A Complete Characterization of Mixed State Entanglement using Probability Density Functions

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We propose that the entanglement of mixed states is characterised properly in terms of a probability density function \( P(\mathcal{E}) \). There is a need for such a measure since the prevalent measures (such as concurrence and negativity) are rough benchmarks, and not monotones of each other. Considering the specific case of two qubit mixed states, we provide an explicit construction of \( P(\mathcal{E}) \) and show that it is characterised by a set of parameters, of which concurrence is but one particular combination. \( P(\mathcal{E}) \) is manifestly invariant under \( SU(2) \times SU(2) \) transformations. It can, in fact, reconstruct the state up to local operations - with the specification of at most four additional parameters. Finally the new measure resolves the controversy regarding the role of entanglement in quantum computation in NMR systems.

Quantum entanglement is a unique resource for novel (nonclassical) applications such as quantum algorithms \([1]\), quantum cryptography \([2]\), and more recently, metrology \([3]\). Thus, it has a pivotal role in quantum information theory. It is also central to the study of the foundations of quantum mechanics \([4]\). However, while pure state entanglement is well defined, mixed state entanglement (MSE) is still rather poorly understood. Currently used definitions such as entanglement of formation (EOF) \([5]\) and separability \([6]\) are based on the emphasis given to a particular quantum feature. These definitions are not equivalent \([7]\) and are operational in a limited sense. Thus, concurrence as a characteristic of EOF \([8]\) is defined only for a two qubit system; negativity as a criterion for separability \([9, 10]\) is necessary and sufficient only for two qubit systems and a qubit-qutrit system. Likewise, majorization \([11]\) is a necessary condition for separability. Further, concurrence and negativity are not relative monotones, although the former bounds the latter from above. In particular, states with the same negativity may have different concurrence and vice versa. Note that real systems are almost always in a mixed state. Indeed, NMR quantum computers (NMR QC) \([12, 13]\) are prepared in the so called pseudo pure states which are highly mixed. Their concurrence (and hence negativity) is zero, and yet nontrivial nonclassical gate operations with up to eight qubits have been reported \([14]\). More recently, a 12-qubit pseudopure state has been reported for a weakly coupled NMR system \([15]\). To unravel the sense in which the entanglement is a resource in these systems, there is a clear need to go beyond the above mentioned benchmarks. We address this problem here, and propose an alternative definition of MSE.

To motivate our approach, we recall that a mixed state is required to describe an ensemble of quantum systems each of which is in a pure state. Entanglement has a sharp value in each pure state; Thus, MSE may be expected to acquire a statistical character, and be characterized by a suitably defined probability density function (PDF). We propose below a definition of MSE, in terms of one such PDF, which is strictly operational and applicable to any bipartite system. The definition does not require any new notion of entanglement other than that for pure states. We proceed to give an explicit construction of the PDF for the important case of two qubit systems. For these systems, we show that the PDF has some striking morphological features which completely encode the information on MSE: these features appear as a few points of discontinuity of various orders in the PDF. These points are shown to allow an almost complete reconstruction of the state, up to local operations (LO). It is shown how concurrence gets reinterpreted as a benchmark. Finally, the issue of entanglement in NMR QC gets naturally resolved.

We now posit a probability density function for entanglement, \( P_\rho(\mathcal{E}) \). The definition will be given in several steps: Let the state \( \rho \) of a two qubit system be characterised by its eigenvalues \( \lambda_i \), with respective eigenstates \( |\psi_i\rangle \) which are orthonormal; the notation implies that the eigenvalues are arranged in a non increasing order. The choice of \( |\psi_i\rangle \) is non unique if the eigenvalues are degenerate, but it is of no concern to us here. (i) As the first step, we define a sequence of projection operators

\[
\Pi_i = \sum_{j=1}^{i} |\psi_j\rangle\langle\psi_j|; \quad \Pi_i \subset \Pi_{i+1}, \quad \Pi_4 \text{ being the full Hilbert space.}
\]

It is a trivial identity that

\[
\rho = (\lambda_1 - \lambda_2)\Pi_1 + (\lambda_2 - \lambda_3)\Pi_2 + (\lambda_3 - \lambda_4)\Pi_3 + \lambda_4\Pi_4.
\]

The above equation resolves \( \rho \) into an incoherent sum of a hierarchy of the subspaces \( \Pi_i \), with the weights given by the nonnegative vector \( \Lambda = (\lambda_1 - \lambda_2, \lambda_2 - \lambda_3, \lambda_3 - \lambda_4, \lambda_4) \), whose norm is a measure of the purity of the state. In a sense, the vector represents the manner in which the state “spills over” to successively higher dimensional spaces. (ii) As the next step, observe that if \( \rho \) is a projection \( \Pi_i \) of dimension \( i \), the ensemble would be uniformly distributed over states in \( \Pi_i \): \( \langle \psi | \rho | \psi \rangle = 1 \forall |\psi\rangle \in \Pi_i \). A Probability
Density Function (PDF) may be naturally defined thus:

$$P_\rho(\mathcal{E}) = \frac{\int \int dH_i \delta(\mathcal{E}' - \mathcal{E})}{\int dH_i}$$

with $dH_i$ being the appropriate Haar measure. (iii) As the last step, rescale $\rho \rightarrow \rho_s$ and rewrite it in terms of the difference in relative weights $\mu_i = (\lambda_i - \lambda_{i+1})/\lambda_1$ as $\rho_s = \sum \mu_i \Pi_i$. The definition of the PDF is then given by the simple superposition

$$P(\mathcal{E}) = \sum_\alpha \mu_i P_\alpha(\mathcal{E}).$$

The rest of the paper is devoted to an elucidation of Eqns. 2 and 3. We choose the pure state concurrence $2|\alpha_{\parallel} + \alpha_{\perp} |\alpha_{\perp} - \alpha_{\parallel}|\alpha_{\parallel}$, in terms of the coefficients of expansion of $|\psi\rangle = |\alpha_{\parallel} |\uparrow\rangle + |\alpha_{\perp} |\downarrow\rangle + |\alpha_{\parallel} |\downarrow\rangle + |\alpha_{\perp} |\uparrow\rangle$, as the measure of pure state entanglement. Although the definition is given for the simplest case, the generalization to higher spin systems is straightforward, and we do not discuss it any further in this paper.

**TWO QUBIT PROBABILITY DENSITY FUNCTIONS: DESCRIPTION OF SUBSPACES**

We first consider the situation when $\rho$ is a projection, case by case. We then move on to discuss the general case (displayed in Eqn.3). Since the normalization is provided by dividing by the total volume of the group space, the trace factors will be dropped. We employ LO on the subspaces freely, since the PDF remains unaffected.

**The pure state:** Consider $\rho = \Pi_1 = \langle \phi | \phi \rangle$. The probability density function $P_1(\mathcal{E})$ is simply $\delta(\mathcal{E} - \mathcal{E}_0)$, in terms of the the entanglement of $|\phi\rangle$. The PDF is singular, and specified by a single number.

**Two dimensional projection:** $\rho = \Pi_2$ is the most complicated and the most interesting case. Suppose $|\psi\rangle \in \Pi_2$. Let $|\chi_1\rangle, |\chi_2\rangle$ be orthonormal and span $\Pi_2$. We have, $|\psi\rangle = |\chi_1\rangle \cos \theta e^{i\phi/2} + |\chi_2\rangle \sin \theta e^{-i\phi/2}$. The Haar measure is simply read off as $dH = \sin \theta d\theta d\phi$. By a suitable LO, we can choose $|\chi_1\rangle$ to be separable, in its canonical form $(1,0,0,0)$ in a separable basis, i.e., $|\chi_1\rangle = |\uparrow\rangle$. $|\chi_2\rangle$ can be further chosen to be of the form $(0,x,y,z)$, where $x,y \geq 0$. The entanglement distribution is, therefore, characterized by two non-negative parameters, and is implicitly determined by Eqn.2.

The generic form of the PDF in $\Pi_2$ is shown in FIG. 1 (the solid curve). We observe that it has three markers, (i) $\mathcal{E}_{cusp}$, the entanglement at which the probability density diverges, invariably as a cusp, (ii) $\mathcal{E}_\max$, the maximum entanglement allowed, and (iii) $P_2(\mathcal{E}_\max)$, the probability density at $\mathcal{E}_\max$. In fact, any two of them suffice to characterize the PDF completely. One may specify e.g., $(\mathcal{E}_\max, P_2(\mathcal{E}_\max))$, or equivalently, $P(\mathcal{E}_{cusp}, P_2(\mathcal{E}_\max))$ for characterizing the curve. A straightforward computation establishes the relations

$$\begin{align*}
\mathcal{E}_\max &= xy + \sqrt{x^2 + y^2} \\
\mathcal{E}_{cusp} &= \frac{z^2}{\mathcal{E}_\max} = \mathcal{E}_\max \cos \mu \\
\mu &= \sin^{-1}\left(\frac{1}{\mathcal{E}_\max P_2(\mathcal{E}_\max)}\right) \\
&= \sin^{-1}\left(\frac{2\sqrt{xy(x^2y^2 + z^2)}}{c^{3/2} \mathcal{E}_\max}\right)
\end{align*}$$

which allow us to determine the parameters $x,y$ that define $\Pi_2$. $\mu$ is well defined by virtue of the inequality, $P_2(\mathcal{E}_\max) \geq 1/\mathcal{E}_\max$. Note that unlike with the other measures, the state itself can be reconstructed up to LO.

Two extreme cases occur when $\mathcal{E}_{cusp} = 0$ and $\mathcal{E}_{cusp} = \mathcal{E}_\max$. In the first case, the PDF is a step function, terminating at some $\mathcal{E}_\max$. In the second case, the density increases monotonically, diverging at $\mathcal{E}_\max$ (FIG. 1). The relative abundance of entangled states is more in the latter case. One may per se expect that the associated concurrence should also be larger. Interestingly, however, the concurrence is related to the new parameters by $\mathcal{C} = (\mathcal{E}_\max - \mathcal{E}_{cusp})/2$, vanishing when $\mathcal{E}_{cusp} = \mathcal{E}_\max$. In other words, it is not sensitive to the relative abundance at zero (or small entanglements) at all. In any case, $\mathcal{C}$ emerges as a particular benchmark of the probability density, characterizing it only partially. We note that if $\rho = \Pi_3$, or $\Pi_4$, then its concurrence is zero. By the convexity of the concurrence, we conclude that the

FIG. 1: Some Typical probability density functions for $\Pi_2$. Note the solid curve, which shows all the features of $P_2(\mathcal{E})$. It has a cusp at $\mathcal{E}_{cusp} = 0.8$ and goes to zero at $\mathcal{E}_\max = 0.89$. The step function is an extreme example, where $\mathcal{E}_{cusp} = 0$, and the other dotted curve, has $\mathcal{E}_{cusp} = \mathcal{E}_\max = 1$.
concurrency $C_\rho$ is bounded by

$$C_\rho \leq (\lambda_1 - \lambda_2)C_{\Pi_1} + (\lambda_2 - \lambda_3)C_{\Pi_2}.$$  

Incidentally, the entanglement distribution of a subspace $\Pi_2$ orthogonal to $\Pi_2$ is the same as that of $\Pi_2$.

**Three dimensional projection:** We now move on to the case $\rho = \Pi_3$, whose PDF has a simpler structure. $\Pi_3$ is completely characterised by its dual, $|\xi\rangle \perp \Pi_3$. Thus, the PDF is characterised by a single parameter $E_{\perp}$, which is the entanglement of the orthogonal state $|\xi\rangle$.

The integrating measure \[16\] may be conveniently written as $dH_3 = \sin 2\beta \sin 2\phi \sin^2 \theta d\alpha d\beta d\gamma d\theta$, when the state is expanded in an orthonormal basis as: $|\psi\rangle = \cos \theta |\chi_1\rangle + e^{i(\alpha+\gamma)} \sin \theta \cos \beta |\chi_2\rangle - e^{i(\alpha-\gamma)} \sin \theta \sin \beta |\chi_3\rangle$, with the integration ranges, $\theta, \beta \in [0, \frac{\pi}{2}]$ and $\alpha, \gamma \in [0, \pi]$. Conveniently, one may choose $\chi_{1,2}$ to be separable, and by a suitable LO, they can be brought to the form $|\uparrow\rangle, |\downarrow\rangle$. We have verified that the resulting probability density can be cast into the simple form

$$P_3(E) = \frac{2E}{\sqrt{1 - E^2}} \cosh^{-1} \left( \frac{1}{E} \right).$$ \hspace{1cm} (7)

where $E_{>} = \max(E, E_{\perp})$.

A typical curve for $P_3(E)$ is shown in FIG. 2, which exhibits the required characteristic. The curve possesses a discontinuity in its derivative at $E_{\perp}$. Significantly, concurrency (being identically zero) fails to distinguish different three dimensional projections, e.g., $E_{\perp} = 0$ or 1, although their PDFs are vastly different.

Lastly, we consider the full space $\Pi_4$, whose PDF is universal. This curve is obtained by using the Haar measure on $SU(4)$ \[17\]. Note that the curve is smooth everywhere, as shown in FIG. 4.

It remains to consider the case when $\rho$ is an incoherent sum of the projections (see Eqn.3), where the weights have been chosen such that the special cases $\rho = \Pi$ are naturally recovered; they also ensure that the results are not artefacts of any basis. If $||\rho_1 - \rho_2||$ is small, the corresponding probability density functions will also be close to each other.

**FIG. 2:** A Typical probability density for $\Pi_3$. Note the point of discontinuity in the derivative at $E = E_{\perp}$.

**FIG. 3:** The probability density $P_4(E)$ for the entire Hilbert space.

**FIG. 4:** The overall probability density $P_4(E)$ for a typical mixed state, $\rho$, with eigenvalues $\{0.385, 0.288, 0.231, 0.096\}$. Note that the features of the individual subspaces are vividly preserved.

FIG. 4 illustrates the PDF for this general case. The important point to be noted is that the superposition of curves does not obliterate the information contained in individual curves; they are retained as points of discontinuity or singularity and each individual PDF may be reconstructed, together with the associated weights. $P(E)$ is by definition invariant under LO. With this, one may ask if the state itself may be reconstructed, up to LO. Before we take up this question, we consider an important application of this prescription, to NMR QC.
NMR QC employs the so called pseudopure states for computation. Since it is experimentally demonstrated that the quantum logic operations used in QC are implementable with NMR, it follows that these states should possess a non vanishing entanglement. Indeed, they have the form $\rho_{\text{pps}} = \frac{1}{2} (1 + \epsilon |\psi\rangle \langle \psi|)$, in our system of expansion. The NMR signal is sensitive only to the pure component, the so called deviation matrix. Accordingly, its $P(\rho,E)$ is given by a weighted Dirac Delta superposed on the PDF coming from the full space. The uniform background is invariant under unitary operations, but the one dimensional fluctuation is not, allowing for non-trivial gate operations. Thus NMR QC exploits the excess of entangled states over the unpolarized background as a resource, and this feature is correctly captured by the PDF of the state. This is in contrast to other measures which attribute a zero entanglement to all PPS with $\epsilon \leq \frac{1}{2}$, while usually in practice in NMR QC $\epsilon \sim 10^{-6}$. This analysis also raises the interesting possibility of QC with more general pseudo projection states.

Lastly, we return to the issue of the reconstructibility of the state (up to LO). If $\rho$ is a projection, the reconstructibility is assured, by construction. When $\rho$ is more general, the reconstruction is partial. For, the action of $SU(2) \times SU(2)$ on $\rho$ produces an orbit of dimension six, characterised by nine invariants. The set of parameters which characterize the entanglement are seven in number (for example: $\{\mu_1, \mu_2, \mu_3, \xi_1, \xi_{\text{cusp}}, \xi_{\text{max}}, \xi_{\text{L}}\}$). Geometrically, $P(\rho,E)$ is invariant under independent LO, $L_i$, acting on the subspaces $\Pi_i$, where $\Pi_i \subset \Pi_{i+1}$. If $\rho$ is to be unique up to a global LO, one needs the additional constraint $L_i = U L_i^{(0)}$, where $L_i^{(0)}$ may be chosen freely. Let us choose $L_2^{(0)} = 1$ (where 1 is the identity operator). The nestedness condition, viz., that $|\psi_1\rangle \in \Pi_2$ and $|\psi_4\rangle \in \Pi_2^c$ entails that $L_1^{(0)}$ and $L_3^{(0)}$ are specified by two parameters each [18].

More explicitly, if we have $\Pi_2$ in the canonical form, it is spanned by $|\chi_1\rangle$ and $|\chi_2\rangle$ given respectively as: $(1,0,0,0)$ and $(0,x,y,z)$. Therefore, we can specify $|\psi_1\rangle = |\chi_1\rangle \cos \frac{\theta}{2} e^{-i\phi/2} + |\chi_2\rangle \sin \frac{\theta}{2} e^{i\phi/2}$ by giving the values of $(\theta, \phi)$. Similarly, $|\psi_4\rangle$ can be specified by $(\theta_1, \phi_1)$ when it is expanded in the canonical basis of $\Pi_2^c = (1 - \Pi_2)$, given by $|\chi_1^c\rangle = (0,0,\sqrt{c^2 + b^2}, -b\sqrt{c^2 + b^2})$ and $|\chi_2^c\rangle = (0,\sqrt{c^2 + b^2}, ab\sqrt{c^2 + b^2}, ac\sqrt{c^2 + b^2})$.

In conclusion, we have given a prescription that describes the entanglement of mixed states by not just a number, but an exhaustive set of parameters which characterize the manner in which the entanglement is distributed over the ensemble. They further permit an almost complete reconstruction of the state up to LO. The prescription may provide a better insight into other measures of entanglement such as entanglement of distillation and entanglement cost. Investigations along these lines, and a further study of the PDFs for higher spins may provide us with a better appreciation of quantum entanglement.