Continuous optimal ensembles II. Reducing the separability condition to numerical equations

Romàn R. Zapatrin*

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Abstract

A density operator of a bipartite quantum system is called robustly separable if it has a neighborhood of separable operators. Given a bipartite density matrix, its property to be robustly separable is reduced, using the continuous ensemble method, to a finite number of numerical equations. The solution of this system exists for any robustly separable density operator and provides its representation by a continuous mixture of pure product states.

1 Introduction

Entanglement is treated as a crucial resource for quantum computation. It plays a central rôle in quantum communication and quantum computation. A considerable effort is being put into quantifying quantum entanglement. Usually the efforts are focused on quantifying entanglement itself, that is, describing the impossibility to prepare a state by means of LOCC (local operations and classical communications). One may, although, go another way around and try to quantify separability rather than entanglement: this turned out to be applicable for building combinatorial entanglement patterns for multipartite quantum systems [2]. Briefly, the contents of this paper is the following.

I dwell on the case of bipartite quantum systems. A state of such system is called separable if it can be prepared by LOCC, and robustly separable if it has a neighborhood of separable operators in the space of self adjoint operators. In terms of density matrices that means that $\rho$, its density

*Friedmann Lab. for Theoretical Physics, SPb EF University, Griboedova 30-32, 191023, St.Petersburg, Russia; e-mail: zapatin at rusmuseum.ru
matrix, can be represented as a mixture of pure product states. I suggest to replace finite sums of projectors by continuous distributions on the set of unit vectors. The case of single particle system is considered in section 2 as an example, the explicit form for the equations for the parameters of the mixture is obtained.

In section 3 the bipartite case is considered. The density operators are represented by distribution on the Cartesian product of unit spheres in subsystems’ spaces. Given a density operator $\rho$, we consider it as an element of the space $L$ of all self adjoint operators in the product space $B = \mathcal{H} \otimes \mathcal{H}$. Then the robust separability of $\rho$ is equivalent (see also [4]) to the solvability of the following vector equation in $L$:

$$\nabla K = \rho$$

for the trace functional $K$ on $L$ whose form is obtained in section 3. When we fix a product basis in $B$, this equation becomes a system of $n^4$ transcendent equations with respect to $n^4$ variables.

2 Smeared spectral decomposition and optimal ensembles

The set of all self-adjoint operators in $\mathcal{H} = \mathbb{C}^n$ has a natural structure of a real space $\mathbb{R}^{2n}$, in which the set of all density matrices is a hypersurface, which is the zero surface of the affine functional $\text{Tr} X - 1$.

Generalizing the fact that any convex combination of density operators is again a density operator, we represent density operators as probability distributions on the unit sphere in the state space $\mathcal{H}$ of the system.

Technical remark. Pure states form a projective space rather than the unit sphere in $\mathcal{H}$. On the other hand, one may integrate over any probabilistic space. For technical reasons I prefer to represent ensembles of pure states by measures on unit vectors in $\mathcal{H}$. I use the Umegaki measure on $\mathbb{C}B_n$— the uniform measure with respect to the action of $U(n)$ normalized so that

$$\int_{\phi \in \mathbb{C}B_n} dS_n = 1$$

Similarly, for bipartite case the integration will be carried out over the Cartesian product of unit spheres in appropriate state spaces.
Now pass to a more detailed account of this issue beginning with the case of a single quantum system. Let $\mathcal{H} = \mathbb{C}^n$ be a $n$-dimensional Hermitian space, let $\rho$ be a density matrix in $\mathcal{H}$. We would like to represent the state whose density operator is $\rho$ by an ensemble of pure states. Let this ensemble be continuous with the probability density expressed by a function $\mu(\phi)$ where $\phi$ ranges over all unit vectors in $\mathcal{H}$ (see the technical remark above). The density operator of a continuous ensemble associated with the measure $\mu(\phi)$ on the set $\mathcal{C}B_n$ of unit vectors in $\mathcal{H}$ is calculated as the following (matrix) integral

$$\rho = \int_{\phi \in \mathcal{C}B_n} \mu(\phi) \langle \phi | \phi \rangle \ dS_n$$

(2)

where $|\phi\rangle\langle \phi|$ is the projector onto the vector $\langle \phi |$. Effectively the operator integral $\rho$ can be calculated by its matrix elements. In any fixed basis $\{|e_i\rangle\}$ in $\mathcal{H}$, each matrix element $\rho_{ij} = \langle e_i | \rho | e_j \rangle$ is the following numerical integral:

$$\rho_{ij} = \langle e_i | \rho | e_j \rangle = \int_{\phi \in \mathcal{C}B_n} \mu(\phi) \langle e_i | \phi \rangle \langle \phi | e_j \rangle \ dS_n$$

(3)

### 2.1 Smeared spectral decomposition

Usual spectral decomposition of a density operator $\rho = \sum p_k |e_k\rangle\langle e_k|$ can be treated as an atomic measure on $\mathcal{C}B_n$ whose density is the appropriate combinations of the delta functions:

$$\mu_{\text{spec}}(\phi) = \sum p_k \delta(\phi - e_k)$$

For further purposes a ‘smeared’ version of the spectral decomposition is needed, begin with some technical setup. Denote by $p_0$ the smallest eigenvalue of the density matrix $\rho$ (recall that $p_0 > 0$ as we restrict ourselves to full-range density matrices). Let $K$ be an integer such that $K + 1 < (1/np_0)$, then the density matrix $\rho$ is represented as a continuous ensemble with positive density:

$$\rho = \sum p_k |e_k\rangle\langle e_k| = \int_{\phi \in \mathcal{C}B_n} \mu(\phi) |\phi\rangle\langle \phi| \ dS_n$$
with
\[
\mu(\phi) = \frac{((K+1)n)!}{K \cdot (Kn)!n!} \sum_k \left( p_k - \frac{1}{(K+1)n} \right) |\langle e_k | \phi \rangle|^{2Kn}
\]  
(4)

Furthermore, the distribution (4) tends to the spectral decomposition of \(\rho\) as \(K\) tends to infinity. See appendix A for the proof of formula (4).

2.2 Optimal entropy ensembles

Let us begin with a single particle case. We need to solve the following variational problem. Given a functional \(Q\) on \(L^1(\mathbb{C}B_n)\) and a density matrix \(\rho\) in \(\mathcal{H}\), find the distribution \(\mu\) on the set \(\mathbb{C}B_n\) of unit vectors in \(\mathcal{H}\) such that
\[
\left\{ \begin{array}{l}
\int_{\phi \in \mathbb{C}B_n} \mu(\phi) |\langle \phi | \phi \rangle| \, dS_n = \rho \\
Q(\mu) \to \text{extr}
\end{array} \right.
\]  
(5)

We choose the differential entropy of the distribution \(\mu\) as the functional \(Q\):
\[
Q(\mu) = -\int_{\phi \in \mathbb{C}B_n} \mu(\phi) \ln \mu(\phi) \, dS_n
\]  
(6)

then, according to (3), the variational problem (5) takes the form
\[
\left\{ \begin{array}{l}
\int_{\phi \in \mathbb{C}B_n} \mu(\phi) \langle e_i | \phi \rangle \langle \phi | e_j \rangle \, dS_n = \rho_{ij} \\
-\int_{\phi \in \mathbb{C}B_n} \mu(\phi) \ln \mu(\phi) \, dS_n \to \text{extr}
\end{array} \right.
\]

Solving this variational problem by introducing Lagrangian multiples \(X_{ij}\) we get
\[
-(1 + \ln \mu(\phi)) - \sum_{ij} X_{ij} \langle e_i | \phi \rangle \langle \phi | e_j \rangle = 0
\]  
(7)

Combining the Lagrange multiples into the operator \(X = \sum_{ij} X_{ij} |e_j \rangle \langle e_i|\) we have
\[
\mu(\phi) = e^{-\langle \phi | X | \phi \rangle - 1}
\]  
(8)
and the problem reduces to finding $\mu$ from the condition

$$\int_{\phi \in \mathbb{C}B_n} \mu(\phi) \langle \phi | \phi \rangle \ dS_n = \rho$$

which according to (8) and (3) and redefining $X := - \mathbb{I} - X$ can be written as

$$\langle e_i | \rho | e_j \rangle = \int_{\phi \in \mathbb{C}B_n} e^{\langle \phi | X | \phi \rangle} \langle e_i | \phi \rangle \langle \phi | e_j \rangle \ dS_n$$

(10)

It follows from (7) that the coefficients $X_{ik}$ can be chosen so that $X_{ik} = \bar{X}_{ki}$.

That means that the problem of finding the optimal ensemble reduces to that of finding the coefficients of a self-adjoint operator, that is, to finding $n^2$ numbers from $n^2$ equations.

2.3 The explicit form for single particle case

In case of single particle system the equation (10) can be given an explicit form. First note that, given a self-adjoint operator $X = \sum x_k | e_k \rangle \langle e_k |$, for any integrable function $f(x)$ the operator integral

$$\int_{\mathbb{C}B_n} f(\langle \phi | X | \phi \rangle) \langle \phi | \phi \rangle \ dS_n$$

is diagonal in the eigenbasis of $X$ (see the appendix in [3] for proof). Therefore, in order to calculate the integral (10), we only need its diagonal elements. Calculate first the functional $K$:

$$K(X) = \int_{\mathbb{C}B_n} e^{\langle \phi | X | \phi \rangle} \ dS_n$$

(11)

for which the following formula holds

$$K(X) = (-1)^n (n - 1)! \frac{W_1(x_1, \ldots, x_n)}{W(x_1, \ldots, x_n)}$$

(12)

where $x_1, \ldots, x_n$ are the eigenvalues of the operator $X$,

$$W(x_1, \ldots, x_n) = \det \begin{vmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{n-1} & x_2^{n-1} & \cdots & x_n^{n-1} \end{vmatrix}$$
is the Vandermonde determinant, and the matrix $W_1$ is defined as

$$W_1(x_1, \ldots, x_n) = \det \begin{vmatrix} e^{x_1} & e^{x_2} & \cdots & e^{x_n} \\ 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ \cdots & \cdots & \cdots & \cdots \\ x_1^{n-2} & x_2^{n-2} & \cdots & x_n^{n-2} \end{vmatrix} \tag{13}$$

We can then explicitly write down the expressions for the functional $K$

$$K = (n-1)! \sum_{k=1}^{n} \prod_{i \neq k}^{n} \frac{e^{x_k}}{(x_k - x_i)} \tag{14}$$

For the operator (10) we have $\langle e_j | \nabla K | e_j \rangle =$

$$= (n-1)! \left[ \sum_{k=1}^{n} \frac{e^{x_k}}{(x_k - x_j) \prod_{i \neq k}^{n} (x_k - x_i)} + \frac{e^{x_j}}{\prod_{i=1}^{n} (x_i - x_j)} \left( 1 - \sum_{k=1}^{n} \frac{1}{x_j - x_k} \right) \right] \tag{15}$$

So, in order to obtain the optimal ensemble for the single particle density matrix $\rho = \sum p_j |e_j \rangle \langle e_j|$ we solve the system of $n$ equations $\langle e_j | \nabla K | e_j \rangle = p_j$.

### 3 The bipartite case

Let $\rho$ be a robustly separable density matrix in the product space $\mathcal{H} \otimes \mathcal{H}'$. Then it can be represented (in infinitely many ways) as a continuous ensemble of pure product states. Carrying out the same reasoning as in section 2.2 we conclude (see section 3.2 for further details) that among those continuous ensembles there exists one having the greatest differential entropy, this will be the ensemble we are interested in. Like in section 2.2 formulate the variational problem. Let $\rho$ be a density operator in a tensor product space $\mathfrak{B} = \mathcal{H} \otimes \mathcal{H}'$. The task is to find a probability density $\mu(\phi' \phi)$ defined on the Cartesian product $\mathcal{Z} = \mathbb{C}B_n \times \mathbb{C}B_n$ of the unit spheres in $\mathcal{H}, \mathcal{H}'$, respectively.

$$\begin{cases} \int_{\phi' \phi \in \mathcal{Z}} \mu(\phi' \phi) |\phi'\rangle \langle \phi'| \, dS_n \, dS'_n = \rho \\
Q(\mu) \rightarrow \text{extr} \end{cases} \tag{16}$$
with
\[ Q(\mu) = -\int_{\phi \in C_B} \mu(\phi \phi') \ln \mu(\phi \phi') \, dS_n \, dS'_n \] (17)

Proceeding exactly in the same way as with single particle, we get the following representation:
\[ \rho = \int_{\phi \phi' \in \mathcal{F}} e^{\langle \phi \phi'|X|\phi \phi' \rangle} \, dS_n \, dS'_n \] (18)

for some self-adjoint operator \( X \) in \( \mathcal{L} \).

### 3.1 Bipartite separability problem

From a formal point of view, the equation (18) provides a solution of bipartite separability problem. In fact, given a product basis \( \{|e_i e'_i|\} \) in the product space \( \mathcal{B} \), (18) is a system of \( n^4 \) numeric equations with respect to \( n^4 \) variables—the matrix elements of the quadratic form \( X \).

\[ \rho_{ii'kk'} = \int_{\phi \phi' \in \mathcal{F}} e^{\langle \phi \phi'|X|\phi \phi' \rangle} \langle e_i | e_i' \rangle \langle \phi \phi' | \phi \phi' \rangle \, dS_n \, dS'_n \] (19)

If the solution exists, (19) provides explicitly an instance of representation of \( \rho \) as a mixture of pure product states.

Although these equations are transcendental. Even in the simple case of a single particle in dimension 2, when the operator \( X \) is proved to commute with \( \rho = p_1 |e_1 \rangle \langle e_1| + p_2 |e_2 \rangle \langle e_2| \), we have two variables \( x_1, x_2 \) which we have to find from the following system of equations, which are a special case of (15):

\[ \begin{cases} \frac{e^{x_1}(x_1-x_2-1)+e^{x_2}}{(x_1-x_2)^2} = p_1 \\ \frac{e^{x_2}(x_2-x_1-1)+e^{x_1}}{(x_1-x_2)^2} = p_2 \end{cases} \] (20)

But the essence of the separability problem is the existence of a solution of (19).
3.2 The existence

In this section I show that the existence of a solution of the equations \(19\) for any robustly separable state follows from the concavity of the functional \(Q\) in \(16\). Begin with a two-dimensional geometrical analogy. Let \(S^2 = \{(x_1, x_2, x_3) \mid x_1 + x_2 + x_3 = 1; x_1, x_2, x_3 \geq 0\}\) be a 2-dimensional simplex in \(\mathbb{R}^3\) and \(K\) be a functional on the plane \(P : x_1 + x_2 + x_3 = 1\) symmetric with respect to \(x_1, x_2, x_3\). If \(K\) is concave, that is, for any \(a, b \in P\) and any point \(q\) lying between \(a\) and \(b\)

\[
K(q) \geq K(a), \quad K(q) \geq K(b)
\]

Let \(K\) be bounded in a domain containing the simplex \(S^2\) and let \(l\) be a line intersecting the interior of \(S^2\). Then \(K\) has a local maximum in the interior of \(S^2\).

Now return to the case of bipartite density matrices. Any such matrix \(\rho\) can be represented as (an infinite) number of pseudomixtures of pure product states (see, e.g. [1] for a discussion). Consider the affine space \(P_1\) of all normalized signed measures on the Cartesian product \(\mathcal{I} = \mathbb{C}B_n \times \mathbb{C}B_n\) of unit spheres (it plays the rôle of the plane \(P\) in the example above). Given a density operator \(\rho\), the collection \(l_1\) of all pseudomixtures representing \(\rho\) is an affine submanifold of \(P_1\). The set of all probability measures on \(\mathcal{I}\) is a simplex \(S^\infty\) in \(P_1\).

A density matrix \(\rho\) is robustly separable if and only if \(l_1\) intersects the interior. This because \(\rho\) can be represented as a mixture of products of full-range density matrices in \(\mathcal{H}, \mathcal{H}'\) each of which can be, in turn, represented by a smeared spectral decomposition [4], that means that there exists a probability measure representing \(\rho\) which does not vanish anywhere on \(\mathcal{I}\).

Therefore the solution of the equations \(19\) always exists for any robustly separable \(\rho\) as the functional \(K\) introduced in \(17\) is concave.

4 Concluding remarks

First sum up the contents of the paper. Given a density operator \(\rho\) in the product of two Hilbert spaces each dimension \(n\), to solve the separability problem is to tell if it has a representation by a mixture of pure product states. In this paper the most smeared distribution on pure product states which yields \(\rho\) rather than their finite mixture is considered.

The separability problem is reduced to \(n^4\) numerical equations which are symbolically written as
\begin{equation}
\n\nabla K = \rho
\end{equation}

whose coordinate form in any product basis in \( \mathcal{B} = \mathcal{H} \otimes \mathcal{H} \) is (19)

\[ \rho_{ii'kk'} = \int_{\phi \phi' \in T} e^{\langle \phi \phi' | X | \phi \phi' \rangle} \langle e_i e_i' | \phi \phi' \rangle \langle \phi \phi' | e_k e_k' \rangle \, dS_n \, dS_n' \]

These equations are transcendental even for non-product case (20), but their solution always exists for any robustly separable density matrix \( \rho \).

That is why one can look for asymptotic methods of finding the solution of the separability problem along these lines. This issue will be addressed in the next paper on optimal ensembles.

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A Smeared spectral decomposition

The formula (4) is derived as follows. Let $\langle e | \phi \rangle$ be a unit vector in $\mathcal{H}$, then for any integer $m$ the following formula holds

$$\int_{\phi \in \mathbb{C}B_n} |\langle e | \phi \rangle|^{2m} |\phi\rangle \langle \phi| \, dS_n = \frac{m!(n-1)!}{(m+n)!} \langle m | e \rangle (e | + \mathbb{I}) \quad (21)$$

which is a direct consequence of a more general formula obtained in [3]. Let $m = Kn$ for some integer $K$. Then it follows directly from (21) that

$$Kn |e\rangle \langle e| + \mathbb{I} = \int_{\phi \in \mathbb{C}B_n} \frac{(Kn+n)!}{(Kn)! (n-1)!} |\langle e | \phi \rangle|^{2Kn} |\phi\rangle \langle \phi| \, dS_n$$

Dividing this equation by $n(K+1)$ we obtain the following continuous representation of the projector $|e\rangle \langle e|$ and the white noise matrix $\Lambda = \mathbb{I}/n$:

$$\frac{K}{K+1} |e\rangle \langle e| + \frac{1}{K+1} \cdot \mathbb{I} = \int_{\phi \in \mathbb{C}B_n} \frac{((K+1)n)!}{(K+1) \cdot (Kn)! n!} |\langle e | \phi \rangle|^{2Kn} |\phi\rangle \langle \phi| \, dS_n$$

(22)

The formula (22) is valid for any eigenvector $\langle e_k |$ of $\rho$. Form a convex combination of the lhs of (22) with (yet unknown) coefficients $q_k$ and require it to be $\rho$:

$$\sum q_k \left( \frac{K}{K+1} \cdot |e_k\rangle \langle e_k| + \frac{1}{K+1} \cdot \frac{1}{n} \right) = \sum p_k |e_k\rangle \langle e_k|$$

When $\mathbb{I}$ is replaced by $\sum |e_k\rangle \langle e_k|$, the second summand in the lhs of the above formula takes the form $\frac{1}{K+1} \cdot \frac{1}{n} \sum |e_k\rangle \langle e_k|$, from which we obtain

$$q_k \cdot \frac{K}{K+1} + \frac{1}{K+1} \cdot \frac{1}{n} = p_k$$

the we get the expression for $q_k$

$$q_k = \frac{K+1}{K} \left( p_k - \frac{1}{(K+1)n} \right) \quad (23)$$

So, we can form the convex combinations of the expressions (22) with the coefficients $q_k$ which yields us $\rho$:
\[
\rho = \sum_k \frac{K+1}{K} \left( p_k - \frac{1}{(K+1)n} \right) \int_{\phi \in \mathbb{C}B_n} \frac{((K+1)n)!}{(K+1) \cdot (Kn)! n!} |\langle \mathbf{e}_k | \phi \rangle|^{2Kn} |\phi\rangle \langle \phi | dS_n
\]

Let \( p_0 \) be the smallest eigenvalue of \( \rho \), then, if \( K+1 < (1/np_0) \), all the coefficients \( q_k \) in (23) are positive.

**B Proof of the formula (14)**

Given a self-adjoint operator \( X \) in \( \mathcal{H} \), consider its eigenbasis \( \{ \mathbf{e}_k \} \) and the integral

\[
F^n(x_1, \ldots, x_n) = \int_{\mathbb{C}B_n} f \left( \langle \phi | X | \phi \rangle \right) dS_n
\]

In order to calculate it denote \( \langle \phi | \mathbf{e}_k \rangle = e^{i\theta} r_k \). Then, taking into account that the integrand does not depend on phases, the above integral (with respect to the normalized measure) reads

\[
F^n(x_1, \ldots, x_n) = \frac{(n-1)!}{2\pi^n} (2\pi)^n \int_{\sum r_k^2 \leq 1} f \left( x_n + \sum_{k=1}^{n-1} (x_k - x_n) r_k^2 \right) \left( \prod_{k=1}^{n-1} r_k \, dr_k \right)
\]

then, introducing the variables \( t_k = r_k^2 \), we reduce the above integral to

\[
F^n(x_1, \ldots, x_n) = (n-1)! \int_{\sum t_k \leq 1} f \left( x_n + \sum_{k=1}^{n-1} (x_k - x_n) t_k \right) \left( \prod_{k=1}^{n-1} dt_k \right)
\]

then, introducing the variables \( t_k = r_k^2 \), we reduce the above integral to

\[
F^n(x_1, \ldots, x_n) = (n-1)! \int_{\sum t_k \leq 1} f \left( x_n + \sum_{k=1}^{n-1} (x_k - x_n) t_k \right) \left( \prod_{k=1}^{n-1} dt_k \right)
\]

For \( f(z) = e^z \) the above equation reads

\[
\frac{F^n(x_1, \ldots, x_n)}{(n-1)!} = e^{x_n} \int_{\sum t_k \leq 1} \prod_{k=1}^{n-1} e^{(x_k - x_n) t_k} dt_k
\]
and we get the following recurrent relation

\[ F^n(x_1, \ldots, x_n) = \frac{n - 1}{x_{n-1} - x_n} \left( F^{n-1}(x_1, \ldots, x_{n-1}) - F^{n-1}(x_1, \ldots, x_{n-2}, x_n) \right) \]

(26)

For \( n = 2 \) we have the explicit expression like (20), for higher \( n \) one can directly verify that the expression (14) satisfies the recurrent relation (26).