REVISTA DE LA
UNIÓN MATEMÁTICA ARGENTINA
Volumen 49, Número 2, 2008, Páginas 111–119

THE PROBLEM OF ENTANGLEMENT OF QUANTUM STATES

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Abstract. We give a brief and incomplete survey of the problem of entanglement of states of composite quantum systems.

1. Quantum mechanics, 1930's

A quantum system is kinematically specified by a complex Hilbert space $\mathcal{H}$ (there are hardly cases where a separable space will not do). The physical "observables" are identified with linear operators on $\mathcal{H}$. Usually the most interesting physical observables for continuous systems are given by unbounded operators; but one avoids this problem by exponentiation and works in $\mathcal{B}(\mathcal{H})$ the bounded linear operators on $\mathcal{H}$. Now $\mathcal{B}(\mathcal{H})$ is a C^*-algebra and a von Neumann algebra. In the 1960's - 1980's there were serious attempts (all of them anticipated by J. von Neumann) to do away with the underlying Hilbert space and work directly with the abstract algebraic structure modeled by C^*-algebras or W^*-algebras (abstract von Neumann algebras)[1, 2, 3]. This was particularly fruitful when dealing with systems of infinitely many degrees of freedom (quantum fields, thermodynamic limits, etc.). The problem of entanglement which we want to address here can be formulated quite straightforwardly in this algebraic framework of quantum theory. But we will stick to the quantum mechanics of the 1930's and keep the Hilbert space. Mainly because the results which are available concern the finite dimensional case. The "states" of the quantum system specified by $\mathcal{H}$ are associated with the linear functionals $f : \mathcal{B}(\mathcal{H}) \to \mathbb{C}$ which are positive (i.e., $f(a) \geq 0$ for all positive $a \in \mathcal{B}(\mathcal{H})$), normalized (i.e., $f(\mathbf{1}) = 1$) and normal (i.e., $f(sup_n\{a_n\}) = sup_n f(a_n)$ for any increasing family of selfadjoint operators $\{a_n : n = 1, 2, \cdots\}$ which is uniformly bounded). It is this normality condition which guarantees that the states are in one-to-one correspondence with positive trace class operators d of unit trace (density operators) via the formula $\mathcal{B}(\mathcal{H}) \ni a \mapsto tr(da)$. This gives an extremely convenient representation of states and one often confuses the state f as a linear functional with the associated density operator d for which $f(a) = tr(da)$. States are automatically continuous, and satisfy $f(a^*) = \overline{f(a)}$. The complex number $f(a)$ is interpreted probabilistically as the expected value of the "observable" associated with the operator a when the system is in the state f. The normalization condition is thus necessary for the consistency of this interpretation and the normality condition is seen as a non-commutative version of the σ-additivity of probability measures.
Clearly states, which we will denote by $\Sigma(\mathcal{H})$, form a convex set which is closed

with respect to the metric induced by the usual norm of linear functionals. Moreover, given any countable set $\{f_j\} \subset \Sigma(\mathcal{H})$ and any countable set $\{\lambda_j\} \subset [0,1]$ such that $\sum_j \lambda_j = 1$, the series $\sum_j \lambda_j f_j$ converges in the norm of functionals to a state of $\mathcal{H}$.
In physical jargon (due to H. Weyl!) the extremal points $ext(\Sigma(\mathcal{H}))$ of $\Sigma(\mathcal{H})$ are called pure states. They are given by

$$f(b) = \langle \psi, b\psi \rangle \ , \quad \text{with } \psi \in \mathcal{H}, \ \|\psi\| = 1 \ ;$$

here $\langle \cdot, \cdot \rangle$ is the scalar product of $\mathcal{H}$. That is: the associated density operator is an orthogonal projection of rank one projecting onto some one-dimensional subspace of $\mathcal{H}$. This orthoprojection is written $|\psi\rangle\langle\psi|$; and $f(b) = tr(|\psi\rangle\langle\psi|b)$.
The representation theorem mentioned, and the spectral theorem for compact operators shows that the states are the closed convex hull of the pure states; in fact each state can be written as an infinite convex sum of extreme states:

$$\Sigma(\mathcal{H}) = \overline{co(ext(\Sigma(\mathcal{H}))} = co_\sigma(ext(\Sigma(\mathcal{H})) \ .$$

But the convex decomposition into extremal elements is never unique. $\Sigma(\mathcal{H})$ is never a (Choquet-) simplex; quite the opposite is true: there are uncountably many convex decompositions and you can choose almost freely the "ingredients" which enter a decomposition. This is a key feature of quantum theory in contradistinction with classical theories whose state spaces are simplices.

Composition, separability and entanglement

If system 1 is described by the Hilbert space $\mathcal{H}_1$ and system 2 by $\mathcal{H}_2$ then the composite system "$1 \cup 2$" is described by $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, the tensor product of the subsystem Hilbert spaces. This is the composition rule of quantum theory, and it is responsible for the most counterintuitive features of the theory. There are no indications from the real world that this rule is in need of change. I will consider mostly composition of two systems, but the definitions can be readily extended to more than two susbsytems. It is important to stress that we are always thinking of distinguishable (sub-) systems 1 and 2. The case of identical systems (bosons or fermions) is more involved and the entanglement issues are only partially understood.

One has $\mathcal{B}(\mathcal{H}) = \mathcal{B}(\mathcal{H}_1) \otimes \mathcal{B}(\mathcal{H}_2)$ although I will not explain what the $\otimes$ on the right means, [8]. Given $f \in \Sigma(\mathcal{H})$, define partial states $f^{(j)} \in \Sigma(\mathcal{H}_j)$, $j = 1, 2$, by

$$f^{(1)}(b) = f(b \otimes \mathbf{1}) \ , \quad b \in \mathcal{B}(\mathcal{H}_1) \ ,$$

$$f^{(2)}(c) = f(\mathbf{1} \otimes c) \ , \quad c \in \mathcal{B}(\mathcal{H}_2) \ .$$

Given $g \in \Sigma(\mathcal{H}_1)$ and $h \in \Sigma(\mathcal{H}_2)$ there is a unique element of $\Sigma(\mathcal{H})$ written $g \otimes h$, such that

$$(g \otimes h)(b \otimes c) = g(b)h(c) \ ,$$

for all $b \in \mathcal{B}(\mathcal{H}_1)$ and all $c \in \mathcal{B}(\mathcal{H}_2)$. A state f of the composite system is *product* if $f = f^{(1)} \otimes f^{(2)}$; that is, if $\forall b \in \mathcal{B}(\mathcal{H}_1)$ and $\forall c \in \mathcal{B}(\mathcal{H}_2)$:

$$f(b \otimes c) = f(b \otimes \mathbf{1}) f(\mathbf{1} \otimes c) .$$

The product states, denoted by $\Sigma_\pi(\mathcal{H})$, not only do not show any correlation whatsoever between product-observables but also (for precisely that reason) the knowledge of the expected values of the observables of subsystem 1 and of the expected values of the observables of subsystem 2 allows one to construct the state of the composite system. Since convex sums of states can be interpreted classically as classical mixtures, the *separable states* or EPR–correlation free states are defined as those in the closed convex hull of the product-states:

$$\Sigma_{sep}(\mathcal{H}) = \overline{co(\Sigma_\pi(\mathcal{H}))} = co_\sigma(\Sigma_\pi(\mathcal{H})) .$$

The states which are not separable are called *entangled* (*verschränkt* was the German word chosen by Schrödinger after his reaction [4, 5, 6] to the Einstein, Podolsky and Rosen paper [7]). In [4, 5], written in english, the words of Schrödinger are the following: *... I would not call that one but rather the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought. By interaction the two representatives [the quantum states] have become entangled.*

A typical entangled state is a pure state f associated to a one-dimensional subspace such that the representative vector ψ in this subspace is not a product vector: $\psi \neq \alpha \otimes \beta$ with $\alpha \in \mathcal{H}_1$ and $\beta \in \mathcal{H}_2$. Entangled states abound (mathematically) and naturally realized physical states are usually entangled (eigenstates of hamiltonians, thermal equilibrium states at low temperatures, etc.).

2. The problem

The problem is then: given a state f of the composite system decide whether f is separable or entangled. That is: are there states $f_j \in \Sigma(\mathcal{H}_1)$, states $g_j \in \Sigma(\mathcal{H}_2)$ and weights $\lambda_j \in [0,1]$ such that $f = \sum_j \lambda_j (f_j \otimes g_j)$? The sum may be an infinite series, in which case it is automatically convergent with respect to the distance associated to the norm of continuous functionals. There is no loss of generality if one restricts to pure states f_j and g_j.
Via the representation theorem for states, one may rephrase the problem purely in terms of positive trace-class operators of unit trace on a Hilbert space tensor product; but the origin and flavor of the problem are then lost.

In the particular case where the given state f is pure, the problem was solved many years ago by, essentially, Schrödinger [4, 5]. For a modern, direct and beautiful presentation of the problem in this particular case the reader is directed to section 11-8 of Jauch's book [9] (a book which can be recommended warmly to any mathematician interested in learning quantum mechanics). The solution is: f pure is separable if and only if $f^{(1)}$ (or alternatively, $f^{(2)}$) is pure. Thus, one has to determine one of the partial states and then check for purity which is easily done in various alternative ways. The simplest is perhaps: take the trace of the square of the associated density operator; if this number is below 1 the state is not pure, otherwise it is pure. This extends readily to the tensor product of any number of Hilbert spaces.

However, when the given state is not pure our knowledge is rather limited. For $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$ there is a criterion due to Wootters [10]; for $\mathcal{H}_1 = \mathbb{C}^2$ and $\mathcal{H}_2 = \mathbb{C}^2$ or $\mathcal{H}_2 = \mathbb{C}^3$, the positive partial transpose criterion of Peres and M. Horodecki, P. Horodecki and R. Horodecki, solves the problem. A recent review is [11]. Gurvits [12], has proved that when the Hilbert spaces involved are finite dimensional, the problem is NP-hard in the hierarchy of computational complexity.
I describe the criteria just mentioned.

2.1. **Wootters' Criterion.** $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$. Given $f \in \Sigma(\mathcal{H})$ let d be the associated density operator, and put

$$w_d := \sqrt{\sqrt{d}\, u^* \,\overline{d}\, u \,\sqrt{d}}\ ,$$

where u is the operator which for any orthonormal basis $\{\psi_1, \psi_2\}$ of $\mathcal{H}_1$ has associated to it the matrix

$$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} ,$$

with respect to the orthonormal basis $\{\psi_j \otimes \psi_k : \ j,k = 1,2\}$ of $\mathcal{H}$. $\overline{d}$ denotes the complex conjugate of d taking the product basis as real. Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ be the eigenvalues of w_d enumerated non-decreasingly according to their multiplicities.

Theorem 1. *f is separable if and only if $\lambda_1 \leq \lambda_2 + \lambda_3 + \lambda_4$ (equivalently: $2\|w_d\| \leq tr(w_d)$).*

2.2. **Positive Partial Transpose Criterion.** $\mathcal{H}_1 = \mathbb{C}^2$, $\mathcal{H}_2 = \mathbb{C}^{2(3)}$. Choose orthonormal bases for $\mathcal{H}_1$ and for $\mathcal{H}_2$. Identify the tensor product such that the matrix associated to $a \otimes b$ in the product orthonormal basis of $\mathcal{H}$ is

$$a \otimes b = \begin{pmatrix} a_{1,1}b & a_{1,2}b \\ a_{2,1}b & a_{2,2}b \end{pmatrix} .$$

The general operator in $\mathcal{B}(\mathcal{H}) = \mathbb{M}_{4(6)}(\mathbb{C})$ has the form

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} ,\ \alpha, \beta, \gamma, \delta \in \mathbb{M}_{2(3)}(\mathbb{C}) .$$

Let

$$T_1 \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} := \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} .$$

This is the partial transpose with respect to the first factor (one could proceed just as well with transposition with respect to the second factor).
Given $f \in \Sigma(\mathcal{H})$, let d be the associated density operator; then

Theorem 2. *f is separable if and only if $T_1(d) \geq 0$.*

For the tensor product of two Hilbert spaces the positivity condition on the partial transpose is always necessary for separability irrespective of dimensions, as observed by A. Peres. The proof of sufficiency given by M. Horodecki, P. Horodecki and R. Horodecki [13], makes heavy use of the classification of positive linear maps of the 2×2 complex matrices $\mathbb{M}_2(\mathbb{C})$ due to E. Størmer and S.L. Woronowicz. For $\mathcal{H}_1 = \mathbb{C}^2$ and $\mathcal{H}_2 = \mathbb{C}^4$ there are counterexamples (P. Horodecki): $T_1(d) \geq 0$ but f is entangled. This happens whenever the dimension of the tensor product Hilbert space $\mathcal{H}$ exceeds 6.

2.3. **Some remarks.**

- In 1964, some thirty years after the EPR paper, J.S. Bell [14] succeeded in capturing and quantifying the separability/entanglement issue in an inequality involving expectation values (correlation inequality).

  Theorem 3. *If $f \in \Sigma_{sep}(\mathcal{H})$, then*

$$\begin{array}{c} |f\,(a_1 \otimes b_1 - a_1 \otimes b_2 + a_2 \otimes b_1 + a_2 \otimes b_2)\,| \\ \{ \quad \leq |f(a_1 \otimes (b_1 - b_2))| + |f(a_2 \otimes (b_1 + b_2)| \quad \} \\ \leq\ 2 \end{array},$$

  for every pair of selfadjoint a_1, a_2 in the unit ball of $\mathcal{B}(\mathcal{H}_1)$ and every pair of selfadjoint b_1, b_2 in the unit ball of $\mathcal{B}(\mathcal{H}_2)$.

  The inequality in brackets is just the triangle inequality and valid for any state. Assume f is a product state, i.e., $f = g \otimes h$; then

$$\begin{aligned} &|f(a_1 \otimes (b_1 - b_2))| + |f(a_2 \otimes (b_1 + b_2)| \\ &= |g(a_1)|\,.\,\underbrace{|h(b_1) - h(b_2)|}_{=:c_1} + |g(a_2)|\,.\,\underbrace{|h(b_1) + h(b_2)|}_{=:c_2} \\ &= c_1|g(a_1)| + c_2|g(a_2)|\,. \end{aligned}$$

  Since $c_1, c_2 \geq 0$, and $|g(a_1)|\,,\,|g(a_2)| \leq 1$, we obtain

$$\begin{aligned} c_1|g(a_1)| + c_2|g(a_2)| &\leq c_1 + c_2 = |h(b_1) - h(b_2)|\ +\ |h(b_1) + h(b_2)| \\ &= 2\max\{|h(b_1)|\ ,\ |h(b_2)|\} \leq 2\,.^* \end{aligned}$$

  If now f is a convex sum of product states, i.e., $f = \sum_{j=1}^n \lambda_j (g_j \otimes h_j)$, then – using the triangle inequality, the positivity of λ_j and the relation $\sum_{j=1}^n \lambda_j = 1$,

$$\begin{aligned} &|f(a_1 \otimes (b_1 - b_2))| + |f(a_2 \otimes (b_1 + b_2)| \\ &\leq \sum_{j=1}^n \lambda_j \left\{|(g_j \otimes h_j)(a_1 \otimes (b_1 - b_2))| + |(g_j \otimes h_j)(a_2 \otimes (b_1 + b_2)|\right\} \end{aligned}$$

*The observant reader will notice that the validity of $|h(b_1) - h(b_2)| + |h(b_1) + h(b_2)| \leq 2\max\{|h(b_1)|\ ,\ |h(b_2)|\}$ depends crucially on the assumption that b_1 and b_2 are selfadjoint so that $h(b_1)$ and $h(b_2)$ are real numbers. For complex z_1 and z_2 in the unit disc $|z_1 - z_2| + |z_1 + z_2| \leq 2\max\{|z_1|, |z_2|\}$ is not true in general ($z_1 = 1$, $z_2 = i$).

$$\leq \sum_{j=1}^{n} \lambda_j \, . \, 2 = 2 \, .$$

Finally, if $f = \lim_\alpha f_\alpha$ is a limit of states f_α which are convex sums of product states, in a topology which makes expectation values continuous, then the inequality persists.

For many years after 1964, "entanglement" was informally identified with "violation of Bell's inequality".

- The next huge leap forward was taken by R.F. Werner in 1989, [15]. For $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^m$, $m = 2, 3, \cdots$, he succeeded in constructing a family of entangled states which satisfy the inequality of Theorem 3 (or any other such correlation inequality which is necessary for separability). He thus showed that Bell-type correlation inequalities could not decide the issue. Werner does this by constructing a so-called "*local* hidden-variable model" for his states. In the present case of operators with discrete spectrum (denoted by σ), this means: Given a state f de $\mathcal{B}(\mathbb{C}^m) \otimes \mathcal{B}(\mathbb{C}^m)$,
  - Find a measurable space (Ω, Σ, μ)
  - For each $a = a^* \in \mathcal{B}(\mathbb{C}^m)$ find a function $\Phi_a : \sigma(a) \times \Omega \to \mathbb{R}$ such that $\Phi_a(x, \omega) \geq 0$, μ a.e. for every $x \in \sigma(a)$ and
  $$\sum_{x \in \sigma(a)} \Phi_a(x, \omega) = 1 \quad , \quad (\mu \text{ a.e.})$$
  - For each $b = b^* \in \mathcal{B}(\mathbb{C}^m)$ find a function $\Psi_b : \sigma(b) \times \Omega \to \mathbb{R}$ such that $\Psi_b(x, \omega) \geq 0$, μ a.e. for every $x \in \sigma(b)$ and
  $$\sum_{x \in \sigma(b)} \Psi_b(x, \omega) = 1 \quad , \quad (\mu \text{ a.e.})$$
  - $$\int_\Omega d\mu(\omega) \Phi_a(x, \omega) \Psi_b(y, \omega) = f(P_x \otimes Q_y) \, ,$$
  where $P_x \in \mathcal{B}(\mathbb{C}^m)$ is the spectral orthoprojector of a associated to the eigenvalue x and $Q_y \in \mathcal{B}(\mathbb{C}^m)$ that of b associated to the eigenvalue y.

  The qualifier "*local*" of the hidden-variable model is expressed by the fact that Φ and Ψ are independent. The correlation inequalities à la Bell are consequences of the integral formula: on the left-hand side we have the expectation of a product with respect to a probability measure.

- Consider the following simple separability/entanglement criterion used by R.F. Werner in his seminal paper just described. If $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{K}$, let V be the continuous linear extension of (the flip):
  $$V(\psi \otimes \phi) := \phi \otimes \psi \; , \quad \psi, \phi \in \mathcal{K}$$
  Consider the pure product state associated to $\psi \otimes \phi$, $\|\psi\| = \|\phi\| = 1$, that is $\mathcal{B}(\mathcal{H}) \ni b \mapsto \langle \psi \otimes \phi, b(\psi \otimes \phi) \rangle_{\mathcal{H}}$. Then, $\langle \psi \otimes \phi, V(\psi \otimes \phi) \rangle_{\mathcal{H}} =$

$\langle\psi \otimes \phi, \phi \otimes \psi\rangle_{\mathcal{H}} = |\langle\psi, \phi\rangle_{\mathcal{K}}|^2 \geq 0$. Then, if $f \in \Sigma_{sep}(\mathcal{H})$, f is a limit of convex sums of pure product states, and thus:

$$f \in \Sigma_{sep}(\mathcal{K} \otimes \mathcal{K}) \implies f(V) \geq 0 \ ;$$

$$f(V) < 0 \implies f \text{ is entangled} \ .$$

However, there are abundant entangled states f with $f(V) \geq 0$. V gives a simple example of a so-called entanglement witness. It is an instance of the Hahn-Banach separation theorem for convex sets: given a closed convex set (e.g., the separable states) a point not in the set can be separated by a hyperplane.
Other, different, criteria have been established (more along the non–geometric lines of the positive partial transpose criterion; see 2.2.) which constitute necessary conditions for separability.
Among these, the range criterion [16] asserts that if the state f is separable, then there are product vectors $\{\psi_j \otimes \phi_j\}$ spanning the range of the density operator d associated to f and such that $\{\overline{\psi_j} \otimes \phi_j\}$ spans that of the partial transpose $T_1(d)$. This criterion is able to detect entanglement of states with positive partial transpose.

Another class of necessary conditions for separability arises from certain maps which are contractive with respect to the trace-norm $\|\cdot\|_1$. Suppose the linear map Λ mapping $\mathcal{B}(\mathcal{H})$ into itself, satisfies $\|\Lambda(|\psi\rangle\langle\psi| \otimes |\phi\rangle\langle\phi|)\|_1 \leq 1$ for all unit vectors $\psi \in \mathcal{H}_1$ and $\phi \in \mathcal{H}_2$. Then if f is separable and d is the associated density operator, one has that $\|\Lambda(d)\|_1 \leq 1$. An example of such a map is the realignment or reshuffling map R for the case $\mathcal{H}_1 = \mathcal{H}_2$, [17], defined by matrix elements with respect to a product basis $\{\psi_j \otimes \phi_\mu\}$ by:

$$\langle\psi_j \otimes \phi_\mu, R(a)(\psi_k \otimes \phi_\nu\rangle = \langle\psi_j \otimes \psi_k, a(\phi_\nu \otimes \phi_\mu\rangle \ .$$

For twenty years now research on the problem has been going strong fueled mainly by the idea that entangled quantum states can be used as carriers of information, and that these q-bits combined to "quantum computers" can overcome some of the limitations of "classical computers". A very good review of the subject of "quantum vs. classical computation" is [18].
Although enormous progress has been made in understanding the subtleties of entanglement the basic problem of deciding whether or not a given state is or isn't entangled remains open.

- When considering entanglement with respect to more than two subsystems, all the possible bipartite entanglement information for a given state is generically useless. A concrete example for $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ with $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}_3 = \mathbb{C}^2$ is given in [19]. For unitary vectors $\alpha, \beta \in \mathbb{C}^2$, with $\alpha \perp \beta$, let $\gamma_\pm = \frac{\alpha \pm \beta}{\sqrt{2}}$. Let p be the orthoprojector onto the subspace spanned by the four pairwise orthogonal vectors: $\alpha \otimes \alpha \otimes \alpha$, $\beta \otimes \gamma_- \otimes \gamma_+$, $\gamma_+ \otimes \beta \otimes \gamma_-$, $\gamma_- \otimes \gamma_+ \otimes \beta$. Now $q = (\mathbf{1} - p)/4$ is a density operator acting on $\mathcal{H}$; the associated state is not separable but it is, nevertheless, separable for each of the three possible bipartitions of the system:

$$\underbrace{\mathcal{H}_1 \otimes \mathcal{H}_2}_{\mathcal{K}_1} \otimes \mathcal{H}_3 \ , \ \mathcal{H}_1 \otimes \underbrace{\mathcal{H}_2 \otimes \mathcal{H}_3}_{\mathcal{K}_2} \ , \ \underbrace{\mathcal{H}_1 \otimes \mathcal{H}_3}_{\mathcal{K}_1} \otimes \mathcal{H}_2 \ .$$

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Recibido: 10 de noviembre de 2008
Aceptado: 26 de noviembre de 2008