# SEPARABLE STATES OF $N$ QUANTUM BITS


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## Abstract

The state of $N$ two-level quantum systems (quantum bits or *qubits*) is called *separable* if it can be represented as a mixture of tensor product states, i.e., if it can be written as a probability distribution over the orientation of $N$ spinning tops. We describe recent results on the separability of $N$ qubits and discuss their relevance for NMR (nuclear magnetic resonance) quantum computing.


## 1 Introduction

Consider the state of a quantum system composed of $N$ subsystems. In the absence of entanglement, i.e., in the absence of any quantum correlations between the subsystems, the state is called separable. Unlike the problem of quantifying $N$-particle entanglement, which is largely unsolved, separability is a well defined property (see below). Nevertheless, a simple separability criterion is known only for the case $N = 2$, i.e., for two subsystems, and even then only if one of the subsystems is a two-level system (qubit) and the other one is at most a three-level system (qutrit) [1, 2].

In this paper we describe recent results [3, 4, 5, 6] on the separability of a class of states of $N$ qubits that are close to the maximally mixed state, $N$ being arbitrary. This class of states includes the so-called pseudo-pure states used in present-day NMR quantum computing [7, 8, 9]. In Sec. 2 we give the necessary mathematical background as well as a formal definition of separability. Section 3 states the main separability results. In Sec. 4 we give a short introduction to the principles of NMR quantum computing and discuss some implications of separability for this method. In Sec. 5 we introduce a superoperator formalism and use it to define a "canonical" continuous representation for an arbitrary density operator. Section 6 develops a method for deriving discrete representations from the continuous representation. Section 7 concludes with a brief discussion.

## 2 States of $N$ qubits

The states of a $D$-level quantum system are described by density operators, i.e., positive Hermitian operators of trace one on a $D$-dimensional Hilbert space. Thus a state $\rho$ is given by a $D \times D$ Hermitian matrix with nonnegative eigenvalues that sum to 1. If there is maximal information about the system, the density operator has exactly one nonzero eigenvalue, $\lambda = 1$, and the density operator is a one-dimensional projection operator, $\rho = |\psi\rangle\langle\psi|$, onto the corresponding eigenvector $|\psi\rangle$. The state of the system is then called a pure state; otherwise, it is called a mixed state.

A qubit is two-level system, for which $D = 2$. There is a one-to-one correspondence between the pure states of a qubit and the points on the unit sphere, or *Bloch sphere*. Any pure state of a qubit can be written in terms of the Pauli matrices,

$$\begin{aligned} \sigma_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \\ \sigma_2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \\ \sigma_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \end{aligned} \tag{1}$$

as

$$\begin{aligned} P_{\vec{n}} = |\vec{n}\rangle\langle\vec{n}| &= \frac{1}{2}(1 + \vec{\sigma}\cdot\vec{n}) \qquad (2) \\ &= \frac{1}{2}(1 + \sigma_1 n_1 + \sigma_2 n_2 + \sigma_3 n_3) , \end{aligned}$$

where $\vec{n} = (n_1, n_2, n_3)$ is a unit vector, and 1 denotes the unit matrix. An arbitrary state $\rho$, mixed or pure, of a qubit can be expressed as

$$\rho = \frac{1}{2}(1 + \vec{S}\cdot\vec{\sigma}) , \tag{3}$$

where $0 \le |\vec{S}| \le 1$. Furthermore, there is an infinite number of ways in which $\rho$ can be expanded as a convex mixture of pure states,

$$\rho = \int d\Omega\, w(\vec{n}) P_{\vec{n}} , \tag{4}$$

where $w(\vec{n}) \geq 0$.

The Hilbert space of $N$ qubits is the $N$-fold tensor product space

$$\mathcal{H}^{\otimes N} \equiv \mathcal{H} \otimes \cdots \otimes \mathcal{H} , \tag{5}$$

where $\mathcal{H}$ is the two-dimensional Hilbert space of a single qubit. A state of $N$ qubits is given by an $2^N \times 2^N$ Hermitian matrix with nonnegative eigenvalues that sum to 1. We define the pure-product-state projector

$$\begin{aligned} P(\tilde{n}) &\equiv P_{\vec{n}_1} \otimes \cdots \otimes P_{\vec{n}_N} \qquad (6) \\ &= \frac{1}{2^N}(1 + \vec{\sigma}\cdot\vec{n}_1) \otimes \cdots \otimes (1 + \vec{\sigma}\cdot\vec{n}_N) , \end{aligned}$$

where $\tilde{n}$ stands for the collection of unit vectors $\vec{n}_1, \ldots, \vec{n}_N$. This state can be interpreted as $N$ classical tops pointing in the directions given by $\tilde{n}$.

**Definition:** A *separable* state $\rho$ of $N$ qubits is one that can be written as a convex mixture of pure-product-state projectors, i.e., as

$$\begin{aligned} \rho &= \int d\Omega_{\tilde{n}}\, w(\tilde{n}) P(\tilde{n}) \\ &\equiv \int d\Omega_{n_1} \cdots d\Omega_{n_N} w(\tilde{n}) P(\tilde{n}) , \end{aligned} \tag{7}$$

where $w(\tilde{n}) \geq 0$.

# 3 Separability results

In the following, we will consider states of the form

$$\rho = (1-\epsilon) M + \epsilon \rho_1 , \tag{8}$$

where $M = 1/2^N$ is the maximally mixed density operator for $N$ qubits and $\rho_1$ is a density operator. These states are of particular interest in NMR quantum computing (see Sec. 4). Any density operator can be written in this form. For small $\epsilon$, the states (8) are close to the maximally mixed state $M$.

It seems intuitively clear that there exist separable states arbitrarily close to $M$. One might imagine, however, that even though $M$ is close to other separable states, these separable states lie in a low-dimensional subspace within the space of all states. By leaving this subspace, even infinitesimally, one could reach entangled states. In [3], this problem is addressed by an existence proof; namely, it is shown that there exists a sufficiently small neighborhood of $M$ inside which all states are separable. In [10], a lower bound on the size of the neighborhood is given.

In Sec. 5 we give a constructive proof that provides an explicit representation of any state sufficiently close to $M$ as a mixture of product states, and we give a much improved lower bound on the size of the neighborhood. We show that states of the form (8) are separable provided that [4]

$$\epsilon \leq \eta \equiv \frac{1}{1+2^{2N-1}} . \tag{9}$$

Although this bound is not optimal (see below), the following upper bound shows that the size of the separable neighborhood decreases exponentially. An upper bound is given by the fact that if

$$\epsilon > \frac{1}{1+2^{N-1}} , \tag{10}$$

then there exist nonseparable states of the form (8). This follows from a result by Dür, Cirac, and Tarrach [5], who have shown that the $N$-qubit state

$$\rho = (1-\epsilon) M + \epsilon |\psi_{\rm cat}\rangle\langle\psi_{\rm cat}| , \tag{11}$$

where

$$|\psi_{\rm cat}\rangle \equiv \frac{1}{\sqrt{2}}\Big(|0\ldots0\rangle + |1\ldots1\rangle\Big) \tag{12}$$

is the $N$-qubit "cat state," is separable if and only if $\epsilon \leq 1/(1+2^{N-1})$.

In the case $N=2$, an exact bound has been found by Życzkowski [3, 11], who has shown that for $N=2$, all states $\rho$ that satisfy the condition

$$R \equiv \frac{1}{\mathrm{tr}(\rho^2)} \geq 3 \tag{13}$$

are separable. For states of the form (8), one finds

$$R = \left(\frac{1-\epsilon^2}{4} + \epsilon^2 \mathrm{tr}(\rho_1^2)\right)^{-1} . \tag{14}$$

Since $\mathrm{tr}(\rho_1^2) \leq 1$, this means that $R \geq 3$ and, hence, $\rho$ is separable if $\epsilon \leq 1/3$. This bound cannot be improved since for $\epsilon > 1/3$ and $N=2$, the state (11) is nonseparable.

# 4 NMR quantum computing

All NMR quantum computing experiments performed so far [12] work according to the following principles. The state of the sample is described by a density operator $\rho$ for the $N$ spins (qubits) in each molecule. The molecules are prepared in an initial state of the form (8), where $\rho_1$ is usually chosen to be the projector onto a pure state in which all spins are aligned with the external magnetic field. The parameter $\epsilon$ scales like

$$\epsilon = \frac{\alpha N}{2^N} , \tag{15}$$

where $\alpha = h\bar{\nu}/2kT$ determines the polarization of the sample, $\bar{\nu}$ being the average resonant frequency of the active spins in the strong magnetic field. If $\rho_1$ is a pure state, $\rho$ is called a pseudo-pure state [7]. A typical value for $\alpha$ is $2 \times 10^{-6}$.

One interpretation of $\epsilon$ is that it specifies the fraction of molecules in the sample that occupy the desired initial state $\rho_1$. This interpretation is not unique, and it is not mandated or even preferred by quantum mechanics. It becomes a physical fact only if one actually prepares a fraction of the molecules in a particular state [10], a situation that does not apply to a high-temperature NMR experiment. The freedom to interpret $\rho$ in terms of different ensembles underlies the results of this paper.

After synthesis of the desired initial state, a sequence of radio-frequency pulses, alternating with continuous evolution, is applied to the sample. We restrict attention to the case where the evolution is described by a unitary transformation $U$. Applying the unitary operator $U$ to $\rho$ results in the state

$$\begin{aligned} \rho^{\text{out}} &\equiv U\rho U^\dagger \\ &= (1-\epsilon)M + \epsilon U\rho_1 U^\dagger \\ &\equiv (1-\epsilon)M + \epsilon\rho_1^{\text{out}} . \end{aligned} \tag{16}$$

The totally mixed part of the state is unaffected by the unitary transformation. The output state retains the form (8) with the same value of $\epsilon$, but—and this is the essence of the bulk-ensemble paradigm for quantum computation—$\rho_1$ undergoes the desired unitary transformation.

The last step in any NMR experiment is the readout. By applying radio-frequency pulses and then measuring the transverse magnetization of the sample, one can determine all expectation values of the form

$$\operatorname{tr}\Big(\rho^{\text{out}}\sigma_{\beta_1}\otimes\cdots\otimes\sigma_{\beta_N}\Big) = \epsilon\operatorname{tr}\Big(\rho_1^{\text{out}}\sigma_{\beta_1}\otimes\cdots\otimes\sigma_{\beta_N}\Big) . \tag{17}$$

The tensor product in this expression includes one operator for each spin; $\sigma_{\beta_k}$ denotes the unit operator 1 for the $k$th spin if $\beta_k = 0$, and it denotes a Pauli matrix if $\beta_k = 1, 2,$ or 3. In writing Eq. (17) and Eq. (18) below, it is assumed that there is at least one Pauli matrix in the tensor product (not all the $\beta$'s are zero). The maximally mixed part of the density operator does not contribute to the measured expectation values, which are determined by the state $\rho_1^{\text{out}}$ that undergoes the desired evolution. The parameter $\epsilon$ appears naturally as a measure of the strength of the magnetization signal (or of the signal-to-noise ratio).

According to the results given above, states of the form (8) are separable, i.e., they can be written in terms of probability distributions (7) over spin orientations for $N$ classical tops, provided that the inequality (9) holds. If we assume that $\alpha = 2\times 10^{-6}$ in Eq. (15), this inequality holds for $N < 16$ qubits.

The importance of separability in this section is that a separable state of $N$ qubits can be interpreted in terms of an ensemble of classical tops, because the expectation values (17) have the standard form for an ensemble with probability distribution $w(\tilde{n})$:

$$\begin{aligned} &\operatorname{tr}\Big(\rho\,\sigma_{\beta_1}\otimes\cdots\otimes\sigma_{\beta_N}\Big) \qquad (18) \\ &= \int d\Omega_{\tilde{n}}\, w(\tilde{n})\, \underbrace{\operatorname{tr}\Big(P(\tilde{n})\sigma_{\beta_1}\otimes\cdots\otimes\sigma_{\beta_N}\Big)}_{=(n_1)_{\beta_1}\cdots(n_N)_{\beta_N}} . \end{aligned}$$

In this expression, $(n_j)_{\beta_j} = 1$ if $\beta_j = 0$, and $(n_j)_{\beta_j}$ is a Cartesian component of the vector $\vec{n}_j$ if $\beta_j = 1, 2,$ or 3.

Moreover, even completely general measurements, described by a positive-operator-valued measure [13] or POVM, $\{E_r\}$, can be interpreted classically, since

$$\operatorname{tr}\big(\rho\, E_r\big) = \int d\Omega_{\tilde{n}}\, w(\tilde{n})\, \underbrace{\operatorname{tr}\big(P(\tilde{n})E_r\big)}_{\equiv w(r|\tilde{n})} . \tag{19}$$

The expression $w(r|\tilde{n})$ is nonnegative and hence can be viewed as a classical probability of observing the outcome $r$ given that the spin directions are $\tilde{n}$. Any measurement on the system, including measurements in entangled bases, can be described by a POVM.

The results in this section suggest that current NMR experiments are not true quantum computations, since no entanglement appears in the physical states at any stage [14]. We stress, however, that we have not proved this suggestion, since we would need to analyze the power of general unitary operations in their action on separable states. For a further discussion of this point, see [15].

# 5 Continuous representation

In order to treat discrete and continuous density operator representations on an equal footing, we introduce the following superoperator formalism [16]. The set of linear operators acting on a $D$-dimensional Hilbert space $\mathcal{H}$ is a $D^2$-dimensional complex vector space $\mathcal{L}(\mathcal{H})$. Let us introduce operator "kets" $|A) = A$ and "bras" $(A| = A^\dagger$, distinguished from vector kets and bras by the use of round brackets. Then the natural inner product on $\mathcal{L}(\mathcal{H})$, the trace-norm inner product, can be written as $(A|B) = \operatorname{tr}(A^\dagger B)$. The notation $\mathcal{S} = |A)(B|$ defines a superoperator $\mathcal{S}$ acting like

$$\mathcal{S}|X) = |A)(B|X) = \operatorname{tr}(B^\dagger X)A . \tag{20}$$

Now let the set $\{|N_j)\}$ constitute a (complete or overcomplete) operator basis; i.e., let the operator kets $|N_j)$ span the vector space $\mathcal{L}(\mathcal{H})$. It follows that the superoperator $\mathcal{G}$ defined by

$$\mathcal{G} \equiv \sum_j |N_j)(N_j| \tag{21}$$

is invertible. The operators

$$Q_j \equiv \mathcal{G}^{-1}|N_j) \tag{22}$$

form a dual basis, which gives rise to the following resolutions of the superoperator identity:

$$\mathbf{1} = \sum_j |Q_j)(N_j| = \sum_j |N_j)(Q_j| . \tag{23}$$

An arbitrary operator $A$ can be expanded as

$$A = \sum_j |N_j)(Q_j|A) = \sum_j N_j \operatorname{tr}(Q_j^\dagger A) \tag{24}$$

and

$$A = \sum_j |Q_j)(N_j|A) = \sum_j Q_j \operatorname{tr}(N_j^\dagger A) . \tag{25}$$

These expansions are unique if and only if the operators $N_j$ are linearly independent.

The set of all pure-state projectors on the Bloch sphere, Eq. (2), forms an overcomplete basis. The corresponding superoperator,

$$\mathcal{G} = \int d\Omega\, |P_{\vec{n}})(P_{\vec{n}}| = \pi\left(|1)(1| + \frac{1}{3}\sum_j |\sigma_j)(\sigma_j|\right) , \tag{26}$$

has normalized eigenoperators $|1)/\sqrt{2}$ and $|\sigma_j)/\sqrt{2}$, with eigenvalues $2\pi$ and $2\pi/3$, respectively. Thus $\mathcal{G}^{-1}$ can be expressed as

$$\mathcal{G}^{-1} = \frac{1}{4\pi}\left(|1)(1| + 3\sum_j |\sigma_j)(\sigma_j|\right) . \tag{27}$$

The dual-basis operators are then given by

$$Q_{\vec{n}} = \mathcal{G}^{-1}|P_{\vec{n}}) = \frac{1}{4\pi}(1 + 3\vec{\sigma}\cdot\vec{n}) . \tag{28}$$

Any density operator $\rho = \frac{1}{2}(1 + \vec{S}\cdot\vec{\sigma})$ for a single qubit can be represented in the form

$$\rho = \int d\Omega\, |P_{\vec{n}})(Q_{\vec{n}}|\rho) = \frac{1}{4\pi}\int d\Omega\, P_{\vec{n}}(1 + 3\vec{S}\cdot\vec{n}) . \tag{29}$$

This representation has been studied by Scully and Wódkiewicz [17].

For $N$ qubits, using the pure-product-state projectors Eq. (6), any density operator can be expanded as

$$\begin{aligned} \rho &= \int d\Omega_{\tilde{n}}\, w^{\rm can}(\tilde{n}) P(\tilde{n}) \\ &\equiv \int d\Omega_{n_1}\cdots d\Omega_{n_N} w^{\rm can}(\tilde{n}) P(\tilde{n}) , \end{aligned} \tag{30}$$

where

$$w^{\rm can}(\tilde{n}) \equiv {\rm tr}\Big(\rho Q(\tilde{n})\Big) \tag{31}$$

is a canonical expansion function, with

$$\begin{aligned} Q(\tilde{n}) &\equiv Q_{\vec{n}_1}\otimes\cdots\otimes Q_{\vec{n}_N} \qquad (32)\\ &= \frac{1}{(4\pi)^N}(1 + 3\vec{\sigma}\cdot\vec{n}_1)\otimes\cdots\otimes(1 + 3\vec{\sigma}\cdot\vec{n}_N) . \end{aligned}$$

If the coefficients $w^{\rm can}(\tilde{n})$ are nonnegative, the density operator $\rho$ is separable, and the representation (30) provides an explicit product-state ensemble for the density operator.

For any $N$-qubit density operator $\rho$, the expansion coefficients (31) obey the bound

$$w^{\rm can}(\tilde{n}) \geq \begin{pmatrix}\text{smallest eigenvalue}\\ \text{of } Q(\tilde{n})\end{pmatrix} = -\frac{2^{2N-1}}{(4\pi)^N} . \tag{33}$$

This follows from the fact that $1 + 3\vec{\sigma}\cdot\vec{n}$ has eigenvalues -2 and 4. The most negative eigenvalue of the product operator (32) is therefore $(4\pi)^{-N}(-2)4^{N-1}$, from which Eq. (33) follows.

Consider now an $N$-qubit density operator $\rho$ of the form (8), and let $w_1^{\rm can}(\tilde{n})$ be the coefficients (31) for the density operator $\rho_1$. The coefficients (31) for $\rho$ are given by

$$w^{\rm can}(\tilde{n}) = \frac{1-\epsilon}{(4\pi)^N} + \epsilon w_1^{\rm can}(\tilde{n}) \geq \frac{1-\epsilon(1+2^{2N-1})}{(4\pi)^N} , \tag{34}$$

which is nonnegative for

$$\epsilon \leq \frac{1}{1+2^{2N-1}} . \tag{35}$$

This bound, derived for the first time in [4], implies that for $\epsilon \leq 1/(1+2^{2N-1})$, all density operators of the form (8) are separable. It sets a lower bound on the size of the separable neighborhood surrounding the maximally mixed state.

# 6 Discrete representations

It is easy to characterize a class of discrete representations whose expansion coefficients are related to the continuous representation. This section discusses discrete representations with the property that the corresponding discrete expansion coefficients can be obtained by evaluating the expansion coefficients (31) for the canonical continuous representation along a set of directions for each qubit and then renormalizing the resulting function.

Consider a discrete set of projection operators,

$$P_{\vec{n}_\alpha} = |\vec{n}_\alpha\rangle\langle\vec{n}_\alpha| = \frac{1}{2}(1+\vec{\sigma}\cdot\vec{n}_\alpha) , \quad \alpha = 1,\ldots,K. \tag{36}$$

The corresponding superoperator,

$$\begin{aligned} \mathcal{G} &= \sum_{\alpha=1}^{K} |P_{\vec{n}_\alpha})(P_{\vec{n}_\alpha}| \\ &= \frac{1}{4}\Big(K|1)(1| + \sum_\alpha\Big(\vec{n}_\alpha\cdot|\vec{\sigma})(1| + |1)(\vec{\sigma}|\cdot\vec{n}_\alpha\Big) \\ &\qquad + \sum_{j,k}|\sigma_j)(\sigma_k|\sum_\alpha (n_\alpha)_j(n_\alpha)_k\Big) , \end{aligned} \tag{37}$$

generates dual-basis operators and expansion coefficients proportional to those for the continuous representation if and only if $\mathcal{G}$ is proportional to the superoperator (26) for the continuous representation, i.e., if and only if

$$0 = \sum_\alpha \vec{n}_\alpha , \tag{38}$$

$$\frac{1}{3}\delta_{jk} = \frac{1}{K}\sum_\alpha (n_\alpha)_j(n_\alpha)_k . \tag{39}$$

The trace of Eq. (39) is satisfied by any collection of unit vectors.

When these conditions are satisfied, the superoperator (37) simplifies to

$$\mathcal{G} = \frac{K}{4}\left(|1)(1| + \frac{1}{3}\sum_j |\sigma_j)(\sigma_j|\right) , \tag{40}$$

with an inverse

$$\mathcal{G}^{-1} = \frac{1}{K}\left(|1)(1| + 3\sum_j |\sigma_j)(\sigma_j|\right) , \qquad (41)$$

which generates dual-basis operators

$$Q_{\vec{n}_\alpha} = \mathcal{G}^{-1}|P_{\vec{n}_\alpha}) = \frac{1}{K}(1 + 3\vec{\sigma}\cdot\vec{n}_\alpha) . \qquad (42)$$

Any density operator $\rho = \frac{1}{2}(1 + \vec{S}\cdot\vec{\sigma})$ for a single qubit can be represented in the form

$$\rho = \sum_\alpha |P_\alpha)(Q_\alpha|\rho) = \frac{1}{K}\sum_\alpha P_\alpha(1 + 3\vec{S}\cdot\vec{n}_\alpha) . \quad (43)$$

The conditions (38) and (39) are satisfied by unit vectors that point to the vertices of any regular polyhedron inscribed within the Bloch sphere—i.e., a tetrahedron, octahedron, cube, icosahedron, or dodecahedron. The 4 projectors for a tetrahedron are linearly independent, making the corresponding tetrahedral representation (43) unique. The regular polyhedra by no means exhaust the possibilities for representations of this sort. One can use simultaneously the vertices from any number of polyhedra. Moreover, one can produce an appropriate set of unit vectors by the following procedure: starting with any set of unit vectors in the first octant, reflect the set successively through the three Cartesian planes to produce a set of vectors that occupies all eight octants.

For more than one qubit, the possibilities for discrete representations that follow from the continuous representation are even more diverse. The simplest possibility is to use the same set of pure-state projectors for each qubit, but this is not necessary. One can use a different set of projectors for each qubit, or more generally, one can use a "tree structure," in which there is a different set of projectors for the $n$th qubit for each projector for the first $n-1$ qubits. There are possibilities more general even than those with a tree structure, analogous to the "domino states" introduced for two qutrits in [18].

We do not dwell here on the myriad of discrete representations of this sort, merely noting that since the expansion coefficients in such representations follow from the expansion coefficients for the continuous representation, all such representations lead to the same general lower bound (9) on the size of the separable neighborhood surrounding the maximally mixed state. Both the continuous and these discrete representations can, however, give better bounds on the separability of *particular* states of the form (8) [6].

## 7 Conclusion

In this paper we describe bounds on the size of the separable neighborhood of the totally mixed state of $N$ qubits. These bounds show that in current NMR quantum computing experiments, no entanglement appears in the physical states at any stage. We emphasize, however, that the question of whether NMR quantum computing is true quantum computing remains open. In order to derive our separability bounds, we have introduced a canonical procedure for constructing representations of density operators in terms of complete or overcomplete sets of pure product projectors. The procedure is useful for investigating the separability of general density operators: if the expansion coefficients in such a representation are nonnegative, they can be interpreted as a probability distribution, with the result that the representation then provides an explicit product ensemble for the density operator.

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