

Entanglement of formation

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1 Density Matrices

Let the two vectors in vector space describing the system be θ_i and θ_j . The wavefunction of the system consisting of these two vectors can also be written as:

$$|\psi\rangle = \sum_i \sum_j C_{ij} |\theta_i\rangle |\theta_j\rangle \quad (1)$$

Consider an observable A in the “pure” state $|\psi\rangle$ with the expectation value given by

$$\langle A \rangle_\psi = \langle \psi | A | \psi \rangle \quad (2)$$

Then we have following definition

The density matrix ρ for the pure state $|\psi\rangle$ is given by

$$\rho = |\psi\rangle \langle \psi| \quad (3)$$

This density matrix has the following properties:

1. $\rho^2 = \rho$ (Projector)
2. $\rho^\dagger = \rho$ (Hermiticity)
3. $Tr \rho = 1$ (Normalization)
4. $\rho \geq 0$ (Positivity)

The first two properties follow immediately from Definition and property 3. can be verified using the definition of the trace operation for an arbitrary operator D :

Defn- The trace of an operator D is given by

$$Tr D = \sum_n \langle n | D | n \rangle$$

where $|n\rangle$ is a constant.

We take the operator $D = |\psi\rangle \langle \phi|$ and calculate its trace.

$$Tr D = \sum_n \langle n | \psi \rangle \langle \phi | n \rangle = \sum_n \langle \phi | n \rangle \langle n | \psi \rangle = \langle \phi | \psi \rangle \quad (4)$$

Property 4. means that the eigenvalues of ρ are greater or equal to zero, which can also be expressed as

$$\langle \varphi | \rho | \varphi \rangle = \langle \varphi | \psi \rangle \langle \psi | \varphi \rangle = |\langle \varphi | \psi \rangle|^2 \quad (5)$$

which is an important property because probabilities are always greater or equal to zero.

We still have to ensure if the expectation value of an observable in the state $|\psi\rangle$ can be reproduced, which we will see in the following theorem:

Theorem- The expectation value of an observable A in a state, represented by a density matrix ρ , is given by $\langle A \rangle_\rho = \text{Tr } \rho A$

Proof-

$$\begin{aligned} \text{Tr } (\rho A) &= \text{Tr } (|\psi\rangle\langle\psi|A) = \sum_n \langle n|\psi\rangle\langle\psi|A|n\rangle \\ &= \sum_n \langle\psi|A|n\rangle\langle n|\psi\rangle = \langle\psi|A|\psi\rangle = \langle A \rangle \end{aligned} \quad (6)$$

If we let $A = 1$, we get $\text{Tr } A\rho = \text{Tr } \rho = \sum_i x_i = 1$, and, $x_i \geq 0$. [1]

So, we get from density matrices, the real eigenvalues and also the orthonormal set of the eigenvectors, where x_i is the probability of finding the system in state $|i\rangle$

The density matrix of pure state $|\psi\rangle$ is another matrix $\rho = |\psi\rangle\langle\psi|$

We also can identify pure states and mixed states as,

For pure states, $\rho = \rho^2$ and $\text{Tr } \rho = 1$

But, for mixed states, $\rho \neq \rho^2$ and $\text{Tr } \rho = 1$

We can't exactly tell if a state is separable (mixed) or not, because there are infinitely many decompositions of a mixed state. So a mixed state can be written in infinitely many ways [3]. For eg.

$$\rho = \sum_{j=1}^N \rho_j |\psi_j\rangle\langle\psi_j| = \sum_{i=1}^m \rho_i |\psi_i\rangle\langle\psi_i| = \dots\dots\dots \quad (7)$$

The problem here is to find if there exists a state which can be written as product states in convex roof.

1.1 Examples of pure and mixed states

We consider a pure state $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

$$\rho = |\psi\rangle\langle\psi| = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

We have $\rho^2 = \rho$ and $\text{Tr } \rho = 1$

Now, consider mixed state 50% $|\uparrow\rangle$ and 50% $|\downarrow\rangle$

$$\rho = \frac{1}{2}(|\uparrow\rangle\langle\uparrow|) + \frac{1}{2}(|\downarrow\rangle\langle\downarrow|) = \frac{1}{2} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

We have $\rho^2 \neq \rho$ and $\text{Tr } \rho = 1$

Consider equal mixture of $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ & $|\theta\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle + |\uparrow\rangle)$

$$\rho = \frac{1}{2}(|\psi\rangle\langle\psi|) + \frac{1}{2}(|\theta\rangle\langle\theta|) = \frac{1}{2} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} + \frac{1}{2} \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

We have $\rho^2 \neq \rho$ and $\text{Tr } \rho = 1$

2 Entropy

Entropy is the degree of the randomness or uncertainty of particle inside a system. We can devise an experiment in which we can see that for systems with high knowledge, we have low entropy, and for systems having low information, we get high entropy.

2.1 Shannon Entropy

We have 4 sets of boxes containing 10 letters each. We need to find the entropy of each boxes

1. [AAAAAAAAAA]
2. [AAAAABBBBB]
3. [AAAABBBCCC]
4. [AAABBBCCDD]

In this problem, we define $P(least)$ as the probability of getting least different letters

For Box 1.

It is known that the probability of A being selected is 1, no matter whichever A is selected.

$$\text{So, probability } P(A) = \frac{10}{10} = 1 \quad P(least) = 1 * 1 * 1 * 1 * 1 * 1 * 1 * 1 * 1 * 1 = 1$$

For Box 2.

$$P(A) = \frac{5}{10} = 0.5, P(B) = \frac{5}{10} = 0.5 \quad P(least) = .5 * .5 * .5 * .5 * .5 * .5 * .5 * .5 * .5 * .5 = .0009765625$$

For Box 3

$$P(A) = \frac{4}{10} = .4, P(B) = \frac{3}{10} = .3, P(C) = \frac{3}{10} = .3 \quad P(least) = .4 * .4 * .4 * .4 * .3 * .3 * .3 * .3 * .3 * .3 = 0.0000186624$$

For Box 4

$$P(A) = \frac{3}{10} = .3, P(B) = \frac{3}{10} = 0.3, P(C) = \frac{2}{10} = .2, P(D) = \frac{2}{10} = .2. \quad P(least) = .3 * .3 * .3 * .3 * .3 * .2 * .2 * .2 * .2 * .2 = .0000007776$$

We have to find entropy but by the way mentioned above we get very high value in decimals. So, the choice to select a function to overcome the problem is to take logarithm since it is monotonous and it has a property $\log(ab) = \log(a) + \log(b)$

Shannon's entropy associated with probability is defined as $H(X) = (P(A), P(B), \dots, P(n)) = -\sum_X P \log_2 P$

Now, we have

Box	$P(least)$	$-\log_2 P$	$H(X) = -\sum_X P \log_2 P$
[AAAAAAAAAA]	1	0	0
[AAAAABBBBB]	0.0009765625	10	5
[AAAABBBCCC]	0.0000186624	15.7095	5.242
[AAABBBCCDD]	0.0000007776	20.2945	4.9841

Binary Entropy

The experiment with 2-outcomes, is termed as binary entropy.

$H_{bin}P = -(p \log_2 p + (1 - p) \log_2 (1 - p))$ which is further used in Eq. (16). The binary entropy function is also shown in Fig. (1)

2.2 Von-neumann entropy

For measuring the uncertainty associated with quantum states can be shown similar to Shannon's entropy[1]. The probability in shannon's entropy is replaced by density matrices. The **Von-Neumann entropy** of any quantum state ρ is defined as

$$S(\rho) = -Tr(\rho \log_2 \rho)$$

If the state ρ has eigenvalues λ_x , the Von-Neumann entropy can be rewritten as

$$S(\rho) = - \sum_x \lambda_x \log_2 \lambda_x$$

3 Entanglement of formation for bipartite systems

Consider two Hilbert spaces H_1 and H_2 with dimensions N_1 and N_2 with orthonormal basis e_i^k , where $i = 1, 2, 3, \dots, N_k$, $k = 1, 2$ respectively. A pure quantum state $|\psi\rangle \in H_1 \otimes H_2$ can be written as the form[4]

$$|\psi\rangle = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} a_{ij} e_i^1 \otimes e_j^2, \quad a_{ij} \in \mathbb{C} \quad (8)$$

Normalizing a_{ij} , we have

$$\sum_{i=1}^{N_1} \sum_{j=1}^{N_2} a_{ij} a_{ij}^* = 1 \quad (9)$$

The entanglement of formation, E is defined as partial entropy of sub Hilbert spaces $H_1 \otimes H_2$

$$E(|\psi\rangle) = -Tr(\rho_1 \log_2 \rho_1) = -Tr(\rho_2 \log_2 \rho_2) \quad (10)$$

We have a mixed state ρ which can be written as decomposition of many states as

$$\rho = \sum_{j=1}^N \rho_j |\psi_j\rangle \langle \psi_j| \quad (11)$$

where $|\psi_j\rangle$ are normalised distinct pure states of bipartite system. and $\sum_{j=1}^n \rho_j = 1$ and are non-negative.

It is required to find the one minimum average entanglement over infinitely many decompositions of the mixed state ρ [4, 3] to find the entanglement of formation as stated in Eq. (13)

$$E_f(\rho) = \min \left(\sum_{j=1}^n \rho_j E(\psi_j) \right) \quad (12)$$

3.1 Entanglement of formation for 2-qubits

There is a quantity termed as 'concurrence' on which the E_f is defined for a pair of qubits. [3, 4]. For now, we assume that concurrence is only defined for a pair of qubits, though possible generalisations may exist for larger systems [3]. The concurrence $C(\psi)$ of a pure state $|\psi\rangle$ can be defined as $C(\psi) = |\langle \psi | \tilde{\psi} \rangle|$, where $|\tilde{\psi}\rangle = (\sigma_y \otimes \sigma_y) |\psi^*\rangle$, ψ^* is complex conjugate of ψ in standard basis. σ_y is the Pauli operator. The $|\tilde{\psi}\rangle$ takes the state of each qubit to orthogonal state, the state diametrically opposite as viewed on Bloch Sphere, when applied to pure product state. So, the concurrence of pure product state is zero, but the entangled state is left as it is by the operation. This does separates pure product state with mixed. For entangled state, the concurrence takes its maximum value, i.e. one. The relation between entanglement and concurrence then becomes

$$E_f(\psi) = \varepsilon(C(\psi)) \quad (13)$$

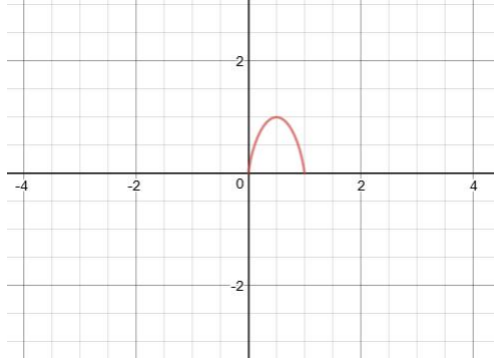


Figure 1: The binary Shannon entropy function ($h(x)$ vs x)

The function ε is defined by [3]

$$\varepsilon(C) = h\left(\frac{1 + \sqrt{1 - C^2}}{2}\right) \quad (14)$$

$$h(x) = -x \log_2 x - (1 - x) \log_2 (1 - x) \quad (15)$$

We see, $h(x)$ obtains a maximum value at $x = 0.5$. Also $x \in (0, 1)$. By plotting the graph of $\varepsilon(C)$ vs C , we get $\varepsilon(C)$ is monotonically increasing, $C \in (0, 1)$. So the entanglement increases when the concurrence increases and takes the maximum value of mixed product state to be 1.

We need to show if $|\psi\rangle$ is factorizable or not. We represent $|\psi\rangle$ in standard basis $|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$. $|\psi\rangle$ is factorizable if $ad = bc$

For calculating the minimum in Eq. (13), we need to find the corresponding minimum of Eq. (17)

$$C(\rho) = \min_{\rho_j \sigma_j} \sum_{j=1}^n \rho_j C(|\psi_j\rangle) \quad (16)$$

A formula for $C(\rho)$ can be found and given in [5, 9]

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\} \quad (17)$$

where λ_i 's represent the square roots of eigenvalues of $\tilde{\rho}\tilde{\rho}$ in decreasing order, $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$

3.2 EOF for isotropic states

A pair of N -dimensional bipartite quantum states A and B , which are invariant under all transformations $U \otimes U^*$ where U^* is the complex conjugate of U in the standard basis are called isotropic states. There is exactly one pure isotropic state in every dimension N [8] given as, $|\psi^+\rangle = \frac{1}{\sqrt{N}} \sum_i |ii\rangle$. The remaining states in N -dimension are a mixture of pure states and mixed states. A choice for labeling isotropic state is $F = \langle \psi^+ | \rho_f | \psi^+ \rangle$, $F \in [0, 1]$. It is found that the state is separable if $F < 1/N$

Convex Hull - The smallest convex polygon containing a set X of points on or inside the boundary of the polygon is referred to as Convex Hull

3.3 EOF for Werner States

A pair of N-dimensional bipartite quantum states A and B, which are invariant under all transformations $U \otimes U$ are called Werner States.[6]

The density matrix of Werner States can be written as

$$\rho_f = \frac{1}{N^3 - N}(N - f)I + (Nf - 1)P \quad (18)$$

Eq. (19) can also be written as $\rho_f = aI + bP$, where I is the Identity operator and P is defined as $P(\phi \otimes \psi) = \psi \otimes \phi$, f is a constant satisfying $-1 \leq f \leq 1$, Werner states are separable iff. $f \geq 0$ shown in [6]

4 Concurrence and its Generalisation

Concurrence quantifies the quantum entanglement and can be used to define how much a state is far from achieving separability. Eg. If concurrence is 0, we define the state as unentangled and if it's non-zero the state is entangled and can't be separated. A formula for Entanglement of formation is given in Eq. (16) for 2-qubits. There are some theories to generalize concurrence to larger systems having more than 2-qubits.

4.1 Arbitrary conjugation

The concurrence for pure state $|\psi\rangle$ is defined as $C(\psi) = |\langle\psi|\tilde{\psi}\rangle|$ where $|\tilde{\psi}\rangle = (\sigma_y \otimes \sigma_y)|\psi^*\rangle$, ψ^* is complex conjugate of ψ in standard basis. σ_y is the Pauli operator. The $|\tilde{\psi}\rangle$ takes the state of each qubit to orthogonal state, the state diametrically opposite as viewed on Bloch Sphere. The **conjugation** means an antiunitary φ such that $\varphi^2 = I$, the identity. The antilinear map is a map from a complex vector space to another complex vector space $f : V \rightarrow W$, satisfying $f(ax + by) = \bar{a}f(x) + \bar{b}f(y)$. Similarly, an antilinear operator φ satisfies

$$\varphi(a|\psi\rangle + b|\omega\rangle) = a^*\varphi|\psi\rangle + b^*\varphi|\omega\rangle \quad (19)$$

An antilinear operator is also antiunitary if it satisfies $\langle\psi|\varphi|\phi\rangle = \langle\phi|\varphi^{-1}|\psi\rangle$

The **skew conjugation** is defined if $\varphi^2 = -I$

The φ - *concurrence* of a pure state $|\psi\rangle$ is defined as

$$C_\varphi(\psi) = |\langle\psi|\varphi|\tilde{\psi}\rangle| \quad (20)$$

The φ - *concurrence* of a mixed state $|\rho\rangle$ is defined as

$$C_\varphi(\rho) = \min \sum_j \rho_j C_\varphi \psi_j$$

We take minimum over all decompositions of ρ . Formula for φ - *concurrence* can be found as [9, 3]

$$C_\varphi(\rho) = \max\{0, \lambda_1 - \sum_{i>1} \lambda_i\}$$

where λ_i 's represent the square roots of eigenvalues of $\rho\tilde{\rho}$ in decreasing order, $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$

4.2 Universal Inverter

The concurrence for an arbitrary pure state of two qubits is based on Wootters' spin-flip operation[3]. In all Hilbert space dimensions, universal operator is defined, which leads to generalised concurrence. Hence, it is needed to generalise spin flip to universal inverter also called as superoperators.[3, 10] Superoperators S_d acts on density matrices in d-dimensions.[3] It satisfies

1. S_d maps hermitian operators to Hermitian operators

2. S_d commutes to all unitary operators
3. For all pure states $|\psi\rangle$ for a bipartite system, $\langle\psi|(S_{d_1}\otimes S_{d_2})(|\psi\rangle\langle\psi|)|\psi\rangle$ is always non-negative and equals zero iff $|\psi\rangle$ is a product state.

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 some of these studies are derived

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. For a pair of qubits this condition is not only necessary but also sufficient for separability, 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. For pure states, one can show directly that the negativity is equal to the concurrence. Eisert and Plenio[12], and later Zyczkowski[13], 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[14]

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[15, 16, 17, 18]. 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

$$C_{max}(\rho) = \max\{0, r_1 - r_3 - 2\sqrt{r_2 r_4}\} \quad (21)$$

5.3 Entanglement of magnetic systems

Finally, concurrence has been used to investigate the entanglement of magnetic systems such as a Heisenberg spin chain.[19] 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. 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[20]. 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.

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