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ENTANGLEMENT OF FORMATION AND CONCURRENCE

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Entanglement of formation is one of three widely studied measures of entanglement of a general bipartite system. This paper reviews our current understanding of entanglement of formation and the related concept of concurrence, including discussions of additivity, the problem of finding explicit formulas, and connections between concurrence and other properties of bipartite states.

Keywords: entanglement, concurrence, quantum information

1. Entanglement of pure and mixed states

In both classical mechanics and quantum mechanics, one can define a *pure* state to be a state that is as completely specified as the theory allows. In classical mechanics a pure state might be represented by a point in phase space. In quantum mechanics it is a vector in a complex vector space. Perhaps the most remarkable feature of quantum mechanics, a feature that clearly distinguishes it from classical physics, is this: for any composite system, there exist *pure* states of the system in which the parts of the system do not have pure states of their own. Such states are called entangled.

One can also define the concept of entanglement for mixed quantum states: a mixed state is entangled if it cannot be represented as a mixture of unentangled pure states.

For both pure and mixed quantum states, there are good measures of the *degree* of entanglement. In the case of pure states of a bipartite system there is a single widely accepted measure of entanglement, whereas for mixed states of such systems there are three measures that have been extensively studied. One of these, entanglement of formation, is the subject of this paper.* After recalling the definition of entanglement of formation and the motivation for the definition, we review some aspects of the current state of our understanding of this entanglement measure. For the special case of a pair of qubits, the entanglement of formation is closely related to a simpler but less physically motivated measure of entanglement called the concurrence, and we devote much of our discussion to this concept and to possible generalizations of it to other bipartite systems.† We begin, though, by discussing the simplest case, the entanglement of pure states.

*The other two are distillable entanglement[1,2] and relative entropy of entanglement.[3]
†Recently some researchers have worked towards generalizing both entanglement of formation[4,5] and concurrence[6] to multipartite systems; in this paper we restrict our attention to the bipartite case.

Consider a general quantum system consisting of two parts labeled A and B. Any pure state $|\Phi\rangle$ of this system can always be written in the form[7]

$$|\Phi\rangle = \sum_{i=1}^{n} c_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle, \tag{1}$$

where $\{|\phi_1^A\rangle, \ldots, |\phi_n^A\rangle\}$ and $\{|\phi_1^B\rangle, \ldots, |\phi_n^B\rangle\}$ are sets of orthonormal states for subsystems A and B, respectively, and the c_i's are a set of positive coefficients. The possibility of entanglement is simply the possibility that there may be more than one term in the above sum. The values c_i are precisely the features of the state $|\Phi\rangle$ that do not change when the parts of the system are subjected to separate unitary transformations. Therefore any reasonable definition of the entanglement of $|\Phi\rangle$ should depend only on those values. Of all the possible functions that one might use, one particular function has, for good reason, been adopted as the standard measure of entanglement for pure states, namely,

$$-\sum_{i=1}^{n} c_i^2 \log_2 c_i^2. \tag{2}$$

This quantity is the von Neumann entropy of the density matrix associated with either of the two subsystems, the values c_i^2 being the non-zero eigenvalues of either of these two density matrices.

The justification for using this particular function comes from the possibility of converting one entangled pure state into another.[8,9] We take a particular entangled state, the singlet state $|\Psi^-\rangle = (1/\sqrt{2})(|01\rangle - |10\rangle)$ of a pair of qubits, as our standard state, and define its entanglement to be one "ebit." The entanglement of any other pure state will then be defined by relating it to the standard state. In particular, suppose that two participants, Alice and Bob, are trying to create n copies of a particular bipartite state $|\Phi\rangle$, such that Alice will hold part A of each pair and Bob will hold part B. They are not allowed any quantum communication between them, but they have at their disposal a large collection of shared singlet pairs. We ask, how many singlet pairs must they use up in order to create n copies of the state $|\Phi\rangle$? The answer[8] is that they need roughly $nE(\Phi)$ singlets, where

$$E(\Phi) = S(\mathrm{Tr}_B|\Phi\rangle\langle\Phi|) = S(\mathrm{Tr}_A|\Phi\rangle\langle\Phi|) = -\sum_{i}^{n} c_i^2 \log_2 c_i^2, \tag{3}$$

S indicating the von Neumann entropy. More precisely, for any $\epsilon > 0$, one can find a large enough n such that from m copies of the singlet state, Alice and Bob can produce n copies of $|\Phi\rangle$, with $m/n \leq (1+\epsilon)E(\Phi)$. This is the justification for using $E(\Phi)$ as the measure of entanglement. For example, if the value of $E(\Phi)$ is $1/2$, then to create 1000 copies of $|\Phi\rangle$, Alice and Bob will need only about 500 singlet pairs; so it is reasonable to say that the state $|\Phi\rangle$ has an entanglement of half an ebit. It is worth noting that this process is reversible, in that Alice and Bob could convert their Φ-pairs back into singlets without any loss (asymptotically).

Let us now extend this idea to mixed states. For a mixed state of a bipartite system the von Neumann entropy of a subsystem is no longer a good measure of entanglement, because each subsystem can now have non-zero entropy on its own even if there is no entanglement. The entanglement of formation is designed to pick out the irreducible entanglement of the mixed state.

We imagine Alice and Bob trying to create n copies of a particular mixed state ρ to be shared between them as before. Again Alice and Bob initially share many singlet states and are allowed no quantum communication. How many singlets must they use up, asymptotically, for each copy of the state ρ that they create? The following rough argument suggests an answer to this question. Suppose that Alice and Bob first write down a decomposition of ρ into pure states. That is, they express ρ as

$$\rho = \sum_{j=1}^{N} p_j |\Phi_j\rangle\langle\Phi_j|, \tag{4}$$

where the $|\Phi_j\rangle$'s are distinct (but not necessarily orthogonal) normalized pure states of the bipartite system and the p_j's are non-negative real numbers that add up to one. Now, for each $j = 1, \ldots, N$, Alice and Bob create np_j copies of the pure state $|\Phi_j\rangle$ by using $np_j E(\Phi_j)$ of their singlet pairs. They will then have created a total of n pairs, which they now collect into a large ensemble. Finally, they discard any records they may have generated that would tell them which value of the index j to associate with each physical pair. At this point, then, each pair could be in any of the states $|\Phi_j\rangle$ with probability p_j; that is, each pair is now in the mixed state ρ. The number of singlets that Alice and Bob had to use up in this process is

$$\text{number of singlets used } = n \sum_{j=1}^{N} p_j E(\Phi_j). \tag{5}$$

Note that this number depends on the particular decomposition of ρ that was chosen. Suppose, for example, that ρ is the state $(|00\rangle\langle 00| + |11\rangle\langle 11|)/2$ of two spin-1/2 particles. We can regard this state either as an equal mixture of $|00\rangle$ and $|11\rangle$, or as an equal mixture of $(1/\sqrt{2})(|00\rangle + |11\rangle)$ and $(1/\sqrt{2})(|00\rangle - |11\rangle)$. To create an ensemble based on the former decomposition requires no singlets at all, since neither $|00\rangle$ nor $|11\rangle$ is entangled. But to create an ensemble based on the latter decomposition requires one singlet pair for each copy of the state ρ. If we want to get a measure of the *minimum* number of singlets required to create ρ, we should look for the decomposition that minimizes the expression in Eq. (5). This line of reasoning motivates the definition of entanglement of formation:[1,2]

$$E_f(\rho) = \inf \sum_j p_j E(\Phi_j), \tag{6}$$

where the infimum is taken over all pure-state decompositions of ρ.[‡]

[‡] In an alternative definition of entanglement of formation, Alice and Bob start with no shared entanglement but are allowed quantum communication. The question then is how many qubits must pass between Alice and Bob in order to create many pairs in the desired state. This approach has been adopted by Nielsen to define a generalization of entanglement of formation for multipartite systems.[4]

There are a number of ways in which the above argument needs to be sharpened. Note in particular that when we imagine creating a mixed state ρ, we must allow the possibility that for finite n, the pairs created will not be *exactly* in the state ρ but will only be approximations to ρ. (For example, we cannot make exactly np_j copies of the pure state $|\Phi_j\rangle$ if p_j is an irrational number.) Therefore the goal must be to create a state whose fidelity to the desired state becomes arbitrarily good as n approaches infinity. A careful treatment of this problem has been carried out by Hayden et al.[13] We discuss their work further in the following section.

One feature of entanglement of formation that distinguishes it from the *distillable entanglement*[1,2] is this: by definition, the entanglement of formation of ρ is zero if and only if ρ is separable, that is, if and only if ρ can be written as a mixture of product states. In contrast, the distillable entanglement, a measure of the amount of pure entanglement that one can *extract* from a given mixed state, can be zero even if the state is non-separable. Entangled states with no distillable entanglement are said to have "bound entanglement":[10] they have entanglement, as measured by the entanglement of formation, but this entanglement cannot be used to create *pure* entanglement, as represented, for example, by a collection of singlet pairs. Thus, in contrast to the case of pure states,[8] the creation of entangled mixed states is not reversible. This irreversibility is not surprising: in creating a mixed state from a pure state, one must discard some information.[11]

Though we can relate entanglement of formation to the creation of an *ensemble of pure states* representing the given mixed state ρ, we cannot yet say that it quantifies in an absolute sense the number of singlets required to create many copies of the state ρ itself. The difference between these two senses of creation is the essence of the "additivity question," which is the subject of the next section.

2. The additivity question

Once again imagine Alice and Bob trying to create n copies of the bipartite state ρ. If n is an even number, this task is the same as creating $n/2$ copies of the bipartite state $\rho \otimes \rho$, where the tensor product indicates the composition of two copies of ρ, each of which is to be shared in the usual way between Alice and Bob. Thus, rather than expressing ρ itself as a mixture of pure states and then creating these pure states by transforming a collection of singlets, Alice and Bob could express $\rho \otimes \rho$ as a mixture of pure states and try to create these pure states. Is there any advantage in doing this? Could they get away with using fewer singlets? This is the beginning of the additivity question. In symbols, the question is whether $E_f(\rho \otimes \rho)$ is equal to $2E_f(\rho)$. More generally, we can ask whether $E_f(\rho^{\otimes N})$ is equal to $NE_f(\rho)$, where $\rho^{\otimes N}$ is the tensor product of N copies of ρ. The answer to this question is not known. It must be the case that $E_f(\rho^{\otimes N})$ is less than or equal to $NE_f(\rho)$, because one can always decompose $\rho^{\otimes N}$ into N copies of the optimal decomposition of ρ. What is not known is whether one can do better.

If it does turn out that there is an advantage in treating many pairs together as a unit, then $E_f(\rho)$ itself is clearly not the proper measure of the quantum resources needed to create the mixed state ρ. Rather, one would want to use the *regularized entanglement of* *formation*, defined as follows:[12]

$$E_f^\infty(\rho) = \lim_{N\to\infty} \frac{E_f(\rho^{\otimes N})}{N}. \tag{7}$$

One has to check, though, (i) that this limit exists and (ii) that there is not some alternative way to create many copies of the state ρ, more efficient than creating the pure states of a decomposition of $\rho^{\otimes N}$. Fortunately, Hayden, Horodecki, and Terhal,[13] using a continuity theorem of Nielsen,[14] have proved that E_f^∞ survives these concerns and does indeed express the asymptotic cost, in singlets, of creating the state ρ.

So far we have been considering the additivity of entanglement for a collection of pairs in the *same* state ρ. The standard notion of additivity is actually more general:[15] we say that entanglement of formation is *additive* if

$$E_f(\rho \otimes \sigma) = E_f(\rho) + E_f(\sigma), \tag{8}$$

where ρ and σ are any two bipartite states, each shared between Alice and Bob. (The states ρ and σ do not have to be states of similar objects. *E.g.*, ρ could be the state of a pair of qubits and σ could be the state of N pairs of qubits.) If entanglement of formation is additive in this sense, then it follows that $E_f^\infty = E_f$. Eq. (8) has been shown to be true for special cases: Benatti and Narnhofer[15] proved it for the case where σ is of the form $\sigma_A \otimes \sigma_B$, and Vollbrecht and Werner[16] extended this result to the case where σ is any separable state, that is, any state for which $E_f(\sigma) = 0$. Beyond this, though, and the fact that no counterexample has ever been found, little is known about the additivity of E_f.

As we will see below, there are some significant analytical results for the entanglement of formation E_f. But E_f^∞ is the more physically interesting quantity, being an expression of the actual asymptotic cost of creating the state ρ. Therefore it would be of great interest to settle the additivity question.

3. Exact Formulas

The definition of entanglement of formation, Eq. (6), requires finding the minimum average entanglement over all possible pure-state decompositions of the given mixed state ρ. Even for a simple system such as a pair of qubits, there is no limit to the number of parameters required to specify a decomposition, because the number of terms can be arbitrarily large. There is, however, a theorem due to Uhlmann[17] guaranteeing that in order to find the minimum average entanglement, it is sufficient to consider decompositions with no more than r^2 terms, where r is the rank of ρ. For a pair of qubits, then, one need never consider mixtures of more than 16 pure states.[a] Moreover a number of researchers have devised efficient methods for minimizing the average entanglement.[22,23,24,25] Nevertheless, one would like if possible to have an explicit expression for E_f that does not require this extremization. Explicit formulas have been found for certain systems and certain classes of states, and they are the subject of this section.

[a] In fact it turns out that for a pair of qubits one never needs more than four terms.[18,19] However, for mixed states of larger systems, the number of terms needed in an optimal decomposition often greatly exceeds the rank of the density matrix.[20,21]

3.1. *Case 1: A pair of qubits*

For a pair of qubits, there exists a general formula for E_f, proved first for special cases[1,26] and later for all states.[19] The formula is based on the quantity called "concurrence," which at this point has a standard definition only for a pair of qubits.[26,19] (But see Section 4 below for possible generalizations to larger systems.)

Let us first consider a pure state $|\Phi\rangle$ of a pair of qubits. The concurrence $C(\Phi)$ of this state is defined to be $C(\Phi) = |\langle\Phi|\tilde{\Phi}\rangle|$, where the tilde represents the "spin-flip" operation $|\tilde{\Phi}\rangle = (\sigma_y \otimes \sigma_y)|\Phi^*\rangle$. Here $|\Phi^*\rangle$ is the complex conjugate of $|\Phi\rangle$ in the standard basis $\{|00\rangle, |01\rangle\, |10\rangle, |11\rangle\}$, and σ_y is the Pauli operator $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. The spin-flip operation, when applied to a pure product state, takes the state of each qubit to the orthogonal state, that is, the state diametrically opposite on the Bloch sphere. The concurrence of a pure product state is therefore zero. On the other hand, a completely entangled state such as the singlet state is left invariant by the spin flip (except possibly for a phase factor), so that for such states C takes the value one, which is its maximum possible value. It is not hard to obtain the following relation between concurrence and entanglement of a pure state.

$$E(\Phi) = \mathcal{E}(C(\Phi)), \tag{9}$$

where the function $\mathcal{E}$ is defined by

$$\mathcal{E}(C) = h\left(\frac{1+\sqrt{1-C^2}}{2}\right); \tag{10}$$

$$h(x) = -x\log_2 x - (1-x)\log_2(1-x). \tag{11}$$

The function $\mathcal{E}(C)$ is monotonically increasing for $0 \le C \le 1$; so the concurrence can be regarded as a measure of entanglement in its own right, though unlike entanglement of formation, it is not a resource-based or information theoretic measure. The connection between concurrence and entanglement is particularly clear if we express the state in the standard basis:

$$|\Phi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle. \tag{12}$$

One can show that $|\Phi\rangle$ is factorizable if and only if $ad = bc$, so that one might take the difference between ad and bc as a measure of entanglement. Indeed, this is what concurrence does: $C(\Phi) = 2|ad - bc|$.

We can define the concurrence of a *mixed* state ρ of two qubits to be the average concurrence of an ensemble of pure states representing ρ, minimized over all decompositions of ρ. That is,

$$C(\rho) = \inf \sum_j p_j C(\Phi_j), \tag{13}$$

where $\rho = \sum_j p_j |\Phi_j\rangle\langle\Phi_j|$. Now it happens that the function $\mathcal{E}(C)$ defined by Eq. (10), in addition to being monotonically increasing, is also convex. It follows that

$$\mathcal{E}(C(\rho)) = \inf \mathcal{E}\Big(\sum_j p_j C(\Phi_j)\Big) \le \inf \sum_j p_j \mathcal{E}(C(\Phi_j)) = E_f(\rho). \tag{14}$$

That is, $\mathcal{E}(C(\rho))$ is a lower bound on $E_f(\rho)$.

At this point we invoke, but do not prove, two remarkable facts about concurrence. First, there always exists a decomposition of ρ that achieves the minimum in Eq. (13) with a set of pure states having the *same* concurrence. This fact makes the inequality in Eq. (14) an equality, so that $\mathcal{E}(C(\rho))$ actually gives us the entanglement of formation. Second, one can find an explicit formula for $C(\rho)$.[19] It is

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{15}$$

where the λ_i's are the square roots of the eigenvalues of $\rho\tilde{\rho}$ in descending order. Here $\tilde{\rho}$ is the result of applying the spin-flip operation to ρ:

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y), \tag{16}$$

and the complex conjugation is again taken in the standard basis.[b] Alternatively, we can say that the λ_i's are the singular values[c] (in descending order) of the symmetric matrix

$$A_{ij} = \sqrt{r_i r_j}\langle\Psi_i|\tilde{\Psi}_j\rangle, \tag{17}$$

where the $|\Psi_i\rangle$'s are the eigenvectors of ρ and the r_i's are the corresponding eigenvalues. One can see that Eq. (15) reduces to the pure state formula $C(\Phi) = |\langle\Phi|\tilde{\Phi}\rangle|$ when ρ is the pure state $|\Phi\rangle\langle\Phi|$. We now have our formula for the entanglement of a pair of qubits in any mixed state ρ:

$$E_f(\rho) = \mathcal{E}(C(\rho)), \tag{18}$$

with C given by Eq. (15) and the function $\mathcal{E}$ given by Eq. (10). The original proof of this formula[19] has been streamlined recently by Audenaert *et al.*[23] on the basis of a theorem of Thompson.[27]

It is a curious fact that for a pair of qubits, one can always find an optimal decomposition of ρ in which all the states have the same entanglement. One might wonder whether this feature will be preserved for larger systems. It is easy to see that the answer is no. Consider, for example, a mixed state of two qutrits (objects with 3 orthogonal states) consisting of an equal mixture of the two pure states

$$|00\rangle \quad \text{and} \quad \frac{1}{\sqrt{2}}(|11\rangle + |22\rangle). \tag{19}$$

One can show that this is the unique optimal decomposition of the given mixed state, and yet its component pure states have quite different entanglements.

In fact, for bipartite systems larger than a pair of qubits, there is no known general formula for the entanglement of formation. However, there do exist formulas for states with special symmetries and we now consider two such cases, Werner states and isotropic states.

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[b] Even though $\rho\tilde{\rho}$ is not necessarily a Hermitian matrix, its eigenvalues are all real and non-negative because it is the product of two non-negative definite matrices.

[c] The singular values of a complex matrix A are the square roots of the eigenvalues of $A^\dagger A$.

3.2. *Case 2: Werner states*

Consider a pair of d-dimensional quantum objects A and B. We assume that we have chosen a correspondence between the states of A and the states of B, so that it would make sense, for example, to say that A and B are in the *same* state. More relevant for our purpose, it makes sense to speak of performing the *same* transformation on A and B. A state ρ of the joint system AB is then called a *Werner state* if it is invariant under all transformations of the form $U \otimes U$, where U is a unitary operator.[16] The most general Werner state is of the form

$$\rho = aI + bF, \tag{20}$$

where a and b are real numbers, I is the identity operator, and F is the operator that interchanges A and B: $F = \sum_{ij} |ij\rangle\langle ji|$. Here the states $|ij\rangle$ are an orthonormal basis of product states for the system AB. The parameters a and b are related by the condition $\mathrm{Tr}\,\rho = 1$; so the Werner states in any given number of dimensions are characterized by a single parameter. A convenient choice for this parameter is $f(\rho) = -\mathrm{Tr}\,\rho F$, which ranges from -1 to 1.

For a pair of qubits, there exists a unique Werner state that is also a pure state, namely, the singlet state $|\Psi^-\rangle\langle\Psi^-|$; the other Werner states are mixtures of the singlet with the completely mixed state. In higher dimensions the Werner states are always mixed states.

By making use of the symmetry of these states, Vollbrecht and Werner[16] found an exact formula for the entanglement of formation, valid in any dimension. I simply state the result here. For $f(\rho) \leq 0$, the state is separable. For $f(\rho) \geq 0$, we have

$$E_f(\rho) = \mathcal{E}(f(\rho)), \tag{21}$$

where $\mathcal{E}$ is the function we defined in Eq. (10) in connection with the entanglement of a pair of qubits. Thus f, when it is non-negative, plays exactly the role of the concurrence; indeed, in the case $d = 2$, $\max\{0, f\}$ is equal to the concurrence.

Notice that the maximum possible entanglement of a Werner state is 1 ebit, regardless of the value of d, even though the maximum possible entanglement of a general state in d dimensions is $\log_2 d$. The maximally entangled Werner states are mixtures of orthogonal singlet states. For example, for $d = 3$ the unique maximally entangled Werner state is an equal mixture of $(1/\sqrt{2})(|01\rangle - |10\rangle)$, $(1/\sqrt{2})(|02\rangle - |20\rangle)$, and $(1/\sqrt{2})(|12\rangle - |21\rangle)$.

3.3. *Case 3: Isotropic states*

Again let us consider two d-dimensional systems A and B for which we have made a correspondence between state spaces. The *isotropic* states of the system AB are those states that are invariant under all transformations of the form $U \otimes U^*$, where the asterisk denotes complex conjugation in a certain fixed basis.[28] In every dimension d, there is exactly one pure state that is an isotropic state, namely, $|\Phi^+\rangle = (1/\sqrt{d})\sum_i |ii\rangle$. The other isotropic states are mixtures of this pure state with the completely mixed state. Thus, these states can, like the Werner states, be labeled in any dimension by a single real parameter. A convenient choice is $g(\rho) = \langle\Phi^+|\rho|\Phi^+\rangle$, which ranges from 0 to 1.

Again by making use of the symmetry, Terhal and Vollbrecht[28] found a formula for the entanglement of formation of a general isotropic state. (This was the first formula obtained for any class of mixed states in arbitrary dimension.) They found that for $g < 1/d$ the state is separable, and for $g \geq 1/d$ the formula is

$$E_f(\rho) = \mathrm{co}\left(h(\gamma) + (1-\gamma)\log_2(d-1)\right), \tag{22}$$

where

$$\gamma = \frac{1}{d}\left(\sqrt{g} + \sqrt{(d-1)(1-g)}\right)^2 \tag{23}$$

and the symbol "co" applied to any function of g indicates the convex hull, that is, the largest convex function that is nowhere larger than the given function.

For $d = 2$, the function inside the "co" symbol is already convex as a function of g—it is in fact $\mathcal{E}(2g-1)$ with $\mathcal{E}$ given again by Eq. (10)—but for other dimensions one needs to find the convex hull. Terhal and Vollbrecht have found the convex hull for $d = 3$ and have conjectured its form for all d. Their conjecture, and their result for $d = 3$, are given by[28]

$$E_f(\rho) = \begin{cases} 0, & g \leq \frac{1}{d}, \\ h(\gamma) + (1-\gamma)\log_2(d-1), & 1/d < g < 4(d-1)/d^2, \\ \left[(g-1)d\log_2(d-1)\right]/(d-2) + \log_2 d, & 4(d-1)/d^2 \leq g \leq 1. \end{cases} \tag{24}$$

The paper of Vollbrecht and Werner[16] shows how to get the entanglement of formation of certain other states that are related to Werner and isotropic states; I refer the reader to that paper for details. We move now to an example that is interesting even though it is not physical.

3.4. *Case 4: A pair of rebits*

Our last example of an explicit formula for entanglement of formation concerns a fictitious object called a "rebit," whose state space is a two-dimensional *real* vector space. This case was investigated by Caves, Fuchs, and Rungta[29] with the aim of seeing how entanglement manifests itself in a theory other than standard quantum mechanics.

A density matrix ρ of a pair of rebits is a 4×4 real symmetric matrix with unit trace and no negative eigenvalues. Following Caves *et al.*, we define the entanglement of formation of a pair of rebits just as in standard quantum mechanics, except that the only decompositions of ρ that we consider are those whose pure-state elements are represented as real vectors. This restriction makes a significant difference, as can be seen in the (real) state

$$\rho_0 = \frac{1}{4}(I \otimes I + \sigma_y \otimes \sigma_y), \tag{25}$$

which is an equal mixture of the two pure entangled states $(1/\sqrt{2})(|00\rangle - |11\rangle)$ and $(1/\sqrt{2})(|01\rangle + |10\rangle)$. In ordinary complex quantum mechanics ρ_0 is separable, because it can also be written as an equal mixture of the two pure product states $(1/2)(|0\rangle + i|1\rangle) \otimes (|0\rangle + i|1\rangle)$ and $(1/2)(|0\rangle - i|1\rangle) \otimes (|0\rangle - i|1\rangle)$. However, these latter states are not allowed in real-vector-space quantum mechanics and it is easy to see that no mixture of real product states can produce the above state ρ_0: any mixture ρ_{sep} of real product states must satisfy

$$\mathrm{Tr}[\rho_{sep}(\sigma_y \otimes \sigma_y)] = 0, \tag{26}$$

since $\langle\psi|\sigma_y|\psi\rangle = 0$ for any real state $|\psi\rangle$. The state ρ_0 does not have zero trace with $\sigma_y \otimes \sigma_y$; so it is not separable in real-vector-space quantum mechanics.

Indeed, for a general mixed state ρ, Caves *et al.* show that the quantity $\mathrm{Tr}[(\rho(\sigma_y \otimes \sigma_y)]$ plays exactly the role of concurrence for a pair of rebits: the entanglement of formation of a pair of rebits is given by $E_f = \mathcal{E}(C)$, where $C = \mathrm{Tr}[(\rho(\sigma_y \otimes \sigma_y)]$ and the function $\mathcal{E}$ is given, as always, by Eq. (10).[29]

Caves *et al.* point out that in real-vector-space quantum mechanics, the state ρ_0 is a *bound* entangled state. It cannot have any distillable entanglement because it has no entanglement at all in the complex world, and any distillation procedure that one could perform in the real case could also be performed in the complex case. This example thus provides an interesting perspective on bound entanglement: bound entanglement can sometimes be a manifestation of a restriction on the pure states that one is allowed to use in building up the given mixed state. Caves *et al.* raise the interesting question whether some bound entangled states in complex quantum mechanics would appear unentangled in quaternionic quantum mechanics.

4. Generalizations of Concurrence

For a pair of qubits, the concurrence is a simple measure of entanglement that provides an analytic formula for the entanglement of formation. It is therefore interesting to ask whether concurrence can be generalized to larger quantum objects. There is no widely accepted definition of concurrence for systems other than a pair of qubits. There are, however, some interesting proposals, which are the subject of this section.

4.1. *Concurrence associated with an arbitrary conjugation*

Recall that the concurrence of a pure state $|\Phi\rangle$ is defined as $C(\Phi) = |\langle\Phi|\tilde{\Phi}\rangle|$, where the tilde operation consists of taking the complex conjugate of $|\Phi\rangle$ in the standard basis and then applying the unitary operator $\sigma_y \otimes \sigma_y$. The tilde operation on a pair of qubits is an example of a *conjugation*, that is, an antiunitary operator whose square is the identity. Uhlmann[30] has generalized the concept of concurrence by considering arbitrary conjugations acting on arbitrary Hilbert spaces.

First let us unpack the definition of "conjugation." An *antilinear* operator Θ is an operator satisfying

$$\Theta(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1^*\Theta|\psi_1\rangle + a_2^*\Theta|\psi_2\rangle. \tag{27}$$

The operator is *antiunitary* if it also satisfies $\langle\psi|\Theta|\phi\rangle = \langle\phi|\Theta^{-1}|\psi\rangle$ for all state vectors $|\psi\rangle$ and $|\phi\rangle$, that is, if the adjoint is the same as the inverse. Finally, an antiunitary Θ is a conjugation if $\Theta^2 = I$. For later reference we also define a *skew conjugation* to be an antiunitary operator θ such that $\theta^2 = -I$.

For any conjugation Θ, one can define the Θ-concurrence of a pure state $|\Phi\rangle$ to be

$$C_\Theta(\Phi) = |\langle\Phi|\Theta|\Phi\rangle|. \tag{28}$$

The Θ-concurrence of a mixed state ρ is then defined as

$$C_\Theta(\rho) = \inf \sum_j p_j C_\Theta(\Phi_j), \tag{29}$$

where the infimum is over all pure-state decompositions of ρ. Uhlmann shows that, just as one can find an explicit formula for the usual concurrence, one can find a very similar formula for the Θ-concurrence:[30]

$$C_\Theta(\rho) = \max\Big\{0, \lambda_1 - \sum_{i>1} \lambda_i\Big\}. \tag{30}$$

Here the λ_i's are the square roots of the eigenvalues of $\rho(\Theta\rho\Theta)$ in descending order. If the system is a pair of qubits and Θ is the tilde operation, this formula reduces to Eq. (15). Thus the formula (15) is a special case of something quite general.

The next question is whether we can use these more general conjugations to get a quantitative handle on entanglement for systems other than a pair of qubits. Uhlmann presents some evidence in that direction as well. In particular, he considers a bipartite quantum system consisting of a qubit and an d-state object (that is, a $2 \times d$ system), where d is even. For that case he obtains the following lower bound on the entanglement of formation:

$$E_f(\rho) \geq \mathcal{E}(\sup_\Theta C_\Theta(\rho)), \tag{31}$$

where Θ is restricted to be the tensor product of two skew conjugations acting on the two subsystems. In the case of a 2×2 system, there is essentially only one such Θ, the two skew conjugations in that case both being the spin flip on a single qubit: $\theta|\phi\rangle = \sigma_y|\phi^*\rangle$.

Partly to deal with *odd* values of d—but we will find this idea useful more generally in the next subsection—Uhlmann suggests using operators that are more general than conjugations in that they send some state vectors to zero. More precisely, he considers arbitrary antilinear operators Θ such that $\Theta^\dagger = \Theta$. One can define the Θ-concurrence for such operators by Eq. (29), and Uhlmann shows that $C_\Theta(\rho)$ is still given by Eq. (30).

For a typical bipartite system larger than a pair of qubits, a single antilinear operator and its associated concurrence will most likely not be enough to capture entanglement. (Hence the "sup" to strengthen the inequality in Eq. (31).) Rather, one will probably need several concurrences. The idea of using many different concurrences leads to the notion of a "concurrence vector," which is the subject of the following subsection.

4.2. *A concurrence vector*

Let ρ be the state of an arbitrary bipartite system, and let $D = \{(|\Phi_i\rangle, p_i)\}$ be a decomposition of ρ into pure states. When the system is a pair of qubits, we can define the average concurrence of the decomposition to be

$$C(D) = \sum_k p_k C(\Phi_k) = \sum_k p_k |\langle\Phi_k|\tilde{\Phi}_k\rangle|. \tag{32}$$

Audenaert, Verstraete, and De Moor[23] generalize this formula in the spirit of Uhlmann's work, by defining for an arbitrary $d_1 \times d_2$ system a specific set of anitlinear operators generalizing the tilde operation.

Following their construction, we begin by choosing once and for all a standard basis for each of the two subsystems. Let (i, i') with $i < i'$ label two specific basis states for the first subsystem, and let j and j' be analogous indices for the second subsystem. For brevity, let α represent the ordered set (i, j, i', j'). There are $[d_1(d_1 - 1)/2][d_2(d_2 - 1)/2]$ possible choices of the two pairs of states, *i.e.*, choices of α. For each such choice, we define an antilinear operator Θ_α by its action on basis vectors: all basis vectors other than the four tensor products formed from the vectors labeled by α are sent to zero by Θ_α , and the action of Θ_α on the four remaining basis vectors is given by

$$\begin{aligned} \Theta_\alpha|ij\rangle &= -|i'j'\rangle, \qquad & \Theta_\alpha|i'j'\rangle &= -|ij\rangle, \\ \Theta_\alpha|ij'\rangle &= |i'j\rangle, \qquad & \Theta_\alpha|i'j\rangle &= |ij'\rangle. \end{aligned} \tag{33}$$

Thus Θ_α projects an arbitrary state of the system onto a "two-qubit subspace" and then performs what amounts to a spin-flip on that subspace.

Now, for any pure state $|\Phi\rangle$ of the system, we define the Θ_α-concurrence of $|\Phi\rangle$ as in Eq. (28): $C_{\Theta_\alpha}(\Phi) = |\langle\Phi|\Theta_\alpha|\Phi\rangle|$. We abbreviate $C_{\Theta_\alpha}(\Phi)$ as $C_\alpha(\Phi)$, and we refer to the ordered set of values $\{C_\alpha(\Phi)\}$ as the *concurrence vector* of the pure state $|\Phi\rangle$. It is not hard to show that a pure state $|\Phi\rangle$ is factorable if and only if $C_\alpha(\Phi) = 0$ for each α. We also note that the squared "length" of the concurrence vector, $\sum_\alpha C_\alpha^2(\Phi)$, is invariant under local unitary transformations of the two separate subsystems.

Returning now to the mixed state ρ with decomposition D, we define a concurrence vector $\{C_\alpha(D)\}$ by analogy with Eq. (32):

$$C_\alpha(D) = \sum_i p_i C_\alpha(\Phi_i). \tag{34}$$

The mixed state ρ is separable if and only if there exists a decomposition D such that every component of the concurrence vector is zero.

Can one use the concurrence vector to express the entanglement of formation of a general $d_1 \times d_2$ system? The answer is not known. However, Audenaert *et al.* use the "vector" of operators Θ_α to formulate an interesting condition for separability. To get to this condition, we first introduce a set of matrices $A^{(\alpha)}$ that are analogous to the matrix A of Eq. (17):

$$A_{ij}^{(\alpha)} = \sqrt{r_i r_j}\langle\Psi_i|\Theta_\alpha|\Psi_j\rangle. \tag{35}$$

Here the r_i's and $|\Psi_i\rangle$'s are again the eigenvalues and eigenvectors of ρ. Let $\{\lambda_i^{(\alpha)}\}$ be the singular values of $A^{(\alpha)}$ in descending order (or alternatively, the square roots of the eigenvalues of $\rho(\Theta_\alpha\rho\Theta_\alpha)$). For any particular α, a necessary and sufficient condition for the existence of a decomposition D such that $C_\alpha(D) = 0$ is the following [see Eq. (30)]:

$$\lambda_1^{(\alpha)} \leq \sum_{i>1} \lambda_i^{(\alpha)}. \tag{36}$$

Thus for each value of α, Eq. (36) is a necessary condition for separability. Note, however, that different values of α may require different decompositions D to make $C_\alpha(D) = 0$, so that even if Eq. (36) is satisfied for every α, there is no guarantee that the state ρ is separable.

One can, however, generate many other necessary conditions for separability simply by starting with a linear combination of the Θ_α's rather than with just one of them. Let $x = \{x_\alpha\}$ be a vector of complex numbers, and define $\{\lambda_i(x)\}$ to be the singular values (in descending order) of the matrix $\sum_\alpha x_\alpha A^{(\alpha)}$. Then for any vector x the following is a necessary condition for separability:

$$\lambda_1(x) \leq \sum_{i>1} \lambda_i(x). \tag{37}$$

Finally, we choose a vector x that makes the separability condition strongest, thus arriving at the condition

$$\max_x \frac{\lambda_1(x)}{\sum_{i>1} \lambda_i(x)} \leq 1. \tag{38}$$

Audenaert *et al.* demonstrate numerically that Eq. (38) is quite a stringent test for separability.[23] In particular it identifies non-separable states of a 3×3 system that are missed by the "partial transpose condition" introduced by Peres.[31] These authors raise the question whether Eq. (38) may even be a *sufficient* condition for separability. If so, this would be a great success for the concurrence-vector approach.

4.3. *Universal state inversion*

The standard definition of concurrence is based on the spin-flip operation, which takes any product state of a pair of qubits to an orthogonal state. Rungta *et al.*[32] have taken this fact as the starting point for another generalization of concurrence, somewhat different in spirit from the ones in the preceding subsections. Rather than working with operations on state vectors (such as conjugations), they look for a *superoperator* S_d—it will act on density matrices in a space of d dimensions—satisfying the following three conditions:

1. S_d maps Hermitian operators to Hermitian operators.
2. S_d commutes with all unitary operators.
3. If $|\Phi\rangle$ is a pure state for a bipartite system, then $\langle\Phi|(S_{d_1} \otimes S_{d_2})(|\Phi\rangle\langle\Phi|)|\Phi\rangle$ is always non-negative, and is equal to zero if and only if $|\Phi\rangle$ is a product state.

They find that up to a constant factor there is only one such superoperator in any dimension, namely,

$$S_d(\rho) = I - \rho, \tag{39}$$

where I is the identity operator. For a pair of qubits, the concurrence of a pure state $|\Phi\rangle$ can be written in terms of S_2 as

$$C(\Phi) = \sqrt{\langle\Phi|(S_2 \otimes S_2)(|\Phi\rangle\langle\Phi|)|\Phi\rangle}. \tag{40}$$

Rungta *et al.* therefore propose an analogous definition of pure-state concurrence in any dimension:

$$C(\Phi) = \sqrt{\langle\Phi|(S_{d_1} \otimes S_{d_2})(|\Phi\rangle\langle\Phi|)|\Phi\rangle} = \sqrt{2[1 - \mathrm{tr}(\rho_A^2)]}, \tag{41}$$

where ρ_A is the density matrix of one of the two parts of the system.

This generalized concurrence turns out to be closely related to the pure-state concurrence vector of the preceding subsection. One can show that it is in fact the *length* of the concurrence vector:

$$C^2(\Phi) = \sum_\alpha C_\alpha^2(\Phi). \tag{42}$$

It is interesting and rather satisfying that these two different approaches to generalizing concurrence are related in such a simple way.

For pure states, the usual entanglement given by Eq. (3) is not a function of the generalized concurrence of Eq. (41): except in the case of two qubits, the two functions give different entanglement orderings for the pure states.[33] So one would not expect to find a formula for entanglement of formation based on Eq. (41). On the other hand, this generalized concurrence may prove valuable either in the search for bounds on the various measures of mixed-state entanglement or in other contexts, such as the entanglement sharing problem (see subsection 5.2 below).

5. Investigations Using Concurrence

Because the concurrence of a pair of qubits is easy to compute for an arbitrary mixed state, it has been used in a number of investigations of the properties of entanglement. In this section I describe some of these studies.

5.1. *Comparison of entanglement measures*

It is interesting to compare concurrence to other quantities related to entanglement. One simple measure of entanglement for a pair of qubits is based on the Peres criterion for separability: a bipartite state ρ is separable only if the partial transpose of ρ, that is, the result of applying the transpose operation to only one of the two subsystems, has no negative eigenvalues.[31] For a pair of qubits this condition is not only necessary but also sufficient for separability,[34] so that if ν is the smallest eigenvalue of the partial transpose of ρ, we can take $N(\rho) = 2\max\{0, -\nu\}$, called the negativity, to be a measure of ρ's entanglement.[35] For pure states, one can show directly that the negativity is equal to the concurrence. Eisert and Plenio,[36] and later Zyczkowski,[22] numerically investigated the relationship between $N(\rho)$ and $C(\rho)$ for many randomly generated mixed states of a pair of qubits and found that the following inequality seemed always to hold: $N(\rho) \leq C(\rho)$. This inequality was later proved by Audenaert *et al.*[35]

Another natural measure of entanglement for a pair of qubits is based on what is called the best separable approximation to a bipartite density matrix, introduced by Lewenstein and Sanpera.[37] Given a density matrix ρ of any $d_1 \times d_2$ system, one can always write ρ as a weighted average of a separable density matrix ρ_s and another, possibly entangled, density matrix ρ_r such that the weight w of ρ_s is maximal. The state ρ_s is then called the best separable approximation to ρ. When the system is a pair of qubits, the best separable approximation is unique and the residual density matrix ρ_r (if such a residual state is required) always represents an entangled pure state.[37,38] One can therefore define the following measure of entanglement for a pair of qubits:[37]

$$R(\rho) = (1 - w)E(\Phi), \tag{43}$$

where $|\Phi\rangle$ is the residual pure state and E is the usual pure-state entanglement given by Eq. (3).

In a recent paper, Wellens and Kuś[39] have found a remarkable connection between $R(\rho)$ and $C(\rho)$, namely, that if the best separable approximation to ρ has full rank (rank 4), then the concurrence is equal to $1 - w$ and the residual pure state $|\Phi\rangle$ is maximally entangled, so that $R(\rho) = C(\rho)$. It follows that when the best separable approximation is of full rank, the Lewenstein-Sanpera procedure generates a pure-state decomposition of ρ that minimizes the average concurrence: the decomposition consists of a single pure state with $C = 1$ and weight R, together with other states all having $C = 0$. This result may sound surprising, since the optimal decompositions we discussed in Section 3 always *equalize* the concurrences of the pure states. But in fact it is typically the case that many different decompositions achieve the same minimum concurrence, so that the above result is not paradoxical.[a]

5.2. *Entanglement under constraints*

A number of authors have studied the relationship between the entanglement of a state ρ and some measure of the purity of the state.[22,40,41] In general, entanglement becomes less likely as the purity diminishes. One formulation of this problem is to ask what the maximum possible entanglement is for a fixed set of eigenvalues of the density matrix. The answer to this question is now known for a pair of qubits. Let ρ be any state of a pair of qubits, and let (r_1, r_2, r_3, r_4) be the eigenvalues of ρ in descending order. Then the maximum possible concurrence of ρ is

$$C_{max}(\rho) = \max\{0, r_1 - r_3 - 2\sqrt{r_2 r_4}\}. \tag{44}$$

A special case of this result was proved by Ishizaka and Hiroshima[42] and the general case by Verstraete, Audenaert, and De Moor.[43] It follows from Eq. (44) that any state ρ for which $\mathrm{Tr}\,\rho^2$ does not exceed 1/3 cannot be entangled, a result that appears also in the work of Zyczkowski *et al.*[40] and Munro *et al.*.[41]

Fixing the purity or the eigenvalues of ρ is one sort of constraint on the state that can limit entanglement. Another limitation arises when entanglement must be shared among several quantum objects.[44] Consider, for example, a system of three qubits A, B, and C. *A priori*, the concurrence C_{AC} between A and C could have any value between 0 and 1. However, if there is some entanglement between A and B, this will limit the entanglement

[a]On the other hand, if one wants to minimize the average *entanglement* as given by Eq. (3), rather than the average *concurrence*, then for a pair of qubits one *must* choose a decomposition in which all the entanglements are equal, because the function $\mathcal{E}$ of Eq. (10) is strictly convex.

between A and C. Coffman *et al.*[45] showed that the two concurrences C_{AB} and C_{AC} are constrained by the following inequality:

$$C_{AB}^2 + C_{AC}^2 \leq 1. \tag{45}$$

Moreover, the bound is a tight one in that for any values of C_{AB} and C_{AC} satisfying the corresponding equality, one can find a quantum state having those values of the concurrences.

In a system of n qubits there can be many more constraints on the sharing of entanglement. Suppose, for example, that one wants each pair of qubits to be as entangled as possible. This goal will require some compromising, since increasing the entanglement between one pair will work against the entanglements of other pairs. One might choose, then, to maximize the *smallest* pairwise entanglement in the system. The evidence so far suggests that the smallest concurrence between any pair cannot exceed $2/n$. This bound has been proved for the case of three qubits by Dür *et al.*[46] and is suggested for n qubits by the work of Koashi *et al.*[47]

In a different problem involving n qubits, one imagines the qubits arranged in a *ring* and tries to maximize the nearest neighbor concurrences. O'Connor and Wootters[48] have shown that the optimal nearest-neighbor entanglement in this problem does not approach zero as the number of qubits goes to infinity but instead approaches a value no smaller than 0.434.

5.3. *Entanglement of magnetic systems*

Finally, concurrence has been used to investigate the entanglement of magnetic systems such as a Heisenberg spin chain.[49,50,51,52] Perhaps the most interesting result of this work is the observation that under certain circumstances, entanglement—say the entanglement between nearest neighbors—can *increase* as the temperature rises from absolute zero.[49] This happens, for example, if an external field forces the ground state to be a product state, each spin being aligned with the field. In that case, raising the temperature allows certain entangled energy eigenstates, which are suppressed at $T = 0$ by the external field, to have nonzero probability so that the thermal mixed state can be entangled. Of course for large enough temperature the entropy becomes too large for entanglement (that is, the purity becomes too small), and all entanglements must vanish because of the considerations of Subsection 5.2.

As is clear from the dates of many of the references in the present article, we are in the midst of a very active period of research on entanglement. In the near future, not only are we likely to make progress in finding formulas or bounds for entanglement of formation; we will probably also see more connections between entanglement and other areas of physics. The current work on magnetic systems is an interesting example, being a bridge between quantum information theory and the physics of condensed matter.

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