Negativity vs entropy in entanglement witnessing

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In this work, we prove that while all measures of mixedness can be used to witness entanglement, no measure of mixedness is more sensitive than the negativity of the partial transpose. However, computing either the negativity or differences between von Neumann entropies to witness entanglement requires complete knowledge of the joint density matrix (and is therefore not practical at high dimension). In light of this, we examine joint vs marginal purities as a witness of entanglement, (which can be obtained directly through interference measurements) and find that comparing purities is actually more sensitive at witnessing entanglement than using von Neumann entropies while also providing tight upper and lower bounds to it in the high-entanglement limit.

I. INTRODUCTION

Quantum entanglement is the principal resource consumed in many applications of quantum information such as quantum computing, communication, and enhanced quantum metrology. Understanding its fundamental nature goes hand in hand with developing adequate techniques to fully characterize it in the exceptionally high-dimensional systems being employed today, such as quantum computations on 53-qubit states [1], or in pairs of particles entangled in high-dimensional degrees of freedom [2].

In this article, we use the quantum Renyi entropy of order \( \alpha \) to look at measures of mixedness as a hallmark of quantum entanglement. In doing this, we find that the von Neumann entropy (i.e., Renyi for \( \alpha = 1 \)) is both less sensitive and requires more resources to witness entanglement than measuring the state purity (a function of the Renyi entropy for \( \alpha = 2 \)). Moreover, the state purity can be used to bound the value of the von Neumann entropy, which is more valuable in quantum information. Along the way, we discover that when there are no resource limitations to determining the full quantum state, the negativity of the partial transpose \( N \) supersedes all measures of mixedness at witnessing entanglement.

II. FOUNDATION: ENTANGLEMENT FROM MIXEDNESS AND MAJORIZATION

In classical probability, joint distributions are never less mixed than the marginal distributions obtained from them [3]. In the language of Shannon entropy, the joint entropy is never less than the marginal entropy; two random variables never take less information to communicate than one. However, this need not be the case when comparing the mixedness of joint and marginal quantum states.

To quantify the mixedness of quantum states, we measure the mixedness of the probability distribution generated by the eigenvalues of the density matrix. This is the least mixed ensemble of pure states that can constitute the state being measured. What makes quantum states special is that it is possible for the joint state of two parties \( AB \) to be less mixed than the marginal state of either \( A \) or \( B \). For example, \( AB \) can be in a pure quantum state such as a Bell state, while the reduced states of \( A \) and \( B \) are both maximally mixed. This can only happen however, if the joint state is entangled [4]. Indeed, it was proven in [4] that given a separable state, the joint density matrix of \( AB \) cannot be less mixed than either that of \( A \) or \( B \) because the probability eigenvalues of \( AB \) are majorized by those of both \( A \) and \( B \). This is known as the majorization criterion of separability.

Majorization is a relation between two probability distributions (or density matrices) in which one can be obtained from the other through a series of mixing operations. Given two density matrices \( \hat{\rho} \) and \( \hat{\sigma} \), we say that \( \hat{\rho} \) majorizes \( \hat{\sigma} \) (denoted \( \hat{\rho} \succ \hat{\sigma} \)) when the sum of the \( n \) largest eigenvalues of \( \hat{\rho} \) is greater than or equal to the sum of the \( n \) largest eigenvalues of \( \hat{\sigma} \) for all \( n \). When \( \hat{\rho} \succ \hat{\sigma} \), there exists a series of Robin-Hood [5] mixing operations that will convert \( \hat{\rho} \) into \( \hat{\sigma} \), but not the other way around. Although measures of mixedness are well-defined functions over all density matrices, it is possible (and common) for two density matrices to be incomparable with respect to each other (i.e., where neither density matrix majorizes the other). This begs the question whether there are states whose entanglement cannot be witnessed by comparing one measure of mixedness, but can by another, motivating this study.

III. QUANTUM STATE PURITY AS A SUPERIOR ENTANGLEMENT WITNESS TO VON NEUMANN ENTROPY

In this section, we examine measures of mixedness based on the second-order moment of the density matrix (i.e., \( \text{Tr}[\hat{\rho}^2] \)), in comparison to the von Neumann entropy given as \( -\text{Tr}[\hat{\rho}\ln(\hat{\rho})] \). In particular, we show how comparing the joint and marginal state purities is generally more sensitive at witnessing entanglement than comparing joint and marginal von Neumann entropies,

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FIG. 1: (Left to right) Scatter plots and respective purity histograms for $10^6$ 2-quDit systems for $D = \{2, 3, 5, 10\}$ and normalizing exponents $\{3, 4, 6, 9\}$, respectively. For each state, the second-order conditional entropy $S_2(A|B)$ is plotted against the first-order conditional entropy $S_1(A|B)$. The red dotted line is where $S_1(A|B) = S_2(A|B)$, and all points in the lower right quadrant are states whose entanglement is witnessed by $S_2(A|B) < 0$, but not by $S_1(A|B) < 0$. (Bottom) This table gives the percentages of the total number of generated states whose entanglement was witnessed with the entropy function (and the negativity $N$) in the first column. Here, we measured the percentages both by sampling the eigenvalues uniformly on the probability simplex, and on the redistributed set of eigenvalues obtained by raising them by the normalizing exponent and renormalizing.

A. Monte Carlo simulations of random density matrices

In order to compare the effectiveness of comparing von Neumann entropies to comparing state purities as witnesses of entanglement, we performed Monte-Carlo simulations on 1 million 2-quDit systems, for $D = \{2, 3, 5, 10\}$. The fair sampling of random density matrices is accomplished by the algorithm in [8, 9] to generate an ensemble of eigenvalues uniform on the probability simplex (given by the set of vectors $\vec{\lambda}$ such that $\{\lambda_i\} \geq 0$ and $\sum \lambda_i = 1$). Although uniform on the simplex, this ensemble is biased against pure states at high dimension simply because the fraction of the total hypervolume occupied by states near the corner vertices (representing nearly pure states) decreases exponentially with dimension [10]. In order to better cover the full range of values that the quantum entropy can take, we created a second ensemble by raising the generated probability eigenvalues to a fixed power (dependent on dimension) and renormalizing to produce a different set of eigenvalues less biased against pure states. Once we have both ensembles of randomly sampled diagonal density matrices, we rotate them by taking randomly selected unitary transformations uniform according to the Haar ensemble. This distribution

\begin{align}
S_\alpha(A) &= S_\alpha(\hat{\rho}_A) = \frac{1}{1-\alpha} \log \left( \mathrm{Tr}[\hat{\rho}_A^\alpha] \right), \quad (1) \\
\lim_{\alpha \to 1} S_\alpha(A) &= S_1(A) \equiv -\mathrm{Tr}[\hat{\rho}_A \log(\hat{\rho}_A)], \quad (2) \\
\lim_{\alpha \to \infty} S_\alpha(A) &= S_\infty(A) = -\log \left( \max_i \{\lambda_{Ai}\} \right), \quad (3) \\
S_\alpha(A|B) &= S_\alpha(AB) - S_\alpha(B). \quad (4)
\end{align}

Here we see that $S_1(A)$ is the von Neumann entropy of system $A$, and $S_2(A)$ is a monotonically decreasing function of $\mathrm{Tr}[\hat{\rho}_A^2]$ known as the quantum collision entropy. Ironically, $S_\infty(A)$ is known as the min-entropy. We define the Renyi conditional entropy $S_\alpha(A|B)$ for convenience. Whenever $S_\alpha(A|B)$ is negative, the joint state of $AB$ is less mixed than the marginal state of $B$, witnessing entanglement.
of unitary transformations is uniform in that the ensemble remains invariant under any additional unitary transformation. In the table at the bottom of Fig. 1 we show that the percentages of randomly generated states whose entanglement is witnessed, either by different measures of mixedness or by the negativity of the partial transpose $N$, increase when renormalized and dramatically so at higher dimension.

In Fig. 1, we show scatter plots of the von Neumann conditional entropy $S_1(A|B)$ vs the second-order Renyi conditional entropy $S_2(A|B)$. In all situations, we find that there are substantially more states where $S_2(A|B) < 0$ but $S_1(A|B) > 0$ instead of the other way around. From this, we see that for most states, comparing purities will be a more sensitive witness of entanglement than comparing von Neumann entropies. Moreover, the fraction of states whose entanglement is witnessed by von Neumann entropy but not by purity relative to the opposite case appears to shrink, possibly towards zero at high dimension (see last scatter plot in Fig. 1). However, it is worth pointing out that the number of randomly generated states required to fill the state space to a given average density increases exponentially with dimension, which makes the scatter plots more diffuse at higher dimension for a constant number of points.

B. Side note: Increased sensitivity when using higher-order moments

Using higher-order moments of the density matrix may yield more sensitive entanglement witnesses than the purity, but at the expense of becoming progressively more difficult to obtain directly from experiment. In particular, the direct measurement of $\text{Tr}[^p] \rho^n$ requires interfering $n$ copies of the state $\hat{\rho}$, which becomes impractical as $n$ grows large.

That said, it is straightforward to show that for all states with maximally mixed marginal systems, every state whose entanglement is witnessed by $S_\alpha(A|B) < 0$ must have its entanglement witnessed with any entropy of higher order $\alpha' > \alpha$. This comes from the fact that the Renyi entropy of order $\alpha$ is a monotonically decreasing function of $\alpha$.

As a particularly striking example of how sensitive these higher-order entropies can be, we consider the case of the $N \otimes 1$ Werner state, which is a mixture of the Bell state $|\Phi\rangle \langle \Phi|$ and the maximally mixed state:

$$\rho^{(Werner)}_{AB} = p|\Phi\rangle \langle \Phi| + (1 - p) \frac{1}{N^2}, \quad (5)$$

$$|\Phi\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^N |i\rangle |i\rangle. \quad (6)$$

The probability eigenvalue vectors for the Werner state are:

$$\vec{\lambda}(AB) = \left( p + \frac{1-p}{N^2}, \frac{1-p}{N^2}, \ldots, \frac{1-p}{N^2} \right), \quad (7)$$

$$\vec{\lambda}(A) = \vec{\lambda}(B) = \left( \frac{1}{N}, \ldots, \frac{1}{N} \right). \quad (8)$$

The entanglement of the Werner state is witnessed whenever $S_\alpha(A|B) < 0$. For constant $p$, $S_\alpha(A|B)$ decreases as $\alpha$ increases; and for constant $\alpha$, $S_\alpha(A|B)$ decreases as $p$ increases. To keep the value of $S_\alpha(A|B)$ constant at increasing $\alpha$, there must be a corresponding decrease in $p$. The threshold Bell state fraction $p$ for which $S_\alpha(A|B) = 0$ must also decrease as $\alpha$ increases.

Clearly for Werner states, higher-order Renyi entropies make for more sensitive witnesses of entanglement than lower-order. Indeed, if one uses $S_1(A|B)$, one finds that the threshold value of $p$, $(p_c)$, does not scale favorably at high dimension $N$. Instead, $p_c$ asymptotically approaches $1/2$ as $N \to \infty$. On the other hand, using $S_2(A|B)$ scales more favorably, and has an analytic value of $p_c = 1/\sqrt{N+1}$, decreasing toward zero for large dimension. Going beyond second order, using $S_\alpha(A|B)$ scales better still, with an analytic value of $p_c = 1/(N+1)$, a quadratic improvement over the collision entropy. Even here, the favorability of the scaling is understated. Recall that the 53-qubit state has dimension of $2^{53} \approx 9.0 \times 10^{15}$, and a Werner state of such a dimension can still have its entanglement witnessed by comparing purities for any Bell state fraction greater than $1.05 \times 10^{-8}$.

IV. THE SUPREMACY OF THE NEGATIVITY

In 1998, the Horodeckis [11] showed that all states with a positive partial transpose are undistillable, being either separable or bound-entangled [12]. In 2003, Tohya Hiroshima proved [13] that if a joint state $\hat{\rho}_{AB}$ is undistillable, then it must satisfy the majorization criterion. Together, this proves that all states with a positive partial transpose satisfy the majorization criterion. Therefore, any state violating the majorization criterion must have a negative partial transpose (NPT). In this way, we see that by computing the negativity (a measure sensitive to NPT states), the entanglement present will be witnessed in at least all states that might have otherwise been witnessed by comparing measures of mixedness. That does not mean however, that comparing measures of mixedness is obsolete.

Although the negativity is a tractable measure of entanglement (not suffering the NP-hardness [14] of faithful entanglement measures) the difficulty in reconstructing a density matrix from experimental data becomes intractable at high dimension due to the sheer number of elements that a density matrix may contain. Although tomography is not too challenging for a state made of one or two qubits, the number of elements to be determined increases exponentially with the number of qubits. Indeed,
a 53-qubit state (realizable on state-of-the-art quantum computing experiments [1]) has a total of $4.06 \times 10^{31}$ density matrix elements, a number so large that it is intractable to store, let alone compute with. In particular, $4.06 \times 10^{31}$ bits is over ten billion zettabytes, exceeding the world’s estimated data storage capacity by approximately nine orders of magnitude [15].

V. CONCLUSION: MERITS OF DIFFERENT ENTANGLEMENT WITNESSES

In our investigations, we examined how well comparing the mixedness of a joint quantum state to the mixedness of its subsystems witnesses entanglement. While the von Neumann entropy is a popular measure of mixedness, we find that even comparing the joint and marginal purities (i.e., $\text{Tr}[\hat{\rho}^2]$ as measured by second-order Renyi entropy) witnesses entanglement in more quantum states than when using the von Neumann entropy. This is good news, as there exist direct measurements of $\text{Tr}[\hat{\rho}^2]$ by interfering two copies of a quantum state [6, 16], so that full state tomography is unnecessary. In addition, straightforward upper and lower bounds exist for the von Neumann entropies given a constant state purity. The maximum entropy distribution for constant purity is uniform except for one outcome, while the corresponding minimum entropy distribution is a discrete top-hat distribution with one non-uniform nonzero outcome (see [17] for details). When full state tomography is possible, however, computing the negativity of the partial transpose is more sensitive than comparing any measure of mixedness.

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