# Entanglement: Quantum Weirdness Gets Serious

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Warning Regarding Notation: For a product state of two sub-systems A and B, $|\phi\rangle_A|\psi\rangle_B$, the bra formed from this ket will be written here as $\langle\phi|_A\langle\psi|_B$, i.e. the left-to-right ordering of A-then-B is maintained between bra and ket. Many authors invert the order on forming the bra, preferring to write $\langle\psi|_B\langle\phi|_A$. Of course, when the sub-scripts $_A$ and $_B$ are included it makes little difference since which state refers to which sub-system is clear anyway. But we shall generally omit these sub-scripts, and rely on the ordering of the states to define the sub-system to which they refer.

## 1. Recognising Entangled Pure States

One of the defining features of quantum mechanics is the possibility of forming new pure states as superpositions (additions) of state vectors. This feature gives rise to the 'wavelike' properties of quantum mechanics, such as interference effects. But the weirdest things happen when superposing combined states. Consider bipartite states formed from the direct product of two Hilbert spaces, $H_A \otimes H_B$. This should not be misunderstood to consist only of states of the form $|\psi_A\rangle|\psi_B\rangle$. The product space can be spanned by states of this form, but the general product space vector is not a product of vectors. Rather it is $\sum_{i,j} a_{ij}|\psi_i\rangle_A|\psi_j\rangle_B$, where $a_{ij}$ are complex numbers with suitable normalisation. For example $[|\psi_1\rangle_A|\psi_1\rangle_B + |\psi_2\rangle_A|\psi_2\rangle_B]/\sqrt{2}$ cannot be expressed as the direct product of an A-state and a B-state. This contrasts with, for example, $[|\psi_1\rangle_A|\psi_1\rangle_B + |\psi_2\rangle_A|\psi_2\rangle_B - |\psi_1\rangle_A|\psi_2\rangle_B - |\psi_2\rangle_A|\psi_1\rangle_B]/2$ which *is* a product state, namely $[(|\psi_1\rangle_A - |\psi_2\rangle_A)(|\psi_1\rangle_B - |\psi_2\rangle_B)]/2$.

We have already remarked that a state like $[|\psi_1\rangle_A|\psi_1\rangle_B + |\psi_2\rangle_A|\psi_2\rangle_B]/\sqrt{2}$ has the peculiar property that there is no measurement on particle 1 which can result in a determinate outcome. The same is true for particle 2. And yet the combined state is a pure state. This leads to the non-classical result that the entropy of particle 1, considered as a sub-system, is 1, as is that of particle 2. But the combined state has zero entropy. The entropy of the combined state is less than that of either of its components, an impossible situation classically. This fact is intimately connected with the EPR paradox.

This behaviour does not occur for the product state $[(|\psi_1\rangle_A - |\psi_2\rangle_A)(|\psi_1\rangle_B - |\psi_2\rangle_B)]/2$, since a change of basis means this can be written simply $|\psi'_A\rangle|\psi'_B\rangle$. Hence there are measurements on the sub-systems A and B which have deterministic outcomes, and both the sub-systems and the combined state have zero entropy.

In contrast, states like $[|\psi_1\rangle_A|\psi_1\rangle_B + |\psi_2\rangle_A|\psi_2\rangle_B]/\sqrt{2}$ are said to be "entangled".

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It is worth considering how this appears in terms of the density matrix. A useful concept is the "reduced density matrix". This is what you get if you form the sum of the expectation values of the density matrix over all states of one of the sub-spaces. Thus,

$$\hat{\rho}_A = \sum_i \langle \psi_{iB} | \hat{\rho} | \psi_{iB} \rangle = Tr_B(\hat{\rho}) \qquad \text{(QM7.1)}$$

This is also referred to as "tracing out" the B-states. The state $[(|\psi_1\rangle_A - |\psi_2\rangle_A)(|\psi_1\rangle_B - |\psi_2\rangle_B)]/2$ results in a reduced density matrix for the A subspace of $(|\psi_1\rangle_A - |\psi_2\rangle_A)(\langle\psi_1|_A - \langle\psi_2|_A)/2 = |\psi'_A\rangle\langle\psi'_A|$. This confirms that such a product state corresponds to a pure state when reduced to a one-particle state by "tracing out" (i.e. averaging over) the other particle.

This is not the case for an entangled state. The state $[|\psi_1\rangle_A|\psi_1\rangle_B + |\psi_2\rangle_A|\psi_2\rangle_B]/\sqrt{2}$ gives a reduced density matrix, $[|\psi_{1A}\rangle\langle\psi_{1A}| + |\psi_{2A}\rangle\langle\psi_{2A}|]/2$. This is a mixed state, with the maximum 2D entropy, i.e. 1. This confirms that, if we interpret these as spin states, no spin measurement, wrt any axis, will produce deterministic outcomes. And yet this arises from a pure state simply by averaging over the other particle state. In contrast to product states, entangled states become mixtures when one part is traced out.

Since pure product states give rise to pure states when one part is traced out, it follows that the vN entropy of the composite state and the reduced state are both zero. In contrast, an entangled pure state gives rise to a mixture when one part is traced out. Hence, whilst the vN entropy of the composite state is zero, the vN entropy of the reduced state is non-zero. The signature of entanglement in a pure state is therefore that,

Entangled pure state: $$S_{vN}(\hat{\rho}_{AB}) = 0 < S_{vN}(\hat{\rho}_A) = S_{vN}(\hat{\rho}_B) \neq 0 \qquad \text{(QM7.2)}$$

In fact, for pure bipartite states, the von Neumann entropy of the reduced state defines the degree of entanglement of the bipartite state, noting that it does not matter which sub-system is traced out. Hence, the entanglement of a pure state is defined as,

$$E(\hat{\rho}_{AB}) = S_{vN}(\hat{\rho}_A) = S_{vN}(\hat{\rho}_B), \text{ where, } \hat{\rho}_A = Tr_B(\hat{\rho}_{AB}) \text{ and } \hat{\rho}_B = Tr_A(\hat{\rho}_{AB}) \qquad \text{(QM7.0)}$$

**1.1 The Most General Maximally Entangled Two Qubit State**

A state is maximally entangled if its entanglement is 1. For pure states of two qubits, the most general maximally entangled state is a superposition of Bell states with real coefficients. The Bell states of two qubits are conventionally defined as,

$$|\Phi_\pm\rangle = (|0\rangle|0\rangle \pm |1\rangle|1\rangle)/\sqrt{2} \quad \text{and} \quad |\Psi_\pm\rangle = (|0\rangle|1\rangle \pm |1\rangle|0\rangle)/\sqrt{2} \qquad \text{(QM7.0a)}$$

The reduced density matrix for all four of these bipartite states is $\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$, and hence the entanglement of the Bell states is maximum, i.e. 1. Are there any other two qubit states with maximal (unity) entanglement? The answer is "yes". The condition for maximal entanglement is very simple to state when expressed in terms of a basis slightly modified from the Bell basis, i.e. the e-basis defined by,

$$|e_1\rangle = |\Phi^+\rangle \ , \quad |e_2\rangle = i|\Phi^-\rangle, \quad |e_3\rangle = i|\Psi^+\rangle, \quad |e_4\rangle = |\Psi^-\rangle \qquad \text{(QM7.0b)}$$

The necessary and sufficient condition for maximal entanglement of a pure two qubit state is that it has ***real*** coefficients when expressed in the e-basis, i.e.,

$$|\psi_{AB}\rangle = \sum_{i=1}^{4} \alpha_i |e_i\rangle \qquad \text{(QM7.0c)}$$

where the four coefficients αi are real, and obviously required to obey $\sum_{i=1}^{4} \alpha_i^2 = 1$. This will now be proved.

The general two qubit state can be written,

$$|\psi_{AB}\rangle = a|0\rangle|0\rangle + b|0\rangle|1\rangle + c|1\rangle|0\rangle + d|1\rangle|1\rangle \qquad \text{(QM7.0d)}$$

where a, b, c and d will, in general, be complex. Hence,

$$\begin{aligned} \hat{\rho}_A &= (a|0\rangle + c|1\rangle)(a^*\langle 0| + c^*\langle 1|) + (b|0\rangle + d|1\rangle)(b^*\langle 0| + d^*\langle 1|) \\ &= \begin{pmatrix} |a|^2 + |b|^2 & ac^* + bd^* \\ ca^* + db^* & |c|^2 + |d|^2 \end{pmatrix} \end{aligned} \qquad \text{(QM7.0e)}$$

To find the vN entropy of this mixed reduced state we need to find the eigenvalues of the above matrix. Elementary manipulation shows these to be,

$$\lambda = \frac{1}{2}\left\{1 \pm \sqrt{1 - 4|ad - bc|^2}\right\} \qquad \text{(QM7.0f)}$$

The coefficients are subject to the normalisation $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$. It must be that $|ad - bc| \le \frac{1}{2}$ since the eigenvalues of an Hermetian matrix must be real. When this inequality is saturated both eigenvalues are ½ and hence the vN entropy of the reduced state is maximum (i.e. 1), and hence the entanglement of the bipartite state is maximum (i.e. 1). Hence, the problem reduces to finding the most general coefficients which have $|ad - bc| = ½$ .

The simplest way of solving this is to note that the state (QM7.0d) can alos be written in terms of the e-basis, as in (QM7.0c). The relationship between the coefficients is then,

$$a = \frac{1}{\sqrt{2}}(\alpha_1 + i\alpha_2), \quad d = \frac{1}{\sqrt{2}}(\alpha_1 - i\alpha_2), \quad b = \frac{1}{\sqrt{2}}(\alpha_4 + i\alpha_3), \quad c = -\frac{1}{\sqrt{2}}(\alpha_4 - i\alpha_3) \qquad \text{(QM7.0g)}$$

From this it follows that,

$$|ad - bc| = \frac{C}{2}, \text{ where, } C = \alpha_1^2 + \alpha_2^2 + \alpha_3^2 + \alpha_4^2 \qquad \text{(QM7.0h)}$$

Now the normalisation requirement for the state (QM7.0d) is that $\sum_{i=1}^{4}|\alpha_i|^2 = 1$. So, if all the $\alpha_i$ are real, (QM7.0h) has C = 1 and hence becomes $|ad - bc| =$ ½ , as required.

The converse also follows: maximal entanglement requires $|ad - bc| =$ ½ and hence C=1, but this is only possible if all the $\alpha_i$ are real since otherwise $\sum_{i=1}^{4}|\alpha_i|^2$ would be less than 1. QED.

The other important result which follows from (QM7.0d) is that the entanglement is zero iff $|ad - bc| = 0$, because this is equivalent to the eigenvalues of the reduced density matrix being 0 and 1 (which gives zero vN entropy). We will see in Section 4, below, that the condition $|ad - bc| = 0$ is precisely that which ensures that the bipartite state can be factorised as a product state of the two sub-systems. Hence, this establishes that the entanglement measure defined by (QM7.0) is sensible in that it produces zero entanglement for product states.

## 2. Recognising Entangled Mixed States

What do we mean by an entangled mixture? The most obvious definition is that an entangled mixture is a mixture of pure states at least one of which is entangled. However this will not do at all. The reason is that it is possible for entanglement to effectively 'cancel out' between two entangled pure states which contribute to a mixture. A simple example is to consider a 50/50 mixture of the two maximally entangled 'Bell' states, $(|0\rangle|0\rangle + |1\rangle|1\rangle)/\sqrt{2}$ and $(|0\rangle|0\rangle - |1\rangle|1\rangle)/\sqrt{2}$. The density matrix of this mixture is,

$$\begin{aligned}\hat{\rho} &= \frac{1}{4}\left[(|0\rangle|0\rangle + |1\rangle|1\rangle)(\langle 0|\langle 0| + \langle 1|\langle 1|) + (|0\rangle|0\rangle - |1\rangle|1\rangle)(\langle 0|\langle 0| - \langle 1|\langle 1|)\right] \\ &= \frac{1}{2}\left[|0\rangle|0\rangle\langle 0|\langle 0| + |1\rangle|1\rangle\langle 1|\langle 1|\right]\end{aligned} \qquad \text{(QM7.2a)}$$

The 'entangled' parts (the cross-products) have cancelled between the two contributing states. Hence, this mixture is, in fact, separable, i.e. it has no entanglement. This is unambiguous because this state is clearly a mixture of pure states.

Hence, the correct definition is that a non-entangled mixture (called a "separable state") is a mixture of pure product states. The most general pure product state is $|\psi\rangle_A|\phi\rangle_B$, and hence the most general separable mixture can be written $\hat{\rho}_{AB} = \sum_i p_i |\psi_i\rangle_A |\phi_i\rangle_B \langle\psi_i|_A \langle\phi_i|_B$. The states $|\psi_i\rangle_A$ and $|\phi_i\rangle_B$ are any pure states of the A and B sub-systems, labelled by some index i, and need not be orthogonal. Also there can be an arbitrary number of them in the sum, subject only to $\sum_i p_i = 1$. Since we can write $\hat{\rho}_{Ai} = |\psi_i\rangle_A \langle\psi_i|_A$ for each contributing sub-system, A, state, it follows that a separable mixture can equivalently be defined by the existence of a decomposition of the density matrix as a sum over direct products of reduced density matrices, i.e., $\hat{\rho}_{AB} = \sum_i p_i \hat{\rho}_{Ai} \otimes \hat{\rho}_{Bi}$. This defines a separable mixture. Conversely, an entangled mixture is any mixed state which cannot be cast into this form. Recall that the range of the index i is arbitrary (i.e. it is not related to the number of orthogonal states).

Another example is a 50/50 mixture of two other Bell states, $|\psi_1\rangle = (|0\rangle|0\rangle + |1\rangle|1\rangle)/\sqrt{2}$ and $|\psi_2\rangle = (|0\rangle|1\rangle + |1\rangle|0\rangle)/\sqrt{2}$. It is less obvious that this is separable because there are no cancellations in this case. However, writing single particle density matrices as,

$$\hat{\rho}_1 = \frac{1}{\sqrt{2}}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right) \qquad \text{and} \qquad \hat{\rho}_2 = \frac{1}{\sqrt{2}}\left(|0\rangle\langle 1| + |1\rangle\langle 0|\right) \qquad \text{(QM7.2b)}$$

it is readily seen that the 50/50 mixture of the above two Bell states can be written as,

$$\frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2| = \frac{1}{2}\hat{\rho}_{1A} \otimes \hat{\rho}_{1B} + \frac{1}{2}\hat{\rho}_{2A} \otimes \hat{\rho}_{2B} \qquad \text{(QM7.2c)}$$

This may be expressed in matrix form, adopting the conventional 'computational basis' for the product states, defined by,

| **1** | **2** | **3** | **4** |
|---|---|---|---|
| $|0\rangle_A|0\rangle_B$ | $|0\rangle_A|1\rangle_B$ | $|1\rangle_A|0\rangle_B$ | $|1\rangle_A|1\rangle_B$ |

Hence, $$\frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{(QM7.2d)}$$

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The most general pure bipartite state can be written in terms of some orthonormal basis as $\sum_{I,J} a_{IJ} |I\rangle_A |J\rangle_B$ , where I and J span the number of possible states (the dimensionality of the Hilbert sub-spaces). It follows that the most general mixture can be written $\sum_{I,J,I',J',k} p_k a_{kIJ} a^*_{kI'J'} |I\rangle_A |J\rangle_B \langle I'|_A \langle J'|_B$ where the range of k is arbitrary (simply the number of states which are being mixed). Thus, in the product basis, $|I\rangle_A |J\rangle_B$ , the mixed state has a filled density matrix with off-diagonal elements.

However, the mere fact that the density matrix has off-diagonal terms, $\sum_{I,J,I',J'} C_{IJI'J'} |I\rangle_A |J\rangle_B \langle I'|_A \langle J'|_B$ , does not mean that it is inseparable (entangled). A separable density matrix will have off-diagonal elements when expressed in an arbitrary basis. Thus, if we write $|\psi_k\rangle = \sum a_{kI} |I\rangle_A$ and $|\phi_k\rangle = \sum b_{kJ} |J\rangle_B$ then the most general ***separable*** density matrix is seen to be $\sum_{I,J,I',J',k} p_k a_{kI} a^*_{kI'} b_{kJ} b^*_{kJ'} |I\rangle_A |J\rangle_B \langle I'|_A \langle J'|_B$ .

Hence, the problem of the separability of an arbitrary density matrix, which can be specified by the coefficients $C_{IJI'J'}$ , is whether these coefficients can be written in the form $C_{IJI'J'} = \sum_k p_k a_{kI} a^*_{kI'} b_{kJ} b^*_{kJ'}$ . If such coefficients $a_{kI}$, $b_{kJ}$ and $p_k$ exist, then the mixture is separable. If it seems like a tricky problem to determine whether such $a_{kI}$, $b_{kJ}$ and $p_k$ exist, that's because it is. Before saying more about attempts at the general solution, firstly we remark on an obvious hypothesis which fails.

**2.1 Entropy Does Not Identify Entanglement for Mixed States**

Following (QM7.2) we may be tempted to identify entangled states with any state whose entropy has the non-classical property of being less than that of its parts. Classically the Shannon entropy obeys $S^{AB}_{Shannon} \geq MAX\left(S^{A}_{Shannon}, S^{B}_{Shannon}\right)$. One might guess, therefore, that the signature of entanglement in a general mixed state might be that,

Sufficient for entanglement: $$S_{vN}(\hat{\rho}_{AB}) < MAX[S_{vN}(\hat{\rho}_A), S_{vN}(\hat{\rho}_B)] \qquad \text{(QM7.3)}$$

Would it were that simple! It is not. The condition (QM7.3) is indeed a sufficient condition to ensure that the composite state is entangled. But it is not necessary. Entangled states exist which violate this inequality.

Nevertheless, (QM7.3) is important since it may well identify the majority of entangled states in a given situation, and it will tend to fail only for those states which are rather less entangled (assuming some quantification of the degree of entanglement which we have not yet defined).

Note that the condition (QM7.3) lies within the range permitted by the triangle inequality, (3.2.4.2) [see Part 6 of these Notes, QM6], which requires for any bipartite state that

$$\left|S_{vN}^{A} - S_{vN}^{B}\right| \le S_{vN}^{AB} \le S_{vN}^{A} + S_{vN}^{B} \qquad (3.2.4.2)$$

Hence, the non-classical, definitely entangled, regime is,

$$\left|S_{vN}^{A} - S_{vN}^{B}\right| \le S_{vN}^{AB} < MAX[S_{vN}^{A}, S_{vN}^{B}] \qquad (QM7.4)$$

and the remaining regime, which may or may not be entangled, is,

$$MAX[S_{vN}^{A}, S_{vN}^{B}] \le S_{vN}^{AB} \le S_{vN}^{A} + S_{vN}^{B} \qquad (QM7.5)$$

The residual problem of identifying entangled mixed states therefore consists of sorting the entangled from the separable states in the regime (QM7.5).

**2.2 Rigorous Theorems Identifying Entangled Mixtures**

In (QM7.3) we have a sufficient, but not a necessary, condition for a mixture to be entangled. We are still seeking a necessary *and* sufficient condition. Actually, we already have one. The most general density matrix for a bipartite system is,

$$\hat{\rho}_{AB} = \sum_{I,J,I',J'} C_{IJI'J'} \left|I\right\rangle_A \left|J\right\rangle_B \left\langle I'\right|_A \left\langle J'\right|_B \qquad (QM7.6)$$

The necessary and sufficient condition that this is entangled is that there exists coefficients $a_{kI}$, $b_{kJ}$ and $p_k$ such that,

$$C_{IJI'J'} = \sum_k p_k a_{kI} a_{kI'}^{*} b_{kJ} b_{kJ'}^{*} \qquad (QM7.7)$$

and also such that, $0 \le p_k \le 1$ with $\sum_k p_k = 1$, and $\sum_I \left|a_{kI}\right|^2 = \sum_J \left|b_{kJ}\right|^2 = 1$, where k runs over the arbitrary number of terms in the mixture, and I and J run over the dimension of the A and B Hilbert sub-spaces.

Unfortunately, whilst this is a correct necessary and sufficient condition, it does not provide an effective algorithm for deciding whether a given density matrix is separable. As far as I am aware, no effective decision algorithm for the general case has yet been devised. Is this true?

However, Asher Peres (1996) devised a criterion which he showed to be another sufficient condition to ensure that a mixture is entangled. It was then shown by Horodecki et al (1996) that the Peres criterion is also a necessary condition for a mixture to be entangled in the special case of systems of two qubits, and also systems comprising a qubit and a three-state sub-system. The Peres criterion provides a simple effective algorithm, so a simple decision procedure exists for the 2 x 2 and 2 x 3 cases. Unfortunately, Horodecki et al (1996) also showed that the Peres criterion is ***not*** necessary for Hilbert spaces of larger dimensions.

Despite its limited range of applicability as a necessary and sufficient condition, the Peres criterion is important in practice, since two-qubit systems are of wide applicability. We have seen that the density matrix of the most general bipartite mixture can be written $\hat{\rho} = \sum_{I,J,I',J',k} p_k a_{kIJ} a^*_{kI'J'} |I\rangle_A |J\rangle_B \langle I'|_A \langle J'|_B$ in terms of an orthonormal basis. Its components wrt this basis are obviously $\rho_{I\,J\,I'\,J'} = \sum_k p_k a_{kIJ} a^*_{kI'J'}$. Peres considers the matrix formed by "partial transposition", i.e. by transposing only the indices of the A sub-system but not the B subsystem. This defines $\sigma_{I'\,J\,I\,J'} = \rho_{I\,J\,I'\,J'}$. If the original state is separable, the partially transposed matrix must necessarily have only non-negative eigenvalues. In other words, the existence of one or more negative eigenvalues of the partially transposed matrix is sufficient to imply that the original mixture is entangled.

Even for systems of higher dimension than 2 x 2 or 2 x 3, the Peres criterion may be of assistance in identifying entangled states which are not identified by the entropy criterion, (QM7.3).

## 3. Example: The Lowest Excited State of N Identical Bosons

A bipartite mixture can be formed by starting with a state of N identical bosons, and then tracing-out N-2 of the particles. This will provide an example of a mixture which is clearly entangled but which fails the entropy test, (QM7.3), i.e. the entropy of the bipartite state is greater than that of its individual particles. However, we shall show that the Peres criterion does successfully identify the state as entangled.

Suppose the single particle states are, (i)a ground state $|0\rangle$, and, (ii)a lowest excited state $|e\rangle$, together with possibly more highly excited states which will not be relevant here. Consider initially the pure state of three of these identical bosons in which just one particle is in the first excited state, and the others are in the ground state. It is,

$$|\psi\rangle = \frac{1}{\sqrt{3}}\left\{|0\rangle_A|0\rangle_B|e\rangle_C + |0\rangle_A|e\rangle_B|0\rangle_C + |e\rangle_A|0\rangle_B|0\rangle_C\right\} \qquad \text{(QM7.8)}$$

Hence we see that,

$${}_C\langle 0|\psi\rangle\langle\psi|0\rangle_C = \left(|0\rangle_A|e\rangle_B + |e\rangle_A|0\rangle_B\right)\left({}_A\langle 0|_B\langle e| + {}_A\langle e|_B\langle 0|\right)/3 \qquad \text{(QM7.9a)}$$

Similarly,

$${}_C\langle e|\psi\rangle\langle\psi|e\rangle_C = \left(|0\rangle_A|0\rangle_B\right)\left({}_A\langle 0|_B\langle 0|\right)/3 \qquad \text{(QM7.9b)}$$

The reduced density matrix for the bipartite state consisting of particles A and B only is the sum of (QM7.9a) and (QM7.9b), i.e.,

$$\hat{\rho}_{AB}^{(3)} = \frac{1}{3}\left(|0\rangle_A|e\rangle_B + |e\rangle_A|0\rangle_B\right)\left({}_A\langle 0|_B\langle e| + {}_A\langle e|_B\langle 0|\right) + \frac{1}{3}\left(|0\rangle_A|0\rangle_B\right)\left({}_A\langle 0|_B\langle 0|\right) \qquad \text{(QM7.10)}$$

We suspect that this mixture must be entangled since the state (QM7.9a) is clearly entangled, and the state (QM7.9b) involves only different states and hence cannot combine with (QM7.9a) to 'cancel' the entanglement. We adopt the obvious matrix notation in which the indices are defined as representing the product states of A and B as follows,

| **1** | **2** | **3** | **4** |
|---|---|---|---|
| $\|0\rangle_A\|0\rangle_B$ | $\|0\rangle_A\|e\rangle_B$ | $\|e\rangle_A\|0\rangle_B$ | $\|e\rangle_A\|e\rangle_B$ |

The density matrix of the bipartite AB system is thus,

$$\hat{\rho}_{AB}^{(3)} = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(QM7.11a)}$$

By considering the same development for 4, 5, etc particles it is readily seen that for N particles, tracing out all but particles A and B results in,

$$\hat{\rho}_{AB}^{(N)} = \frac{1}{N}\begin{pmatrix} N-2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(QM7.11b)}$$

Tracing out particle B to leave the density matrix for particle A alone yields,

$$\hat{\rho}_{A}^{(N)} = \mathrm{Tr}_B\left(\hat{\rho}_{AB}^{(N)}\right) = \frac{N-1}{N}|0\rangle\langle 0| + \frac{1}{N}|e\rangle\langle e| \equiv \frac{1}{N}\begin{pmatrix} N-1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{(QM7.12)}$$

The vN entropy of the reduced (single particle) state is therefore,

$$S_{vN}\left(\hat{\rho}_{A}^{(N)}\right) = \frac{N-1}{N}\log_2\frac{N}{N-1} + \frac{1}{N}\log_2 N \qquad \text{(QM7.13)}$$

The vN entropy of the 2-particle mixture, (QM7.11b), is simply found by diagonalising the matrix (QM7.11b), which gives,

$$\hat{\rho}_{AB}^{(N)} \to \frac{1}{N}\begin{pmatrix} N-2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(QM7.14)}$$

Hence,

$$S_{vN}\left(\hat{\rho}_{AB}^{(N)}\right) = \frac{N-2}{N}\log_2\frac{N}{N-2} + \frac{2}{N}\log_2\frac{N}{2} \qquad \text{(QM7.15)}$$

Thus we find that $S_{vN}\left(\hat{\rho}_{AB}^{(N)}\right) \geq S_{vN}\left(\hat{\rho}_{A}^{(N)}\right)$, as follows,

| N | $S_{vN}\left(\hat{\rho}_{AB}^{(N)}\right)$ | $S_{vN}\left(\hat{\rho}_{A}^{(N)}\right)$ |
|---|---|---|
| 3 | 0.9183 | 0.9183 |
| 4 | 1 | 0.8113 |
| 5 | 0.9710 | 0.7219 |
| 6 | 0.9183 | 0.6500 |
| 10 | 0.7219 | 0.4690 |
| 100 | 0.1414 | 0.0808 |

Hence, the entropy test fails to identify the state (QM7.11b) as entangled.

We now investigate the Peres criterion to see if that is successful in identifying the entanglement of the bipartite state, (QM7.11b). To do so we first note that the partial transpose matrix is given in term of the matrix elements in (QM7.11b) as follows,

$$\sigma = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{31} & \rho_{32} \\ \rho_{21} & \rho_{22} & \rho_{41} & \rho_{42} \\ \rho_{13} & \rho_{14} & \rho_{33} & \rho_{34} \\ \rho_{23} & \rho_{24} & \rho_{43} & \rho_{44} \end{pmatrix} = \frac{1}{N}\begin{pmatrix} N-2 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(QM7.16)}$$

For all $N \geq 3$ this matrix has one negative eigenvalue. For N=3 it is -0.2060, for N=10 it is -0.0123, for N=100 it is -0.0001. The existence of a negative eigenvalue is sufficient to guarantee that the 2-particle state, (QM7.11b), is entangled – as indeed we already know. So the Peres criterion succeeds in identifying the entanglement in this case, whereas the entropy criterion fails to do so. However, the Peres criterion will not always work either if the dimensions exceed 2 x 2 and 2 x 3.

## 4. The Entanglement of Random States (Algebraic Proofs)

If we choose a state at random, how likely is it to be entangled? The answer depends crucially upon whether we mean a randomly chosen pure state or a random mixture. The answer is,

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- If a pure state is chosen at random from a Hilbert space describing a bipartite system, then it is essentially certain to be entangled;
- If a very large number of pure states are chosen at random and combined with random probabilities to form a mixture, then the resulting mixture will be separable (i.e., not entangled) in almost all cases.

In the first bullet, "essentially certain" means that the product states form a set of measure zero in the Hilbert space. In the second bullet, "almost all cases" tends to "all cases" in the limit that the number of contributing states to the mixtures becomes infinite. Both of these observations surprised me when I first stumbled across them.

These claims will now be proved. Firstly consider the case of a randomly chosen pure state. It suffices to consider a pair of qubits. The most general product state of two qubits can be written $(\alpha|0\rangle + \beta|1\rangle)(\gamma|0\rangle + \delta|1\rangle)$, where α, β, γ, δ are arbitrary complex numbers apart from having to obey $|\alpha|^2 + |\beta|^2 = 1$ and $|\gamma|^2 + |\delta|^2 = 1$. Consequently there are six continuum degrees of freedom involved in the choice of a random pair of qubits: four phase angles, and two magnitudes.

The most general state in the 2 x 2 product Hilbert space is,

$$a|0\rangle|0\rangle + b|0\rangle|1\rangle + c|1\rangle|0\rangle + d|1\rangle|1\rangle \qquad \text{(QM7.17)}$$

This is required to respect only the one constraint: $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$. Hence, there are seven continuum degrees of freedom involved in choosing a random state from the 2 x 2 product space of two qubits. It is clear, therefore, that it would be a fluke if a randomly chosen state happened to be a product state. Specifically, the random a, b, c, d would have to be such that $a = \alpha\gamma, b = \beta\delta, c = \alpha\delta$ and $d = \beta\gamma$ . It is easily seen that this can be true only if ab – cd = 0. Choosing a, b, c and d at random, this relation will "almost never" be exactly obeyed. Hence, essentially all random 2 x 2 states are entangled.

Does this generalise to a Hilbert space of arbitrary dimension? Yes it does. Suppose the dimensionality is $D_1$ x $D_2$. Consider the general product state. The number of phases is $D_1 + D_2$. The number of magnitudes is $D_1 + D_2 – 2$, because of the two constraint equations. Hence, the total number of degrees of freedom is $2(D_1 + D_2 – 1)$. Now consider the most general state from the product space. There are $D_1D_2$ terms, and hence $2D_1D_2 – 1$ degrees of freedom, because of the one constrain equation. But it is clear than $2D_1D_2 – 1 > 2(D_1 + D_2 – 1)$ for $D_1$ and $D_2$ both $\geq 2$. Hence, essentially all random states, of any dimensionality, are entangled.

The morale of this story is that the natural state of pure quantum states of bipartite systems is to be entangled.

Now let us consider the case of a random mixture of N randomly chosen states from our two qubit Hilbert space. We now know that all N pure states contributing to the mixture will be entangled. How come the mixture can end up being un-entangled, then? The answer is that entanglement can, in effect, cancel out between contributing states. A simple example is to consider a 50/50 mixture of the two entangled 'Bell' states, $(|0\rangle|0\rangle+|1\rangle|1\rangle)/\sqrt{2}$ and $(|0\rangle|0\rangle-|1\rangle|1\rangle)/\sqrt{2}$. The density matrix of this mixture is,

$$\begin{aligned}\hat{\rho} &= \frac{1}{4}\left[(|0\rangle|0\rangle+|1\rangle|1\rangle)(\langle 0|\langle 0|+\langle 1|\langle 1|)+(|0\rangle|0\rangle-|1\rangle|1\rangle)(\langle 0|\langle 0|-\langle 1|\langle 1|)\right] \\ &= \frac{1}{2}\left[|0\rangle|0\rangle\langle 0|\langle 0|+|1\rangle|1\rangle\langle 1|\langle 1|\right]\end{aligned} \quad \text{(QM7.18)}$$

Hence, this mixture is, in fact, separable, i.e. it has no entanglement. The 'entangled' parts (the cross-products) have cancelled between the two contributing states. Note that this phenomenon is not always caused by cancelling *per se*. The second example in Section 2 shows that it can also come about due to the two mixed states combining in such a way to become factorisable.

Consider a set of arbitrary pure states of a bipartite system, $\{|\psi_i\rangle\}$, where i runs from 1 to some arbitrary number of contributing states in the mixture, N. Each state can be written as $|\psi_i\rangle = \sum_{j,k}^{D1,D2} C_{ijk}|j\rangle|k\rangle$, where D1 and D2 are the dimensions of the sub-system Hilbert spaces. If these states contribute to a mixture with respective probabilities $p_i$, the mixed state is,

$$\hat{\rho} = \sum_{i,j,k,m,n} p_i C_{ijk} C^*_{imn} |j\rangle|k\rangle\langle m|\langle n| \quad \text{(QM7.19)}$$

where i runs from 1 to N, and j and m run from 1 to D1, and k and n from 1 to D2. This can be simplified as,

$$\hat{\rho} = \sum_{i,j,k,m,n} D_{jkmn}|j\rangle|k\rangle\langle m|\langle n| \quad \text{where, } D_{jkmn} = \sum_i p_i C_{ijk} C^*_{imn} \quad \text{(QM7.20)}$$

The coefficients $C_{ijk}$ are arbitrary except for the requirement that $\sum_{j,k}|C_{ijk}|^2 = 1$, for each value of i. The probabilities, $p_i$, are also arbitrary except for requiring that $\sum_i p_i = 1$. Consequently, for given values of i, j, k, m and n, the two numbers $C_{ijk}$ and $C^*_{imn}$ will be uncorrelated, except when j = m and k = n. Consequently, provided that there are enough randomly chosen terms in the sum over i, it is to be expected that,

$$D_{jkmn} = \sum_i p_i C_{ijk} C^*_{imn} \propto \delta_{jm}\delta_{kn} \quad \text{(QM7.21)}$$

Of course, this is only true in the sense of being an expectation value. For any finite sum, the value of $D_{jkmn}$ will be non-zero. But its typical magnitude is expected to reduce as the number of states contributing to the mixture increases (proportional to 1/√N). Substituting (QM7.21) into (QM7.19) shows that the mixture is expected to tend to become separable, i.e.,

$$\hat{\rho} \to \sum_{i,j,k} p_i \left| C_{ijk} \right|^2 |j\rangle |k\rangle \langle j| \langle k| \qquad \text{(QM7.22)}$$

This prediction has been explored numerically (using MATLAB), and this is described in the next Section.

## 5. The Entanglement of Random States (Numerical Exploration)

We have considered mixtures composed of random two-qubit states. The software randomly combines a specified number, N, of random pure two-qubit states into a mixture. It is important to realise that, for a fixed small value of N, the resulting density matrix is not random. It is biased because it is constrained to be composed of exactly N pure states. The most obvious example is N = 1, for which the density matrix is not even a mixture, it is a pure state.

For each value of N considered, a large number (Nt) of trials (i.e., randomly generated density matrices) were run, typically the order of thousands. For each trial the vN entropy of the mixture and its reduced density matrices were found, as were the corresponding linear entropies, concurrence and Entanglement of Formation. These latter terms are defined in Sections 6.1 and 6.2. The Peres criterion (Section 2.2) was also deployed, which, for this 2 x 2 Hilbert space, is guaranteed to identify separable and inseparable mixtures.

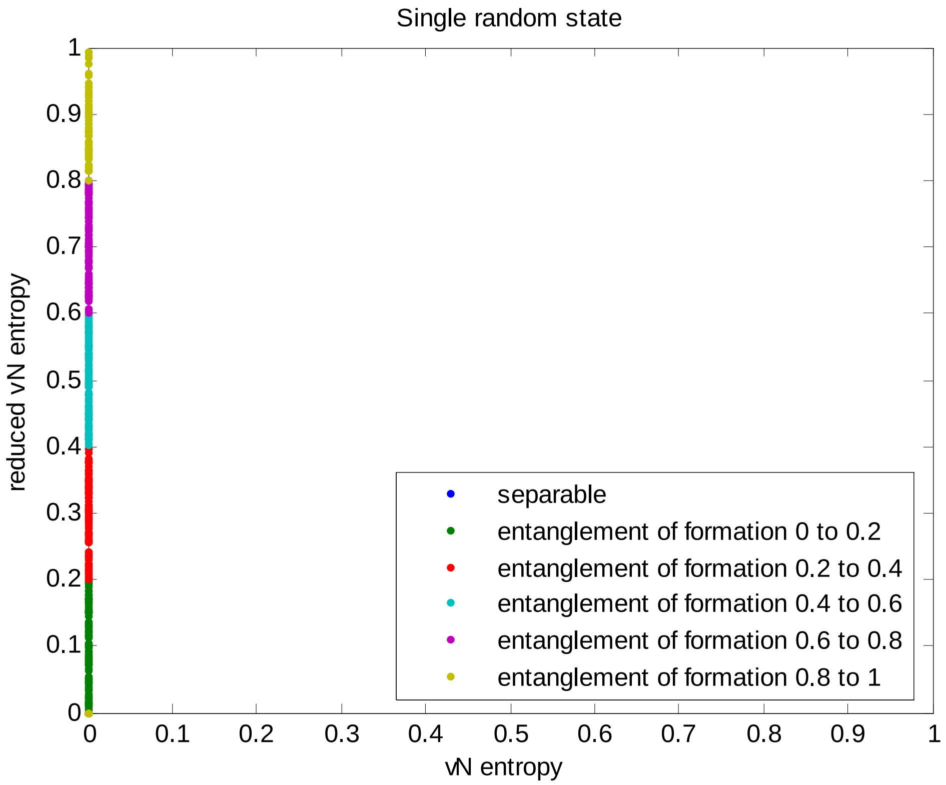
The sub-additivity inequality (see Part 6 of the QM Notes, QM6) says that the von Neumann entropy of the combined state does not exceed the sum of the von Neumann entropies of its parts: $S_{vN}^{AB} \le S_{vN}^{A} + S_{vN}^{B}$. In this Section we have used a variant definition of the von Neumann entropy in which the dimension of the Hilbert space in question is used as the base of the logarithm,

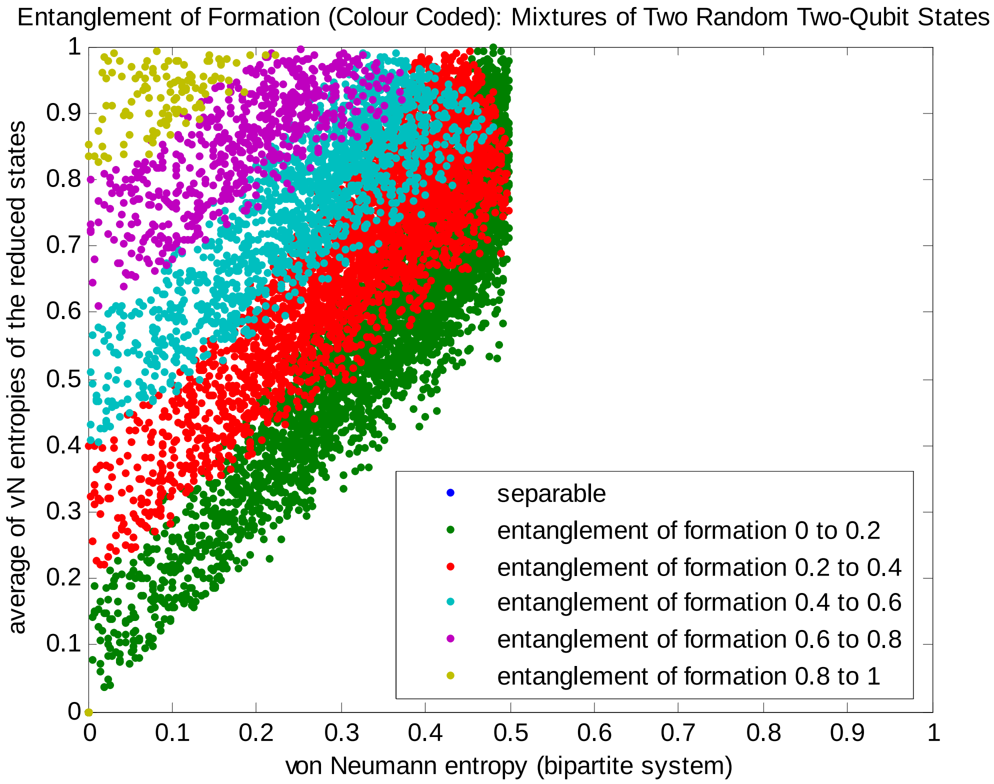
$$S_{vN} = -\sum_i p_i \log_D p_i$$

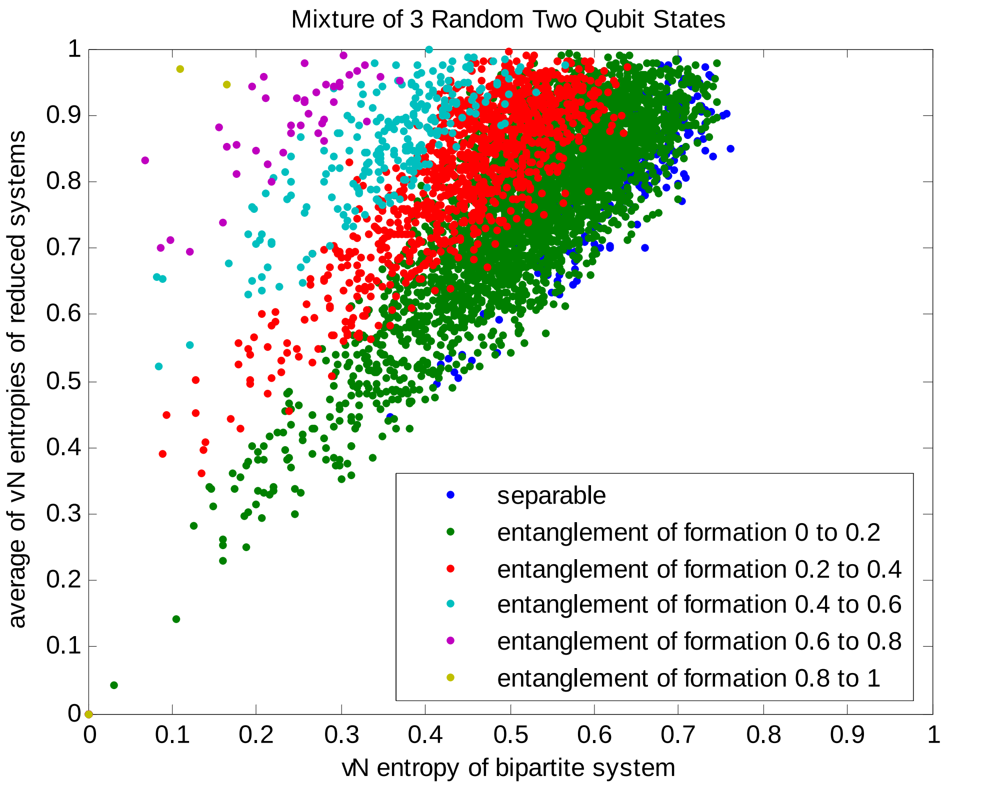
The resulting vN entropy is less than the $\log_2$ definition by a factor of $\log_2 D$. This makes no difference to the reduced density matrices, since these are one-qubit (D=2) spaces. The only other space is the 2 qubit space, D=4, so the vN entropy of the combined states is reduced by a factor of 2. Hence, with this definition, the sub-additivity inequality becomes $S_{vN}^{AB} \le \left(S_{vN}^{A} + S_{vN}^{B}\right)/2$. We have plotted the outcomes of our trials as the average of the reduced state vN entropies, $S_{vN}^{av} = \left(S_{vN}^{A} + S_{vN}^{B}\right)/2$, against the combined state vN entropy, $S_{vN}^{AB}$. All the data necessarily lie, therefore, above the line of equality. Note that with this definition of vN entropy, all of $S_{vN}^{AB}, S_{vN}^{A}$ and $S_{vN}^{B}$ lie in the range [0, 1].

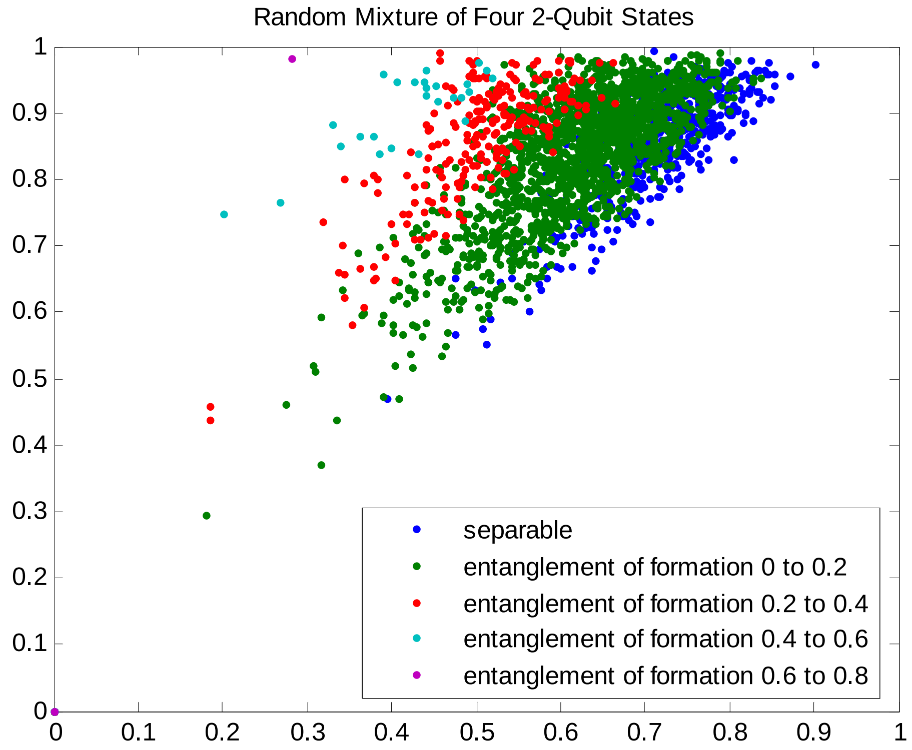
The Figures below show these plots, for N = 1, 2, 3, 4, 5, 6, 7 and 10 respectively. For N = 1 the vN entropy of the combined state is zero, because these are pure states. The reduced states, however, are mixed and can have average entropies, $S_{vN}^{av}$, anywhere from 0 to 1. The Figures are colour coded to distinguish, (a)the separable states (deep blue), and, (b)entangled states, with varying magnitudes of the Entanglement of Formation (EoF). Five ranges of EoF are distinguished, from 0 to 0.2 (green) to 0.8 to 1 (mustard). The EoF is one possible measure of the degree of entanglement (see Section 6).

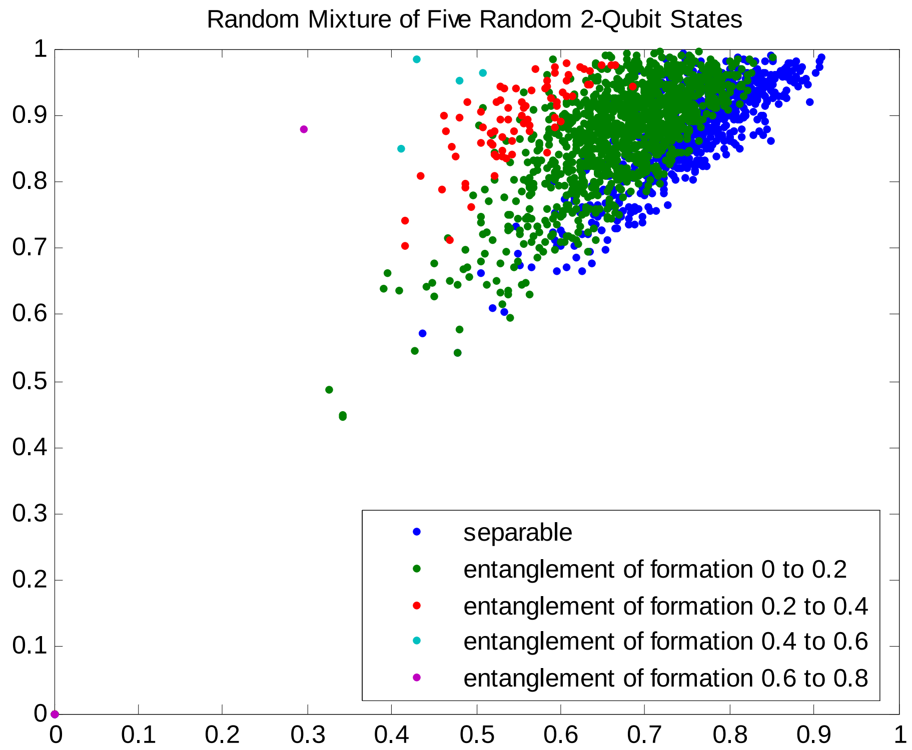
We already know, from the previous Section, that there will be no separable states in the N=1 plot. However, we find that all the N=2 states are entangled also.

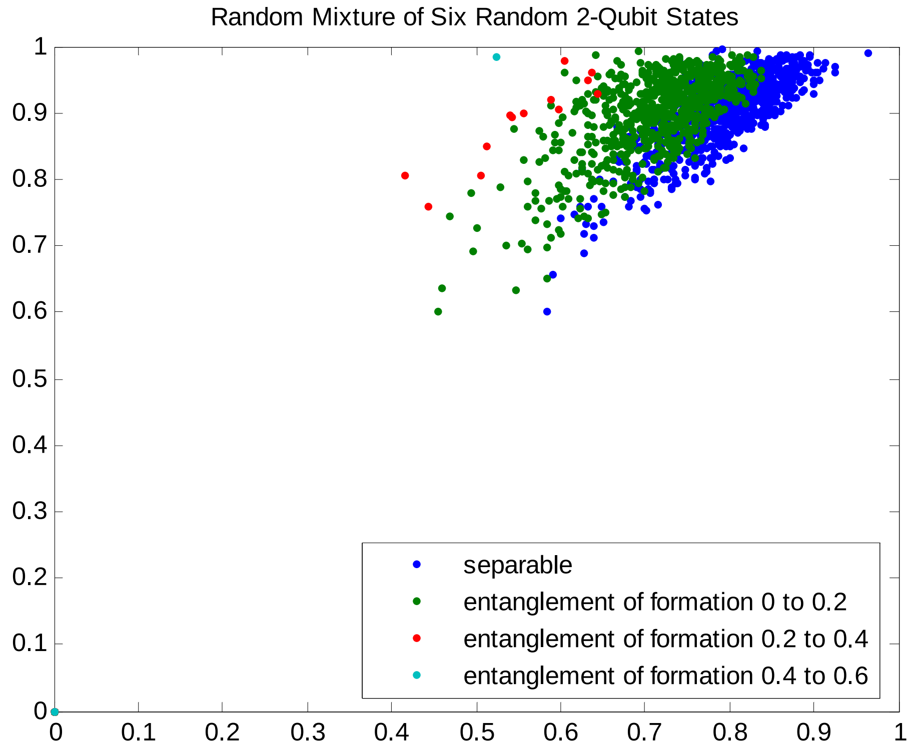


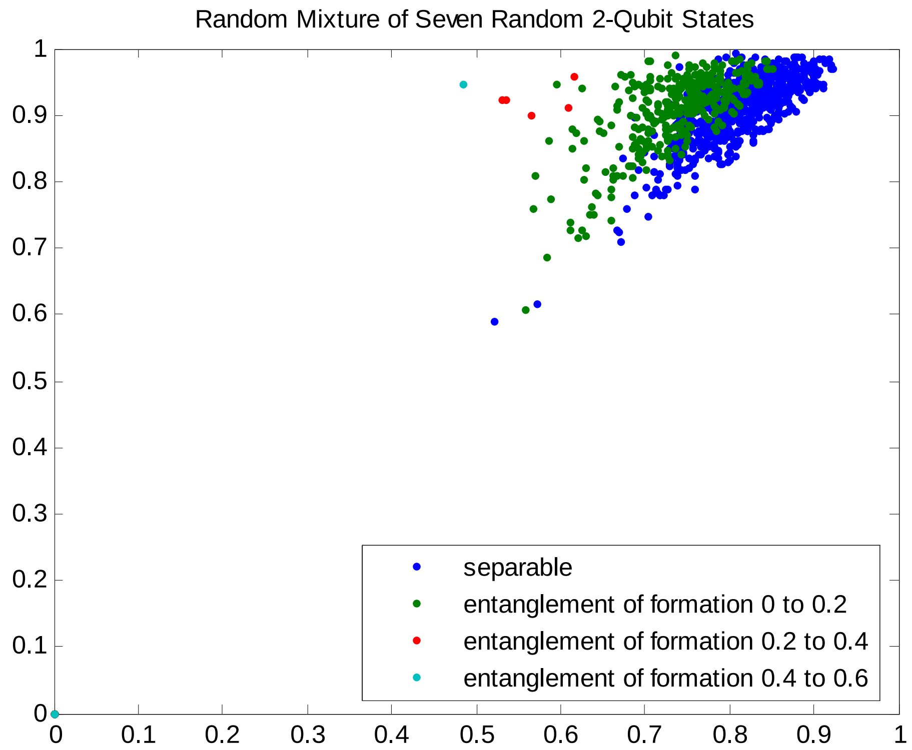

Entanglement of Formation (Colour Coded): Mixtures of Two Random Two-Qubit States
average of vN entropies of the reduced states
von Neumann entropy (bipartite system)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
separable
entanglement of formation 0 to 0.2
entanglement of formation 0.2 to 0.4
entanglement of formation 0.4 to 0.6
entanglement of formation 0.6 to 0.8
entanglement of formation 0.8 to 1

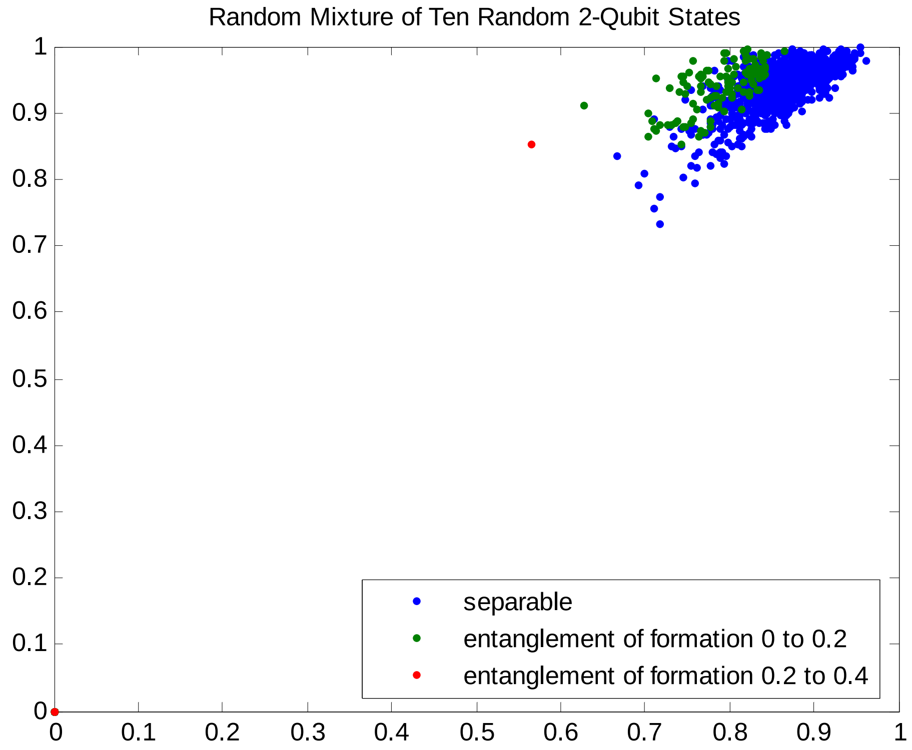

Mixture of 3 Random Two Qubit States
average of vN entropies of reduced systems
vN entropy of bipartite system
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
separable
entanglement of formation 0 to 0.2
entanglement of formation 0.2 to 0.4
entanglement of formation 0.4 to 0.6
entanglement of formation 0.6 to 0.8
entanglement of formation 0.8 to 1


Random Mixture of Four 2-Qubit States
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
separable
entanglement of formation 0 to 0.2
entanglement of formation 0.2 to 0.4
entanglement of formation 0.4 to 0.6
entanglement of formation 0.6 to 0.8


Random Mixture of Five Random 2-Qubit States
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
separable
entanglement of formation 0 to 0.2
entanglement of formation 0.2 to 0.4
entanglement of formation 0.4 to 0.6
entanglement of formation 0.6 to 0.8


Random Mixture of Six Random 2-Qubit States
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
separable
entanglement of formation 0 to 0.2
entanglement of formation 0.2 to 0.4
entanglement of formation 0.4 to 0.6


Random Mixture of Seven Random 2-Qubit States
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
separable
entanglement of formation 0 to 0.2
entanglement of formation 0.2 to 0.4
entanglement of formation 0.4 to 0.6

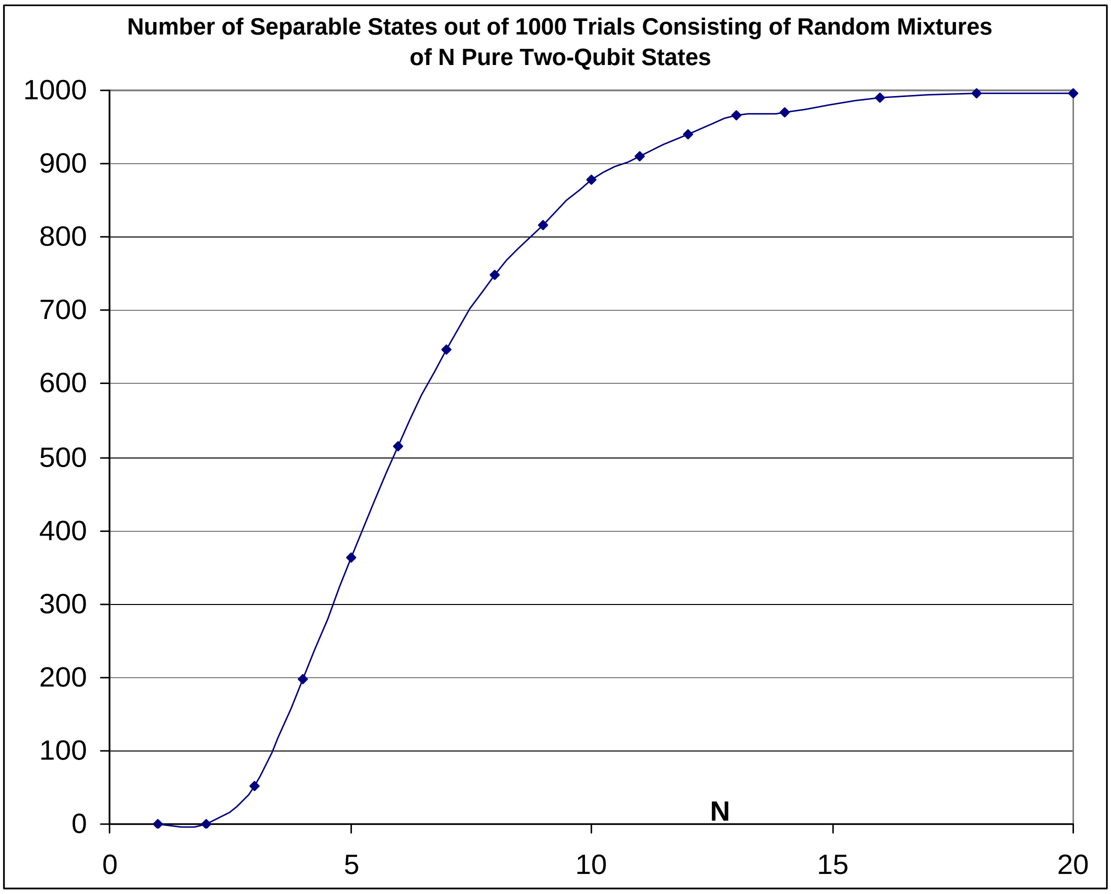



Separable states first occur for N = 3, and become increasingly common as N increases further.

As N increases, the proportion of states which have small vN entropies (combined or reduced) diminishes rapidly. At the same time, the proportion of states with large entanglements of formation also diminishes rapidly. For N=10 there was only one state with EoF > 0.2. Hence, as $N \to \infty$, we have $S_{vN}^{AB}, S_{vN}^{A}$ and $S_{vN}^{B}$ all $\to 1$, whereas EoF $\to 0$, and the plots become increasingly dominated by the deep blue points which cluster at the top right hand corner. In other words, for a sufficiently large number of states contributing to the mixture, the resulting mixed state becomes separable. This is just as deduced algebraically in the previous Section.

The number of separable states out of 1000 trials for N from 1 to 20 is shown below. Each N has been run three times to indicate the spread in results obtained. The average of these three results is plotted in the graph which follows.

| **N** | **Number of Separable States (out of 1000 trials)** | | |
|---|---|---|---|
| 1 | 0 | 0 | 0 |
| 2 | 0 | 0 | 0 |
| 3 | 53 | 44 | 61 |
| 4 | 204 | 199 | 190 |
| 5 | 375 | 356 | 358 |
| 6 | 515 | 515 | 517 |
| 7 | 663 | 664 | 616 |
| 8 | 761 | 734 | 750 |
| 9 | 831 | 800 | 819 |
| 10 | 881 | 866 | 887 |
| 11 | 905 | 913 | 915 |
| 12 | 939 | 947 | 935 |
| 13 | 971 | 966 | 962 |
| 14 | 974 | 977 | 962 |
| 16 | 991 | 990 | 992 |
| 18 | 997 | 993 | 997 |
| 20 | 996 | 999 | 995 |




## 6. Attempts to Quantify the Degree of Entanglement for Mixtures

Previous Sections have discussed recognising whether a state or mixture is entangled or separable. However, there are degrees of entanglement. For pure states we have seen that 'almost all' states, chosen at random, are entangled in the sense of being non-separable. However, the degree of entanglement varies widely, as illustrated by the first of the preceding graphs (the colour coding, the Entanglement of Formation, being a measure of the degree of entanglement).

There is a widely adopted entanglement measure for pure states. The entanglement of a bipartite state $\hat{\rho}_{AB}$ is defined as the von Neumann entropy of the reduced state, noting that it does not matter which sub-system is traced out,

$$E(\hat{\rho}_{AB}) = S_{vN}(\hat{\rho}_A) = S_{vN}(\hat{\rho}_B), \text{ where, } \hat{\rho}_A = Tr_B(\hat{\rho}_{AB}) \text{ and } \hat{\rho}_B = Tr_A(\hat{\rho}_{AB}) \qquad \text{(QM7.0)}$$

Unfortunately, there is no single, universally agreed, measure of the degree of entanglement for mixed states. Moreover, some entanglement measures, whilst well-defined, are hard to evaluate in the general case. In this Section we present some of the more common entanglement measures that are in use for mixed states, though the subject is large and this is by no means a complete survey. One of the seminal papers in this area is Bennett et al (1996), which is strongly recommended.

**6.1 Purity, Linear Entropy and Entanglement of Formation for Mixtures**

The Purity of a mixture, μ, is defined as,

$$\mu = \mathrm{Tr}\left(\hat{\rho}^2\right) \qquad \text{(QM7.6.1)}$$

Recall that any pure state has $\mathrm{Tr}\left(\hat{\rho}^2\right) = 1$, and hence the purity is unity for pure states. The minimum purity is obtained for maximum vN entropy, when all the eigenvalues of the density matrix equal 1/D, where D is the dimension of the Hilbert space. Hence the minimum purity is 1/D.

The Linear Entropy is defined by,

$$S_L = (1-\mu)\cdot\frac{D}{D-1} \qquad \text{(QM7.6.2)}$$

Hence the linear entropy ranges from 0 (when the purity is 1) to 1 (when the purity is 1/D).

Entanglement of Formation (EoF) of a mixed state is defined as the optimised weighted sum of the von Neumann entropies of the states contributing to the mixture,

$$\mathrm{EoF} = \mathrm{MIN}\left[\sum_i p_i E\left(|\psi_i\rangle\langle\psi_i|\right)\right] \qquad \text{(QM7.6.3)}$$

where the entanglement of a pure bipartite state, $E\left(|\psi_i\rangle\langle\psi_i|\right)$, is defined as the von Neumann entropy of the reduced state, $E\left(|\psi_i\rangle\langle\psi_i|\right) = S_{vN}\left[\mathrm{Tr}_A\left(|\psi_i\rangle\langle\psi_i|\right)\right]$, noting that it does not matter which sub-system, A or B, is chosen. For a pure state, the EoF reduces to the usual definition of the entanglement of a pure state, (QM7.0).

The set of states $\{|\psi_i\rangle\}$ such that $\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is not unique. The Entanglement of Formation is defined by (QM7.6.3) by minimising the result with respect to any $\{p_i\}$ and $\{|\psi_i\rangle\}$ for which $\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ equals the density matrix in question. In general this is a difficult optimisation to perform. However, a simple algorithm for EoF exists for an arbitrary mixture of two qubits. This is given below.

Before giving this algorithm, it is worth emphasising how crucial is the minimisation of (QM7.6.3). Choosing an inappropriate (i.e. non-optimal) basis, $\{|\psi_i\rangle\}$, will give a grossly misleading result. A simple example is provided by the 50/50 mixture of Bell states,

$|\psi_\pm\rangle = (|0\rangle|0\rangle \pm |1\rangle|1\rangle)/\sqrt{2}$. We know that this is a separable mixture (see Section 2), since the density matrix is $\hat{\rho} = \frac{1}{2}\left[|0\rangle|0\rangle\langle 0|\langle 0| + |1\rangle|1\rangle\langle 1|\langle 1|\right]$. In this latter, computational, basis, the reduced density matrices corresponding to the two terms are

$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ respectively. These both have zero vN entropy, and hence $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$ evaluated in this basis is zero. This is obviously the minimum and hence the EoF (which measures the entanglement) is zero, as it should be for a separable state. However, if we evaluated $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$ in the Bell basis, we have,

$Tr_A(|\psi_\pm\rangle\langle\psi_\pm|) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \rightarrow \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$. The vN entropy of these states is 1, and hence $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$ is also unity. So, evaluating in the wrong (i.e. non-optimal) basis gives a grossly misleading result. It suggests that the state is maximally entangled, when in fact it is separable.

Incidentally, this example may give the false impression that the reduced density matrix is basis dependent. Of course that is not true. The reduced density matrix is basis independent because,

$$Tr_A(\hat{\rho}_{AB}) = \sum_i \langle i|_A \hat{\rho}_{AB} |i\rangle_A = \sum_{i,I,J} U^*_{iJ} \langle J|_A \hat{\rho}_{AB} |I\rangle_A U_{iI} = \sum_{I,J} \langle J|_A \hat{\rho}_{AB} |I\rangle_A \delta_{IJ} = \sum_I \langle I|_A \hat{\rho}_{AB} |I\rangle_A$$

The two bases used above do lead to the same reduced density matrix, but expressed as the sum of different terms, as follows,

$$\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \text{ compared with } \frac{1}{2}\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

Thus, whilst both give the same total reduced density matrix, the expression on the RHS of the definition of EoF, $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$, involves evaluating the $S_{vN}$ for each term in the sum *separately*. This is how the difference arises.

### 6.2 Algorithm for Finding EoF for an Arbitrary Two-Qubit Mixed State and Definition of Concurrence, C

The Entanglement of Formation is a good entanglement measure. Unfortunately it is difficult to evaluate in the general case because of the optimisation needed. However, for two qubit states there is an effective algorithm for EoF, first stated by Wootters (1997), as follows:-

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2 x 2 Hilbert space: $$\text{EoF} = g\left(\frac{1}{2}\left[1+\sqrt{1-C^2}\right]\right) \quad \text{(QM7.6.4a)}$$

where, $$g(x) = -x\log_2 x - (1-x)\log_2(1-x) \quad \text{(QM7.6.4b)}$$

and where C is the Concurrence.

The Concurrence, C, of a 2 x 2 state, is defined by,

$$C = \text{MAX}(0, \xi) \quad \text{(QM7.6.5a)}$$

where, $$\xi = \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4} \quad \text{(QM7.6.5b)}$$

and the $\lambda i$ are the eigenvalues, in descending order, of the matrix,

$$\rho(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y) \quad \text{(QM7.6.5c)}$$

where $(\sigma_y \otimes \sigma_y)$ is the direct product of the y-component Pauli matrix, i.e.,

$$(\sigma_y \otimes \sigma_y) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \quad \text{(QM7.6.5d)}$$

The square of the concurrence is called the "tangle".

The Entanglement of Formation, the concurrence, and the tangle are all measures of entanglement in that they range from 0 for separable states to 1 for maximally entangled states.

Bennett et al (1996) show that the EoF is the number of pure Bell states (e.g. pure singlets) which Alice and Bob would have to share in order to be able to prepare the mixed quantum state without the exchange of further quantum states. This justifies the name "entanglement of formation".

Wootters (1997) also gives an algorithm for explicitly constructing a decomposition of the bipartite density matrix, $\{|\psi_i\rangle, p_i\}$, which gives the minimal value for $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$. Again this is for the 2 x 2 Hilbert space only.

As far as I am aware, no effective algorithm for calculating the entanglement of formation, or explicitly constructing a corresponding decomposition, $\{|\psi_i\rangle, p_i\}$, has yet been devised for Hilbert spaces of arbitrary dimensionality.

Example of 2 x 2 Evaluation of EoF

Consider the bipartite density matrix in the usual computational basis,

$$\rho_{AB} = \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 1/4 & 1/4 & 0 \\ 0 & 1/4 & 1/4 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(QM7.6.5e)}$$

The obvious decomposition is $|\psi_1\rangle = |0\rangle|0\rangle$ with $p_1$ = ½ , plus, $|\psi_2\rangle = (|0\rangle|1\rangle + |1\rangle|0\rangle)/\sqrt{2}$ with $p_2$ = ½ . The first of these states produces a reduced density matrix with vN entropy zero, whilst the reduced density matrix of the second is $\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$ which has a vN entropy of 1. Hence, this decomposition produces a value for $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$ of ½ . The correct EoF cannot exceed this value, since it is, by definition, the minimum possible value of $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$. We will see that the EoF is actually smaller than this.

We follow Wootters' prescription given above. The matrix defined by (QM7.6.5c) evaluates to,

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/8 & 1/8 & 0 \\ 0 & 1/8 & 1/8 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(QM7.6.5f)}$$

The eigenvalues of this matrix are λi = ¼, 0, 0, 0. Hence, from (QM7.6.5a,b), C = ½ . So $\left[1 + \sqrt{1 - C^2}\right]/2 = 0.9330$, and hence EoF = g(C) = 0.3546, using (QM7.6.4b). Hence, the EoF is indeed less than 0.5.

What decomposition achieves this minimum of $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$? Wootters (1997) gives an algorithm for explicitly constructing such a decomposition for 2 x 2 mixed states. Here we shall just write down a minimal decomposition, obtained by a little trial and error for this simple example, i.e.,

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}|0\rangle|0\rangle - \frac{1}{2}(|0\rangle|1\rangle + |1\rangle|0\rangle) \quad \text{and} \quad |\psi_{21}\rangle = \frac{1}{\sqrt{2}}|0\rangle|0\rangle + \frac{1}{2}(|0\rangle|1\rangle + |1\rangle|0\rangle) \qquad \text{(QM7.6.5g)}$$

with $p_1 = p_2 = ½$ . This clear reproduces the density matrix (QM7.6.5e). The reduced density matrices of these states are $\begin{pmatrix} 3/4 & \pm 1/2\sqrt{2} \\ \pm 1/2\sqrt{2} & 1/4 \end{pmatrix}$, which both have the same eigenvalues, i.e. 0.9330 and 1 – 0.9330 = 0.0670. Hence $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$ evaluates to 0.3546, as given by Wootters' prescription. QED.

Note that a useful biproduct of Wootters (1997) is that it shows that the number of states in a minimal decomposition need not exceed the number of non-zero eigenvalues of the bipartite density matrix (i.e. 2 in the above example). I am not sure if this holds for dimensions greater than 2 x 2.

### 6.3 Purity Measure of Entanglement for Gaussian States

Adesso, Serafini & Illuminati (2004) have proposed entanglement measures specific for continuous-variable (CV) Gaussian states. The purity of the bipartite state is denoted $\mu$, whilst the purities of the reduced states are denoted $\mu_A$ and $\mu_B$. For Gaussian states it can be shown rigorously that,

All states are separable in the range: $\mu_A\mu_B < \mu \le \frac{\mu_A\mu_B}{\chi_1}$ (QM7.6.6a)

States may be separable or entangled in the range:

$$\frac{\mu_A\mu_B}{\chi_1} < \mu \le \frac{\mu_A\mu_B}{\chi_2} \quad \text{(QM7.6.6b)}$$

All states are entangled in the range: $\frac{\mu_A\mu_B}{\chi_2} < \mu \le \frac{\mu_A\mu_B}{\chi_3}$ (QM7.6.6c)

where,

$$\chi_1 = \mu_A + \mu_B - \mu_A\mu_B ; \quad \text{(QM7.6.6d)}$$

$$\chi_2 = \sqrt{\mu_A^2 + \mu_B^2 - \mu_A^2\mu_B^2} \quad \text{(QM7.6.6e)}$$

$$\chi_3 = \mu_A\mu_B + |\mu_A - \mu_B| \quad \text{(QM7.6.6f)}$$

I had hoped that, although proved for Gaussian states, this entanglement measure might prove useful for the general discrete state also. However, this appears not to be the case. Take, for example, the 50/50 mixture of the Bell states $|\psi_1\rangle = (|0\rangle|0\rangle + |1\rangle|1\rangle)/\sqrt{2}$ and $|\psi_2\rangle = (|0\rangle|1\rangle + |1\rangle|0\rangle)/\sqrt{2}$ . We have seen already in Section 2 that this is a separable state, $\frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2| = \frac{1}{2}\hat{\rho}_{1A} \otimes \hat{\rho}_{1B} + \frac{1}{2}\hat{\rho}_{2A} \otimes \hat{\rho}_{2B}$, where, $\hat{\rho}_1 = \frac{1}{\sqrt{2}}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ and $\hat{\rho}_2 = \frac{1}{\sqrt{2}}(|0\rangle\langle 1| + |1\rangle\langle 0|)$. In matrix form this is written as,

$\frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Now the square of this two qubit density matrix is $\frac{1}{8}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$, and hence $\mu = ½$. The reduced density matrix is $\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$, and hence $\mu_A = ½$ . The values of the expressions in (QM7.6.6d,e,f) are thus $\chi_1 = \frac{3}{4}$, $\chi_2 = \frac{\sqrt{7}}{4}$, $\chi_3 = \frac{1}{4}$, so that the three ranges defined by (QM7.6.6a,b,c) are respectively, $\frac{1}{4} < \mu \le \frac{1}{3}$; $\frac{1}{3} < \mu \le \frac{1}{\sqrt{7}} = 0.37796$; and, $\frac{1}{\sqrt{7}} = 0.37796 < \mu \le 1$. Thus, our value of $\mu = ½$ is in the last range, which should correspond to a guaranteed entangled state (for Gaussian states). But this is the wrong result. We know this state is separable. So I conclude that these Gaussian state purity measures of entanglement are of no use for general discrete states. (This is unfortunate because they are very simple to evaluate).

**6.4 The Entanglement of Teleportation (Pure States Only)**

Although the most commonly used measure of entanglement for pure states is the von Neumann entropy of the reduced states, it is not the only measure which has been defined. It would appear that the most appropriate measure of entanglement depends upon what physical property is in question. Thus, Rigolin (2005) has defined an "entanglement of teleportation". This was defined specifically to reflect faithfully the usefulness of the state as a quantum teleportation channel. As far as I am aware, the entanglement of teleportation has been defined only for pure states with an even number of orthogonal states (i.e. for bipartite states, each sub-system comprising N qubits). Rigolin's entanglement of teleportation is, in general, different from the entanglement of formation (which reduces to the vN entropy of the reduced states for pure bipartite states). This is best illustrated by example. In these examples we are adopting the convention that maximal entanglement (or entropy) is unity. This means that, for 2-qubit states, the vN entropy is defined using logs to base 4.

Rigolin defines a magic basis for states of 4 qubits, consisting of 16 basis states of which one example is,

$$|g_1\rangle = (|0000\rangle + |0101\rangle + |1010\rangle + |1111\rangle)/2 \qquad \text{(QM7.6.7)}$$

These generalised Bell states have maximal entanglement according to the vN entropy definition, and also maximal entanglement of teleportation. These states will reliably teleport an arbitrary 2-qubit quantum state. [NB: In QM7.6.7, the first pair of qubits is accessible to Alice, and the second pair is accessible to Bob, and the teleportation involves a 2-qubit state].

Consider now the state, defined by Rigolin, as,

$$\left|GHZ^{\pm}\right\rangle = \left(\left|0000\right\rangle \pm \left|1111\right\rangle\right)/\sqrt{2} \qquad \text{(QM7.6.8)}$$

The entanglement of teleportation is ½ [see Rigolin(2005)]. To find the vN based entanglement, note that the reduced density matrix is $\left(\left|00\right\rangle\left\langle 00\right| + \left|11\right\rangle\left\langle 11\right|\right)/2$. Hence the vN entropy of the reduced state, i.e. the entanglement, is 2 x ½ $\log_4(2)$ = ½ . So, the vN entanglement and the entanglement of teleportation are again equal for these states. However the fact that the entanglement of teleportation is not optimal for these states reflects the fact that they can reliably teleport only a subset of 2-qubit states.

As a final example consider Rigolin’s state,

$$\left|W\right\rangle = \left(\left|0001\right\rangle + \left|0010\right\rangle + \left|0100\right\rangle + \left|1000\right\rangle\right)/2 \qquad \text{(QM7.6.9)}$$

The reduced density matrix is $\frac{1}{2}\left|00\right\rangle\left\langle 00\right| + \frac{1}{4}\left(\left|01\right\rangle + \left|10\right\rangle\right)\left(\left\langle 01\right| + \left\langle 10\right|\right)$, i.e. the matrix,

$$\begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 1/4 & 1/4 & 0 \\ 0 & 1/4 & 1/4 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

where the arrow denotes diagonalisation. Hence the vN based entanglement is,
2 x ½ $\log_4(2)$ = ½ . However, Rigolin gives the entanglement of teleportation of this state to be zero. This reflects the fact that this state cannot be used as a reliable teleportation channel for any quantum states. The fact that the vN based entanglement is ½ therefore implies that it is not a good guide to the usefulness of a state as a teleportation channel.

**6.5 Distillable Entanglement**

The entanglement of formation (EoF) measures how many pure Bell states (each defined as having unit entanglement) is needed to prepare the mixed state in question. But it may be more indicative of the usefulness of a mixed state for physical purposes (e.g. quantum computation) to consider the number of pure Bell states which can be *made from* the given mixed state, rather than the reverse. This is the “distillable entanglement”. Bennett et al (1996) define two versions of the distillable entanglement depending upon whether only one-way or two-way classical communication between Alice and Bob are permitted. In neither case is the exchange of quantum states permitted, of course. Unfortunately, the distillable entanglement is even harder to compute in the general case than the EoF. We finish by quoting Bennett et al,

"By distillable entanglement we will mean the asymptotic yield of arbitrarily pure singlets that can be prepared locally from mixed state M by entanglement purification protocols (EPP) involving one-way or two-way communication between Alice and Bob. Distillable entanglement for one and two-way communication will be denoted D1(M) and D2(M), respectively. Except in cases where we have been able to prove that D1 or D2 is identically zero, we have no explicit values for distillable entanglement, but we will exhibit various upper bounds, as well as lower bounds given by the yield of particular purification protocols."

Note that it is physically obvious that D1(M) ≤ D2(M) ≤ E(M), since otherwise we could distill more entanglement out than we put in, which could then be used to create a more entangled state.

## 7. Summary

- The concept of entanglement applies to systems which can be considered as composed of two sub-systems (bipartite), often called Alice and Bob.
- A pure bipartite quantum state is entangled iff it cannot be expressed as the product of quantum states of the two sub-systems.
- A mixed bipartite state is entangled iff its density matrix cannot be written as a weighted sum over direct products of density matrices for the two sub-systems.
- If a pure state is chosen at random from a given Hilbert space describing a bipartite system, then it will almost always be entangled (the separable states are of measure zero);
- If a large number (N) of pure states are chosen at random and combined with random probabilities to form a mixture, then the resulting mixture will be separable (i.e., not entangled) in almost all cases. This becomes 'all cases' as $N \to \infty$.
- A widely used measure of the entanglement of a pure bipartite state is the von Neumann entropy ($S_{vN}$) of the reduced states.
- However, even for pure states, the most appropriate measure of entanglement can depend upon the physical application in mind. Thus, the above $S_{vN}$ based entanglement measure is misleading as an indicator of the functionality of a state as a quantum teleportation channel. For this, Rigolin's entanglement of teleportation is more indicative.
- There is no universally agreed measure of entanglement in mixed states. Though the entanglement of formation is widely used it suffers from the disadvantage of being difficult to calculate for states of dimensionality greater than two qubits (4D). It terms of interpretation, it suffers from the disadvantage of being the entanglement needed to create a given mixed state, as opposed to the amount of entanglement that can be extracted from it (the distillable entanglement).
- There is a simple effective algorithm for the calculation of the entanglement of formation in the case of arbitrary mixtures of two qubit states. This also provides the alternative entanglement measures, the Concurrence and its square, the Tangle.

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- There is also an effective algorithm for constructing a decomposition of the bipartite density matrix into a mixture of states which realises the minimum value of $\sum_i p_i E(|\psi_i\rangle\langle\psi_i|)$ which defines the entanglement of formation – but only for the two qubit case.
- A simple criterion due to Peres provides a necessary and sufficient criterion for the separability of arbitrary mixtures of bipartite states of dimensionality 2 x 2 and 2 x 3.
- The Peres criterion is sufficient to imply entanglement, as is the criterion that the vN entropy of the bipartite mixture exceeds that of either reduced state, but neither of these criteria are necessary in general.

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