{n-1} + 1) \) and concluding the proof that \( W^{+[n]}(s,j) \) is fully separable if and only if \( s \leq 1/(2^{n-1} + 1) \). This result may be compared with those obtained earlier in [11] and [12].

We next use the spin representation to establish a new and general sufficient condition for full separability. We introduce a norm on densities which is expressed in terms of the spin coefficients.

**Theorem 2** If the spin coefficients \( s_{j,k} \) of a density \( \rho \) on \( \mathcal{H}^{[n]} \) satisfy \( ||\rho||_1 \equiv \sum (j,k) \neq (0,0) |s_{j,k}| \leq 1 \), then \( \rho \) is fully separable.

Since \((-1)^{j \odot k} S^{[n]}_{j,k} \) is Hermitian, \( i^{j \odot k} s_{j,k} \) must be real. Now use (17) to write

\[ \rho = (1 - ||\rho||_1) \frac{1}{2^n} S^{[n]}_{0,0} + \sum_{(j,k) \neq (0,0)} |s_{j,k}| \frac{1}{2^n} \left( S^{[n]}_{0,0} + v_{j,k} (-i)^{j \odot k} S^{[n]}_{j,k} \right) , \]

where \( v_{j,k} \) is the sign of \( i^{j \odot k} s_{j,k} \). Again (10) applies and gives full separability for \( \rho \). This guarantees that there is a neighborhood of the completely random state \( S^{[n]}_{0,0}/2^n \) in which all the densities are separable, and in particular that every density with \( |s_{j,k}| \leq 1/(2^{n-1} + 1) \) is fully separable, giving the analogous result in [17] as a corollary.

If \( \rho = W^{+[n]}(s(n),j) \), with \( s(n) = 1/(2^{n-1} + 1) \), then \( ||\rho||_1 = (2^n - 1)/(2^{n-1} + 1) \). Thus condition \( ||\rho||_1 \leq 1 \) is sharp for \( n = 2 \) but may be too restrictive for larger \( n \). One can take advantage of the special structure of a class of densities to obtain more refined conditions. For example (9) is also sufficient for the states in \( \tilde{\mathcal{D}}^{[n]} \) invariant with respect to depolarization. Consider also the following subset of \( \tilde{\mathcal{D}}^{[n]} \). Let \( t^{\pm}(j) = (1-s)/2^{n-1} + su_j^\pm \) so that \( \sum_{j=0}^{\hat{m}} (u_j^+ + u_j^-) = 1 \) (recall \( \hat{m} = 01 \ldots 1 \)), and let \( \mu(s) = (1-s) S^{[n]}_{0,0}/2^n + s \rho(u) \). Using the same approach that was used with the Werner densities, we find that \( \mu(s) \) is fully separable provided \( s \leq 1 + 2^{n-1} \left( \sum_{j=0}^{\hat{m}} |u_j^+ - u_j^-| \right)^{-1} \).

As our final result, we show that for any \( n \geq 2 \) and \( \epsilon > 0 \) there exists a density \( \rho \) on \( \mathcal{H}^{[n]} \) which is not fully separable but which has \( ||\rho||_1 < 1 + \epsilon \). Thus, the bound of the theorem is not only the best possible in general but also the best possible for each value of \( n \). As part of the proof we give necessary and sufficient conditions for full separability for a class of densities \( \tilde{\mathcal{D}}^{[n]} \), each of which satisfies the Peres condition. Define first the subset \( \mathcal{D}^{[n]} \) of \( \tilde{\mathcal{D}}^{[n]} \) with all diagonal elements equal: \( \rho^{[n]}(t) = (t^+(j) + t^-(j))/2 = 1/2^n \). In the computational coordinates \( \rho^{[n]}(t) \) is constant down the main diagonal and the only non-zero entries are on the main negative diagonal. Each such density matrix satisfies (9) and in spin coordinates has the form

\[ \rho^{[n]} = \frac{1}{2^n} \left( S^{[n]}_{0,0} + \sum_{j=0}^{\hat{m}} s_{j,1} S^{[n]}_{j,1} \right) , \]
If $\rho^{[n]}$ is fully separable, it can be expressed in the form (4) with $\rho(a, j_k) = (\sigma_0 + \sigma \cdot m(a, j_k))/2$ where $m(a, j_k)$ is a unit vector in the $x$–$y$ plane. Let $\theta(a, j_k)$ be the angle $m(a, j_k)$ makes with the $x$–axis. Then from (4) the non-zero off-diagonal elements are

$$\rho_{j, j}^{[n]} = \sum_a p(a) \frac{1}{2^n} \exp(i \sum_{r=0}^{n-1} (-1)^r \theta(a, j_r)).$$

(19)

All the matrix elements of the matrices in $\mathcal{D}^{[n]}$ are real, so the densities in $\mathcal{D}^{[n]}_c$ satisfy

$$\sum_a p(a) \frac{1}{2^n} \cos \left( \sum_{r=0}^{n-1} (-1)^r \theta(a, j_r) \right) = \rho_{j, j}^{[n]}.$$  

(20)

It is immediate from (20) that if $\rho_{j, j}^{[n]} = 1/2^n$ for some $j$, then for all $a$

$$\sum_{r=0}^{n-1} (-1)^r \theta(a, j_r) = 0 \mod 2\pi.$$  

(21)

We use (21) to define necessary and sufficient conditions for full separability for a subset $\mathcal{D}^{[n]}_c$ of $\mathcal{D}^{[n]}$. Included in $\mathcal{D}^{[n]}_c$ are non-separable density matrices with $\|\rho\|_1$ arbitrarily close to 1, confirming the assertion that $\|\rho\|_1 \leq 1$ cannot be improved for $n \times n$ densities. To illustrate the ideas with minimal notational clutter, we work with the case $n = 3$. Let $\rho_{000,111} = \rho_{001,110} = 1/8$. Then (21) implies that for all $a$,

$$\theta(a, 1) + \theta(a, 2) + \theta(a, 3) = 0 \mod 2\pi \quad \text{and} \quad \theta(a, 1) + \theta(a, 2) - \theta(a, 3) = 0 \mod 2\pi,$$

so that $\theta(a, 3) = 0$ and $\theta(a, 2) = -\theta(a, 1)$. But then it follows that a necessary condition for full separability is

$$\rho_{010,101} = \rho_{011,100} = \frac{1}{8} \sum_a p(a) \cos(\theta(a, 1)).$$

Define $\mathcal{D}^{[3]}_c$ as the set of states with the additional restrictions: if $c$ and $d$ satisfy $-1/8 \leq c, d \leq 1/8$, then $t^+ (010) = 1/8 \pm c$ and $t^\pm (011) = 1/8 \pm d$. Thus the states in $\mathcal{D}^{[3]}_c$ have the form

$$\rho(t(c, d)) = \begin{bmatrix}
1/8 & 0 & 0 & 0 & 0 & 0 & 1/8 \\
0 & 1/8 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1/8 & 0 & 0 & 0 & c \\
0 & 0 & 0 & 1/8 & d & 0 & 0 \\
0 & 0 & 0 & d & 1/8 & 0 & 0 \\
0 & 0 & c & 0 & 0 & 1/8 & 0 \\
0 & 1/8 & 0 & c & 0 & 0 & 1/8 \\
1/8 & 0 & 0 & 0 & 0 & 0 & 1/8
\end{bmatrix}.$$  

(22)

It follows that $\rho(t(c, d))$ is not fully separable if $c \neq d$. Using spin coordinates, it is easy to establish that $\|\rho(t(c, d))\| = 1 + 4 |c - d|$, and thus $\rho(t(c, d))$ is fully separable if $c = d$. Since $\|\rho(t(c, d))\|$ can be made arbitrarily close to 1, we have shown $\|\rho\|_1 \leq 1$ is sharp for $n = 3$. The argument for larger $n$ is similar, and we omit the details.

**Proposition 3** Let $\mathcal{D}^{[n]}_c$ denote the subset of densities in $\mathcal{D}^{[n]}$ which, in addition to being constant on the main diagonal, have $t^+ = 1/(2^{n-1})$ and $t^- = 0$ for the first (and last) $2^{n-2}$ positions on the main negative diagonal, $t^\pm = 1/2 \pm c$ on the next $2^{n-3}$ positions and $t^\pm = 1/2 \pm d$ on the remaining positions, where $-1/2^n \leq c, d \leq 1/2^n$. Then every density in $\mathcal{D}^{[n]}_c$ satisfies the Peres condition and is fully separable if and only if $c = d$. Given $\epsilon > 0$, there exist densities in $\mathcal{D}^{[n]}_c$ which are not fully separable and $\|\rho\|_1 < 1 + \epsilon$. 

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