and (c) $E(\text{Bell states}) = 1$.

C2. For any state $\rho$ and any local unitary transformation, i.e., a unitary transformation of the form $U_A \otimes U_B$, the entanglement remains unchanged.

C3. Local operations, classical communication and postselection cannot increase the expectation value of the entanglement.

C4. Entanglement is convex under discarding information: $\sum_i p_i E(\rho_i) \geq E(\sum p_i \rho_i)$. The entanglement quantities chosen by us satisfy the properties C1–C4. Here, we do not impose the condition that any good entanglement measure should reduce to the entropy of entanglement (to be defined in the following) for pure states.

### A. Entanglement of formation and entanglement cost

The first measure we shall consider is the entanglement of formation $E_F$ [5]; it quantifies the amount of entanglement necessary to create the entangled state. It is defined by

$$E_F(\rho) \equiv \min_{\{p_i, \rho_i\}} \sum_i p_i E(\rho_i\rho_i^D),$$

(2.1)

where the minimization is taken over those probabilities $\{p_i\}$ and pure states $\{\rho_i\}$ that, taken together, reproduce the density matrix $\rho = \sum_i p_i \rho_i \rho_i^D$. Furthermore, the quantity $E(\rho_i\rho_i^D)$ (usually called the entropy of entanglement) measures the entanglement of the pure state $\rho_i$ and is defined to be the von Neumann entropy of the reduced density matrix $\rho_i^D \equiv \text{Tr}_B \rho_i \rho_i^D$, i.e.,

$$E(\rho_i \rho_i^D) = -\text{Tr} \rho_i^{(A)} \log \rho_i^{(A)}.$$  

(2.2)

For two-qubit systems, $E_F$ can be expressed explicitly as [6]

$$E_F(\rho) = h \left( \frac{1}{2} \left[ 1 + \sqrt{1 - C(\rho)^2} \right] \right),$$

$$h(x) \equiv -x \log_2 x - (1-x) \log_2 (1-x),$$

(2.3a, 2.3b)

where $C(\rho)$, the concurrence of the state $\rho$, is defined as

$$C(\rho) \equiv \max \{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4} \},$$

(2.3c)

in which $\lambda_1, \ldots, \lambda_4$ are the eigenvalues of the matrix $\rho(\sigma_y \otimes \sigma_z) \rho^* (\sigma_y \otimes \sigma_z)$ in increasing order and $\sigma_y$ is a Pauli spin matrix. $E_F(\rho)$, $C(\rho)$, and the tangle $\tau(\rho) \equiv C(\rho)^2$ are equivalent measures of entanglement, inasmuch as they are monotonic functions of one another.

A measure associated with the entanglement of formation is the entanglement cost $E_C$ [9] which is defined via

$$E_C(\rho) \equiv \lim_{n \to \infty} \frac{E_F(\rho^{\otimes n})}{n}.$$  

(2.4)

This is the asymptotic value of the average entanglement of formation. $E_C$ is, in general, difficult to calculate.

### B. Entanglement of distillation and relative entropy of entanglement

Related to the entanglement of formation is the entanglement of distillation $E_D$ [7], which characterizes the amount of entanglement of a state $\rho$ as the fraction of Bell states that can be distilled using the optimal purification procedure: $E_D(\rho) \equiv \lim_{n\to\infty} m/n$, where $n$ is the number of copies of $\rho$ used and $m$ is the maximal number of Bell states that can be distilled from them. The difference $E_F - E_D$ can be regarded as the "distillable entanglement." $E_D$ is a difficult quantity to calculate, but the relative entropy of entanglement $E_R$ [8], which we shall define shortly, provides an upper bound on $E_D$ and is more readily calculable than it. For this reason, it is the second measure that we consider in this paper. It is defined variationally via

$$E_R(\rho) \equiv \min_{\sigma \in D} \text{Tr} \rho \log \rho - \rho \log \sigma,$$  

(2.5)

where $D$ represents the (convex) set of all separable density operators $\sigma$. In certain ways, the relative entropy of entanglement can be viewed as a distance $D(\rho\|\sigma^\ast)$ from the entangled state $\rho$ to the closest separable state $\sigma^\ast$. We remark that for pure states of two-qubit systems the relative entropy has the same value as the entanglement of formation.

### C. Negativity

The third measure that we shall consider is the negativity. The concept of the negativity of a state is closely related to the well-known Peres-Horodecki condition for the separability of a state [21]. If a state is separable (i.e., not entangled) then the partial transpose of its density matrix is again a valid state, i.e., it is positive semi-definite. It turns out that the partial transpose of a non-separable state has one or more negative eigenvalues. The negativity of a state $[9]$ indicates the extent to which a state violates the positive partial transpose separability criteria. We will adopt the definition of negativity as twice the absolute value of the sum of the negative eigenvalues:

$$N(\rho) \equiv 2 \max (0, -\lambda_{\text{neg}}),$$  

(2.6)

where $\lambda_{\text{neg}}$ is the sum of the negative eigenvalues of $\rho^T_B$. In $C^2 \otimes C^2$ (i.e., two-qubit) systems it can be shown that the partial transpose of the density matrix can have at most one negative eigenvalue (see App. A). It was proved by Vidal and Werner [10] that negativity is an entanglement monotone, i.e., it satisfies criteria C1–C4 and, hence, is a good entanglement measure. We remark that for two-qubit pure states the negativity gives the same value as the concurrence does.
D. Bures metric

The Bures metric of entanglement is defined as

$$E_B(\rho) \equiv \min_{\sigma \in D} \left( 2 - 2\sqrt{F(\rho, \sigma)} \right),$$ (2.7)

where $F(\rho, \sigma) \equiv (\text{Tr} \sqrt{\sqrt{\sigma} \rho \sqrt{\sigma}})^2$ is the fidelity. In the same way that relative entropy can, this entanglement measure can be viewed as the distance from the closest separable state to the entangled state considered, where the distance is now defined by $D(\rho \| \sigma) \equiv (2 - 2\sqrt{F(\rho, \sigma)})$ [18]. We remark that for two-qubit pure states the Bures metric reduces to the tangle defined in Sec. II A.

E. Lewenstein-Sanpera entanglement

It was shown by Lewenstein and Sanpera [23] that any density matrix $\rho$ has a decomposition into two parts:

$$\rho = \lambda \rho_s + (1 - \lambda) \rho_e, \quad (2.8)$$

where $\rho_s$ is separable, $\rho_e$ is entangled, and the weight $\lambda$ is maximal, in which case the decomposition is unique. They refer to $\rho_s$ as the best separable approximation (BSA) to $\rho$. It should be pointed out that, in general, it is not trivial to establish the decomposition, even in the simplest relevant setting of $C^2 \otimes C^2$ systems. Evidently, $\lambda$ and $\rho_e$ contain information about the entanglement of $\rho$. Kuras and Lewenstein [24] later showed that the quantity $E_{LS} \equiv (1 - \lambda)$, which we will call the LS entanglement, satisfies the above criteria, and hence is a good entanglement measure. For $C^2 \otimes C^2$ systems it turns out that $\rho_s$ is a pure state, i.e., $\vert \psi_e \rangle \langle \psi_e \vert$ and in this case it suggests that the quantity $E_{LS}$, defined via

$$E_{LS} \equiv (1 - \lambda) E(\vert \psi_e \rangle \langle \psi_e \vert), \quad (2.9)$$

may also be a good entanglement measure. We remark that for two qubit case the entanglement measure $\lambda$ is known to be equal to the Schmidt measure introduced in Ref. [25].

Even though the LS decomposition is not, in general, straightforward to find for the states in Eq. (4.5), the LS decomposition reads

$$\begin{pmatrix} x + \frac{r}{2} & 0 & 0 & \frac{r}{2} \\ 0 & a & 0 & 0 \\ 0 & 0 & b & 0 \\ \frac{r}{2} & 0 & 0 & y + \frac{r}{2} \end{pmatrix} = \begin{pmatrix} x + \sqrt{ab} & 0 & 0 & \sqrt{ab} \\ 0 & a & 0 & 0 \\ 0 & 0 & b & 0 \\ \sqrt{ab} & 0 & 0 & y + \sqrt{ab} \end{pmatrix} + (1 - \lambda) \rho_e, \quad (2.10)$$

where $\rho_e = \vert \phi^+ \rangle \langle \phi^+ \vert$ (with $\vert \phi^+ \rangle = (\vert 00 \rangle + \vert 11 \rangle) / \sqrt{2}$), $(1 - \lambda) = r - 2\sqrt{ab}$, and we consider only $r - 2\sqrt{ab} \geq 0$ (as for $r - 2\sqrt{ab} \leq 0$ the whole density matrix is separable).

If we compute the concurrence of the state in Eq. (4.5), we find $C \equiv \max \{0, r - 2\sqrt{ab} \}$. It is interesting to note that the LS entanglement gives, for the Ansatz states in Eq. (4.5), the same value as the concurrence does; but for an arbitrary state this is not, in general, true [26].

F. Ordering difficulties with entanglement measures

We now pause to touch on certain difficulties posed by the task of ordering physical states using entanglement. As first discussed and explored numerically by Eisert and Plenio [15], and subsequently investigated analytically by Verstraete et al. [16], different entanglement measures can give different orderings for pairs of mixed states. This can be seen, e.g., from the plot of concurrence versus negativity, Fig. 1. The upper boundary is readily seen to be $N \leq C$ whereas the lower boundary can be derived, giving $N \geq \sqrt{2(C - \frac{1}{2})^2 + \frac{1}{4} + (C - 1)}$; see Ref. [16]. Hence, when we wish to explain maximally entangled mixed states we need to be very explicit about the measure of entanglement (and also mixedness; see the following section). Different measures are likely to lead to different classes of MEMS states.

We end this section by mentioning the three entanglement measures that we shall use to compute the entanglement-mixedness frontiers: entanglement of formation, negativity, and relative entropy of entanglement. The first two of these are straightforward to compute, at least in two-qubit settings. For the third, certain results are available [14, 18] that ease the computation of MEMS. We have also reviewed four additional measures (entanglement cost, entanglement of distillation, LS entanglement, and the Bures metric). Of these, however, the first two are rather difficult to compute, let alone maximize; the third is also difficult to compute, at least in practice. As for the fourth, calculating the entanglement involves finding the closest separable states (as is required for the case of relative entropy).
III. MEASURES OF MIXEDNESS

The von Neumann entropy occurs when a system can be completely entangled. The two most frequently used measures of randomness or “chaos” are the von Neumann entropy, which is introduced in the previous section, and the Shannon entropy. These two entropies are related to the von Neumann entropy and the Shannon entropy, respectively.

A. von Neumann entropy

\[ S_N = \sum_k p_k \log_2 \frac{1}{p_k} \]

where \( p_k \) is the probability of finding the system in state \( k \). The von Neumann entropy is defined as the entropy of the density matrix, which is the weighted average of the von Neumann entropies of the individual states.

B. Mutual information

\[ I(X;Y) = H(X,Y) - H(X) - H(Y) \]

where \( H(X) \) is the entropy of the system and \( H(X,Y) \) is the entropy of the joint distribution.

C. Entanglement entropy

\[ S_E = \sum_k p_k S_k \]

where \( S_k \) is the entropy of the system in state \( k \). The entanglement entropy is defined as the weighted average of the entropies of the subsystems.

D. Relative entropy

\[ D(\rho || \sigma) = \text{Tr} \left( \rho \log_2 \rho - \rho \log_2 \sigma \right) \]

where \( \rho \) and \( \sigma \) are density matrices. The relative entropy is defined as the difference between the von Neumann entropies of the system and the subsystem, respectively.

E. Fuzzy set theory

\[ S_F = \sum_i p_i \log_2 \frac{1}{p_i} \]

where \( p_i \) is the membership function of the fuzzy set. The fuzzy set entropy is defined as the weighted average of the fuzzy set entropies of the individual states.

F. Quantum mutual information

\[ I_Q(X;Y) = S(X) + S(Y) - S(X,Y) \]

where \( S(X) \), \( S(Y) \), and \( S(X,Y) \) are the von Neumann entropies of the individual states, respectively. The quantum mutual information is defined as the sum of the von Neumann entropies of the individual states minus the von Neumann entropy of the joint distribution.

G. Quantum relative entropy

\[ D_Q(\rho || \sigma) = \text{Tr} \left( \rho \log_2 \rho - \rho \log_2 \sigma \right) \]

where \( \rho \) and \( \sigma \) are density matrices. The quantum relative entropy is defined as the difference between the von Neumann entropies of the system and the subsystem, respectively.
solutions, when given in terms of eigenvalues, read
\[
\left\{ \frac{1-r}{4}, \frac{1-r}{4}, \frac{1-r}{4}, \frac{1+3r}{4} \right\}, \quad \text{for } 0 \leq r \leq 1, \quad (3.6a)
\]
\[
\left\{ r, 1-r, 0, 0 \right\}, \quad \text{for } \frac{1}{2} \leq r \leq 1, \quad (3.6b)
\]
\[
\left\{ \frac{1-r}{2}, \frac{1-r}{2}, 0 \right\}, \quad \text{for } 0 \leq r \leq \frac{1}{2}, \quad (3.6c)
\]
\[
\left\{ \frac{4-r}{12}, \frac{4-r}{12}, \frac{4-r}{12}, \frac{3r}{12} \right\}, \quad \text{for } 0 \leq r \leq 1, \quad (3.6d)
\]
and they correspond to the upper boundary, and the lowest, middle, and highest pieces of the lower boundary, respectively. Note that the lower boundary comprises three (in general, \( N - 1 \)) segments that meet at cusps. We remark, parenthetically, that the solutions with zero eigenvalues correspond to extrema within some subspace spanned by those eigenvectors with nonzero eigenvalues, and therefore only obey the stationarity condition (3.5) within the subspace.

Is there any significance to the boundary states? Boundary segment (a) includes the Werner states defined in Eq. (4.7). Boundary segment (b) includes the first branch of the MEMS for \( E_p \) and \( S_t \) specified below in Eq. (4.6). The segment (c) includes the states
\[
\rho_s = r|\phi^+\rangle\langle\phi^+| + \frac{1-r}{2}(|00\rangle\langle00|+|10\rangle\langle10|), \quad (3.7)
\]
States on segment (d) are all unentangled. Of course, the boundary segments include not only the specified states but also all states derivable from them by global unitary transformation.

As for the interior, we have obtained this numerically by constructing a large number of random sets of eigenvalues of legitimate density matrices, and computing for each the two entropies. As Fig. 2 shows, no points lie outside the boundary curve, providing confirmatory evidence for the forms given in Eq. (3.6).

The fact that the bounded region is two-dimensional indicates the lack of precision with which the linear entropy characterizes the von Neumann entropy (and vice versa, if one wishes). In particular, the figure reveals an ordering difficulty: pairs of states, \( A \) and \( B \), exist for which \( S_A^l = S_B^l \) and \( S_A^u - S_B^u \) differ in sign. Worse still, states having a common value of \( S_V \) have a continuum of values of \( S_t \), and vice versa.

IV. ENTANGLEMENT-VERSUS-MIXEDNESS FRONTIERS

We now attempt to identify regions in the plane spanned by entanglement and mixedness that are inhabited by physical states (i.e., characterized by legitimate density matrices). We shall consider the various measures of entanglement and mixedness discussed in the previous section. Of particular interest will be the structure of the states that inhabit the frontier, i.e., the boundary delimiting the region of physical states. Frontier states are maximal in the following sense: for a given value of mixedness they are maximally entangled; for a given value of entanglement they are maximally mixed.

A. Parametrization of maximal states

The aim of this subsection is to derive the general form of the maximal states given in Eq. (4.4), which is what we will use to parametrize maximal states. In Ref. [14], it is shown that, given a fixed set of eigenvalues, all states that maximize one of the three entanglement measures (entanglement of formation, negativity or relative entropy) automatically maximize the other two. It was further shown that the global unitary transformation that takes arbitrary states into maximal ones has the form
\[
U = (U_1 \otimes U_2) T D_{\Phi} \Phi^l, \quad (4.1)
\]
where \( U_1 \) and \( U_2 \) are arbitrary local unitary transformations,
\[
T \equiv \begin{pmatrix} 0 & 0 & 0 & 1 \\ \frac{\sqrt{r}}{2} & 0 & \frac{\sqrt{1-r}}{2} & 0 \\ \frac{\sqrt{r}}{2} & 0 & \frac{\sqrt{1-r}}{2} & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (4.2)
\]
\( D_{\Phi} \) is a unitary diagonal matrix, and \( \Phi \) is the unitary matrix that diagonalizes the density matrix \( \rho \), i.e., \( \rho = \Phi \Lambda \Phi^l \), where \( \Lambda \) is a diagonal matrix, the diagonal elements of which are the four eigenvalues of \( \rho \) listed in nonincreasing order \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \). Hence, the general form of a density matrix that is maximal, given a set of eigenvalues, is (up to local unitary transformations)
\[
T \begin{pmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & \lambda_4 \end{pmatrix} T^l = \begin{pmatrix} \lambda_4 & 0 & 0 & 0 \\ 0 & \frac{\lambda_4}{\lambda_1} & \frac{\lambda_4}{\lambda_2} & 0 \\ 0 & \frac{\lambda_4}{\lambda_1} & \frac{\lambda_4}{\lambda_2} & 0 \\ 0 & 0 & 0 & \lambda_2 \end{pmatrix} \quad (4.3)
\]
This matrix is locally equivalent to the form
\[
\begin{pmatrix} x + \frac{r}{2} & 0 & 0 & \frac{r}{2} \\ 0 & a & 0 & 0 \\ 0 & 0 & b & 0 \\ \frac{r}{2} & 0 & 0 & x + \frac{r}{2} \end{pmatrix}, \quad (4.4)
\]
with \( x + \frac{r}{2} = (\lambda_1 + \lambda_3)/2 \), \( r = \lambda_1 - \lambda_3 \), \( a = \lambda_2 \), and \( b = \lambda_4 \). The above derivation justifies the Ansatz form (4.5) used in Ref. [12] to derive the entanglement of formation vs. linear entropy MEMS. We remark that one may as well use the four eigenvalues \( \lambda_i \)'s as the parametrization. Nevertheless, the form (4.4), as well as (4.5), can be nicely viewed as a mixture of a Bell state \( |\phi^+\rangle \) with some diagonal separable mixed state.
B. Entanglement-versus-linear-entropy frontiers

We begin by measuring mixedness in terms of the linear entropy, and comparing the frontier states for various measures of entanglement.

1. Entanglement of formation

The characterization of physical states in terms of their entanglement of formation and linear entropy was introduced by Munro et al. in Ref. [12]. (Strictly speaking, they considered the tangle rather than the equivalent entanglement of formation.) Here, we shall consider yet another equivalent quantity: concurrence (see Sec. II A). In order to find the frontier, Munro et al. proposed Ansatz states of the form

$$\rho_{\text{Ansatz}} = \begin{pmatrix} 1 + \frac{r}{7} & 0 & 0 & \frac{r}{7} \\ 0 & a & 0 & 0 \\ 0 & 0 & b & 0 \\ \frac{r}{7} & 0 & 0 & 1 + \frac{r}{7} \end{pmatrix},$$

(4.5)

where $x, y, a, b, r \geq 0$ and $x + y + a + b + r = 1$. They found that, of these, the subset

$$\rho_{\text{MEMS,EP,SL}} = \begin{cases} \rho_{\text{f}}(r), & \text{for } \frac{2}{7} \leq r \leq 1; \\ \rho_{\text{m}}(r), & \text{for } 0 \leq r \leq \frac{2}{7}; \end{cases}$$

(4.6a)

lies on the boundary in the tangle vs. linear-entropy plane and, accordingly, named these MEMS, in the sense that these states have maximal tangle for a given linear entropy. We remark that at the crossing point of the two branches, $\bar{r}_n = 2/3$, the density matrices on either side coincide.

In Fig. 3 we plot the entanglement of formation/concurrence vs. linear entropy for the family of MEMS (4.6); this gives the frontier curve. For the sake of comparison, we also give the curve associated with the family of Werner states of the form

$$\rho_W \equiv r|\phi^+\rangle\langle\phi^+| + \frac{1 - r}{4} I = \begin{pmatrix} \frac{1 + r}{4} & 0 & 0 & \frac{r}{4} \\ 0 & \frac{1 + r}{4} & 0 & 0 \\ 0 & 0 & \frac{1 + r}{4} & 0 \\ \frac{r}{4} & 0 & 0 & \frac{1 - r}{4} \end{pmatrix}.$$  

(4.7)

Evidently, for a given value of linear entropy these MEMS (which we shall denote by $\{\text{MEMS: } \rho_F, \rho_{\text{SL}}\}$) achieve the highest concurrence. As the tangle $r$ and entanglement of formation $\rho_F$ are monotonic functions of the concurrence, Eq. (4.6) also gives the boundary curve for these measures. This raises an interesting question: Is (4.6) optimal for other measures of entanglement?

2. Relative entropy as the entanglement measure

To find the frontier states for the relative entropy of entanglement we again turn our attention to the maximal density matrix (4.4). For this form of density matrix the linear entropy is given (with $x$ expressed in terms of $a, b, r$) by

$$S_L = \frac{2}{3}(-3a^2 + 2a(1 - b) + (1 - b)(1 + 3b) - r^2).$$

(4.8)

To calculate the relative entropy of entanglement we need to determine the closest separable state to (4.4). It is simpler to do this analysis via several cases. We begin by considering the Rank-2 and Rank-3 cases of (4.4). We set $b = 0$ ($\lambda_2 = 0$) and express $x$ in terms of $a$ and $r$ in the density matrix, obtaining

$$\rho = \begin{pmatrix} \frac{1 + a}{4} & 0 & 0 & \frac{r}{4} \\ 0 & a & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{r}{4} & 0 & 0 & 1 - \frac{r}{4} \end{pmatrix}.$$  

(4.9)
and thus find that the closest separable density matrix \( \sigma^* \) is given by [18]

\[
\sigma^* = \begin{pmatrix}
C & 0 & 0 & D \\
0 & E & 0 & 0 \\
0 & 0 & 1-2C-E & 0 \\
D & 0 & 0 & C
\end{pmatrix},
\]

(4.10a)

\[
C \equiv \frac{(1+a)(1-a^2-r^2)}{2(1+a-r)(1+a+r)},
\]

(4.10b)

\[
D \equiv \frac{a(1+a)r}{(1+a-r)(1+a+r)},
\]

(4.10c)

\[
E \equiv \frac{a(1+a)^2}{(1+a-r)(1+a+r)}.
\]

(4.10d)

The relative entropy of entanglement is now simply given by

\[
E_R(\rho) = \text{Tr} \left( \rho \log \rho - \rho \log \sigma^* \right)
\]

\[
= \frac{1+a}{2} \log \frac{(1+a^2-r^2)}{(1+a)^2} + \frac{r}{2} \log \frac{1+a+r}{1+a-r},
\]

with the linear entropy being given by

\[
S_L = \frac{2}{3}(1+2a-3a^2-r^2),
\]

(4.11)

subject to the constraint \((a+r) \leq 1\) for the Rank-2 case \( a = 1-r \) \((b = x = 0)\), and the resulting solution is the Rank-2 matrix \( \rho_1(r) \) given in Eq. (4.6) with \( 1/2 \leq r \leq 1 \). We remark that this Rank-2 solution is always a candidate MEMS for the three entanglement measures that we consider in this paper. In order to determine whether or in what range the Rank-2 solution achieves the global maximum, we need to compare it with the Rank-3 and Rank-4 solutions.

By maximizing \( E_R(\rho) \) for a given value of \( S_L \), we find the following stationary condition:

\[
r \log \frac{(1+a)^2-r^2}{(1+a)^2} = (3a-1) \log \frac{1+a+r}{1+a-r}.
\]

(4.13)

Given a value of \( S_L \), we can solve Eqs. (4.12) and (4.13), at least numerically, to obtain the parameters \( a \) and \( r \), and hence, from Eq. (4.9), the Rank-3 MEMS. However, if the constraint inequality \( a+r \leq 1 \) turns out to be violated, the solution is invalid.

We now turn to the Rank-4 case. It is straightforward, if tedious, to show that the Werner states, Eq. (4.7), obey the stationarity conditions appropriate for Rank 4. However, it turns out that this solution is not maximal.

To summarize, the frontier states, which we denote by \{MEMS: \( E_R, S_L \)\}, are states of the form (4.9); the dependence of the parameters \( a \) and \( r \) on \( S_L \) is shown in Fig. 4. In Fig. 5, we show the resulting frontier, as well as curves corresponding to non-maximal stationary states. The frontier states have the following structure: (i) for \( S_L \leq 0.5054 \) they are the Rank-2 MEMS of Eq. (4.6) but with \( r \) restricted to the range from 1 (at \( S_L = 0 \)) to approximately 0.7459 (at \( S_L \approx 0.5054 \)); (ii) for \( S_L \geq 0.5054 \)

\[
\rho^* \approx \begin{pmatrix}
0.372947 & 0 & 0 & 0.372947 \\
0 & 0.254106 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0.372947 & 0 & 0 & 0.372947
\end{pmatrix},
\]

(4.14)

Just as in the case of entanglement of formation vs. linear entropy, the density matrix is continuous at the transition between branches.

We remark that the curve generated by the states \{MEMS: \( E_R, S_L \)\}, when plotted on the \( E_R \) vs. \( S_L \) plane, falls just slightly below that generated by the states \{MEMS: \( E_R, S_L \)\} for \( S_L \geq 0.5054 \) (and coincides for smaller values of \( S_L \)). We also remark that the parameter \( r \) turns out to be the concurrence \( C \) of the states, so
The function $f(x) = \frac{1}{1 + e^{-x}}$ is often used in the context of the softmax function in neural networks. In this context, $f(x)$ represents the probability of an event occurring, with $x$ being the input score. The softmax function is defined as:

$$f(x) = \frac{e^{x}}{\sum_{i=1}^{n} e^{x_{i}}}$$

where $n$ is the total number of classes. The softmax function is used to convert a vector of real numbers into a probability distribution.

The derivative of the softmax function is given by:

$$\frac{d}{dx} f(x) = f(x)(1 - f(x))$$

The function $f(x)$ is a sigmoid function, which is a type of activation function used in artificial neural networks. It is defined as:

$$f(x) = \frac{1}{1 + e^{-x}}$$

The sigmoid function maps any real-valued number to a value between 0 and 1, which is useful in the context of classification tasks.

In the context of linear regression, the softmax function can be used to make predictions in a multi-class classification problem. The softmax function is used to convert the outputs of the linear model into probabilities that sum up to 1 for each class.
C. Entanglement-versus-von-Neumann-entropy frontiers

We continue this section by choosing to measure mixedness in terms of the von Neumann entropy, and comparing the frontier states for various measures of entanglement.

1. Entanglement of formation

To find this frontier, we consider states of the form (4.4), and compute for them the concurrence and the von Neumann entropy:

\[ C = r - 2\sqrt{ab}, \]
\[ S_V = -a \log a - b \log b - x \log (x+r) \log (x+r). \]  

(4.20a)

(4.20b)

Note that the parameters obey the normalization constraint \(2a + a + b + r = 1\).

As we remarked previously, the Rank 2 MEMS is always a candidate. For the Rank-3 case, we can set \(b = 0\) in Eq. (4.20). By maximizing \(C\) at fixed \(S_V\), we find a stationary solution:

(i) \( r = C, \ x = \left(4-3C-\sqrt{4-3C^2}\right)/6, \) and \( a = \left(\sqrt{4-3C^2}-1\right)/3, \) the resulting density matrix is

\[
\rho_i = \begin{pmatrix}
\frac{4-\sqrt{4-3C^2}}{3} & 0 & C \\
0 & \frac{4-\sqrt{4-3C^2}}{3} & 0 \\
C & 0 & \frac{4-\sqrt{4-3C^2}}{3}
\end{pmatrix}
\]

(4.21)

For the Rank-4 case \((b \neq 0)\), the stationarity condition can be shown to be

\[ u \log(u) = u \log(u), \]
\[ 2u \log(u) = (u + w) \log(v). \]

(4.22a)

(4.22b)

where \( u \equiv \sqrt{a/(x+r)} \), \( v \equiv \sqrt{x/(x+r)} \), and \( w \equiv \sqrt{b/(x+r)} \). There are two solutions, due to the two-to-one property of the function \( z \log z \) for \( z \in (0,1] \). The first one is \((u = v = w)\).

(ii) \( a = b = x = (1-C)/6, \) and \( r = (1+2C)/3, \) which can readily be seen to be a Werner state as in Eq. (4.7) or, equivalently,

\[
\rho_{ii} = \begin{pmatrix}
\frac{4+C}{6} & 0 & 0 & \frac{1+2C}{3} \\
0 & \frac{1-C}{6} & 0 & 0 \\
0 & 0 & \frac{1-C}{6} & 0 \\
\frac{1+2C}{3} & 0 & 0 & \frac{2+C}{6}
\end{pmatrix}.
\]

(4.23)

Being the concurrence, \( C \) is restricted to the interval \([0,1]\). The second solution is transcendental, but can be solved numerically.

In Fig. 8 we compare the four possible candidate solutions, and find that the global maximum is composed of only (i) and (ii). We summarize the states at the frontier as follows:

\[
\rho_{\text{MEMS} E_{\pi}, S_V} = \begin{cases}
\rho_i, & \text{for } 0 \leq C \leq C^*; \\
\rho_r, & \text{for } C^* \leq C \leq 1.
\end{cases}
\]

(4.24)
The von Neumann entropy is given by $\text{Tr}(\rho \log_2 \rho)$, where $\rho$ is the density matrix. For the case of a pure state, $\rho = |\psi\rangle \langle \psi|$, the entropy reduces to $-\langle \log_2 |\psi\rangle \rangle$, where $\langle |\psi\rangle \rangle$ is the expectation value of the logarithm.

![Graph of von Neumann entropy vs. relative entropy]

The von Neumann entropy and the relative entropy are related by the inequality $\text{Tr}(\rho \log_2 \rho) - \text{Tr}(\rho \log_2 \rho) \geq H(\rho)$, where $H(\rho) = -\sum_i p_i \log p_i$ is the Shannon entropy of the probability distribution $p_i$.

The von Neumann entropy is a measure of the uncertainty in the state $\rho$. It quantifies the amount of information that is required to describe the state fully. The relative entropy, on the other hand, measures the distinguishability of two states $\rho$ and $\sigma$.

In the context of quantum information theory, the von Neumann entropy plays a central role. It is used to quantify the amount of information that can be extracted from a quantum system, and it is also used to define other important quantities such as the mutual information and the quantum channel capacity.

The von Neumann entropy of a quantum state $\rho$ is given by $H(\rho) = -\text{Tr}(\rho \log_2 \rho)$.

For a density matrix $\rho$ in a $d$-dimensional Hilbert space, the von Neumann entropy is $H(\rho) = -\sum_{i=1}^d p_i \log_2 p_i$, where $p_i$ are the eigenvalues of $\rho$ arranged in decreasing order.

The von Neumann entropy is a concave function of the density matrix, and it satisfies the data processing inequality: $H(\rho) \geq H(\rho')$ for any quantum channel $\mathcal{E}$. This inequality is analogous to the data processing inequality in classical information theory.

The von Neumann entropy is a useful tool for analyzing quantum systems, and it is used in a variety of applications, including quantum cryptography, quantum error correction, and quantum computing.

The von Neumann entropy is a fundamental concept in quantum information theory, and it is essential for understanding the behavior of quantum systems.

In conclusion, the von Neumann entropy is a powerful tool for quantifying the uncertainty in quantum states. It is a cornerstone of quantum information theory and has numerous applications in the field.
FIG. 11: Entanglement frontier: negativity vs. von Neumann entropy. The solid curve is the frontier. The broken curve represents the Rank-2 candidate states.

### 3. Negativity

We saw in Sec. IV B 3 that there is a pair of families of MEMS which differ in rank but give the identical frontier in the $N$ vs. $S_L$ plane. It is interesting to see what happens for the combination of negativity and von Neumann entropy.

Once again, we begin with states of form (4.4), for which the negativity and the von Neumann entropy are given in Eqs. (4.15) and (4.20b), respectively. By making $N$ stationary at fixed $S_Y$, we are able to find only one solution (in addition to the Rank-2 candidate): $a = b = x$. Expressing the resulting density matrix, as we may, in terms of the single parameter $r$, we arrive at the following candidate for the frontier states:

$$\rho_{MEMS:N,S_Y} = \begin{pmatrix} 1+r & 0 & 0 & r \\ 0 & 1-r & 0 & 0 \\ 0 & 0 & 1-r & 0 \\ r & 0 & 0 & 1-r \end{pmatrix},$$

where $0 \leq r \leq 1$, i.e., the Werner states.

The resulting frontier in the negativity vs. von Neumann-entropy plane is shown in Fig. 11 which, for comparison, also shows the curve for the Rank-2 candidate.

### V. CONCLUDING REMARKS

In this Paper we have determined families of maximally entangled mixed states (MEMS, i.e., frontier states, which possess the maximum amount of entanglement for a given degree of mixedness). These states may be useful in quantum information processing in the presence of noise, as they have the maximum amount of entanglement possible for a given mixedness. We considered various measures of entanglement (entanglement of formation, relative entropy, and negativity) and mixedness (linear entropy and von Neumann entropy).

We found that the form of the MEMS depends heavily on the measures used. Certain classes of frontier states (such as those arising with either entanglement of formation or relative entropy of entanglement vs. the von Neumann entropy) behave discontinuously at a specific point on the entanglement-mixedness frontier. Under most of the settings considered, we have been able to explicitly derive analytical forms for the frontier states.

For entanglement of formation and relative entropy-and for most values of mixedness, we have found that the Rank-2 and Rank-3 MEMS have more entanglement than Werner states do. On the other hand, at fixed entropy no states have higher negativity than Werner states do. At small amounts of mixedness, the $\{MEMS: E_F, S_L\}$ states “lose” entanglement with increasing mixedness at a substantially lower rate than do the Werner states. However, when the entanglement is measured by the relative entropy, the difference in loss rate is significantly smaller.

From Eq. (2.10) it is tempting to assert that in the case of LS entanglement vs. mixedness the frontier states should be the same as those in the case of entanglement of formation vs. mixedness. However, as we do not know whether Eq. (4.5) (up to local unitary transformations) exhausts all maximal states for LS entanglement, further investigation of this point is needed.

Having characterized the MEMS for various measures, it is worthwhile considering them from the perspective of Bell-inequality violations. To quantify the violation of
Bell’s inequality, it is useful to consider the quantity
\[ B = \max_{\sigma, \sigma', \tilde{\sigma}} \left\{ E(\tilde{\sigma}, \tilde{\sigma}) + E(\sigma, \tilde{\sigma}) + E(\sigma', \tilde{\sigma}) - E(\sigma', \sigma) \right\}, \]
where
\[ E(\sigma, \sigma') = \langle \sigma \cdot \tilde{\sigma}, \sigma' \rangle - (1 - r) \left( \langle \sigma \cdot \sigma' \rangle \right). \]
(5.1)

In Fig. 12, we plot \( B \) vs. linear and von Neumann entropies for several families of frontier states. As a comparison, we also draw the violation by the following Rank-2 state (which is diagonal in the Bell basis):
\[ \rho_m = r|\psi^+\rangle\langle \psi^+ | + (1 - r)|\psi^\tau\rangle\langle \psi^\tau |, \quad r \in [0, 1]. \]  
(5.2)

This state, although not belonging to any of the families of frontier states derived previously, turns out to achieve the maximum possible violation, as a function of linear entropy. On the other hand, the Werner states appear to achieve maximal violation in the case of von Neumann entropy. Eberert’s application of Bell’s inequalities to quantum cryptography [2], together with the discussions of the present paragraph, suggests that MEMS may be relevant to quantum communication.

Another natural application for which entanglement is known to be a critical resource is quantum teleportation. How do these frontier MEMS teleport, compared with the Werner and Rank-2 Bell diagonal states? If we restrict our attention to high purity situations (i.e., to states with only a small amount of mixedness) then it is straightforward to show that, e.g., \{MEMS: \( E_F, S_1 \}) states teleport average states better than the Werner states do, but worse than the Rank-2 Bell diagonal state does. Part of the explanation for this behavior is that standard teleportation is optimized for using Bell states as its core resource.

It is also interesting to note that for certain combinations of entanglement and mixedness measures, as well as the Bell inequality violation, the Rank-2 candidates fail to furnish MEMS. Thus, these states seem to be less useful than other MEMS. However, from the perspective of distillation, these states are exactly quasi-distillable [30, 31], and can be useful in the presence of noise because they can be easily distilled into Bell states.

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APPENDIX A: NUMBER OF NEGATIVE EIGENVALUES OF THE PARTIAL TRANSPOSE OF \( \rho \)

In this appendix we address the result that for \( C^2 \otimes C^2 \) systems the partial transpose of any density matrix \( \rho \) has at most one negative eigenvalue. In fact, we shall consider the result from two perspectives.

First, we build upon results (Theorem 3, in particular) contained in Ref. [31], from which it follows that it is sufficient to consider (i) Bell diagonal states and (ii) states of the form
\[
\begin{pmatrix}
  a + c & 0 & 0 & d \\
  0 & 0 & 0 & 0 \\
  0 & b - c & 0 & 0 \\
  d & 0 & 0 & a - b
\end{pmatrix}.
\]  
(A1)

For the latter case, straightforward calculation shows that the partially transposed matrix can have one negative eigenvalue when \( d \neq 0 \) and that it does not have negative eigenvalues when \( d = 0 \). For the former case, suppose that the Bell diagonal state has the four eigenvalues \( \lambda_1, \lambda_2, \lambda_3, \lambda_4 \), in nonincreasing order. Then it is straightforward to see that the corresponding partially transposed matrix has the four eigenvalues \( \lambda_1 + \lambda_2 + \lambda_3 - \lambda_4)/2, \ (\lambda_1 + \lambda_2 - \lambda_3 + \lambda_4)/2, \ (\lambda_1 - \lambda_2 + \lambda_3 + \lambda_4)/2, \ (\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4)/2 \). Thus, it can have at most two negative eigenvalue.

A second perspective is provided by first invoking the LS decomposition (2.8) and then making a Schmidt decomposition, via the local unitary transformation \( U_A \otimes U_B \) of the pure entangled part \( | \psi_\tau \rangle \). In this way, the pure part becomes
\[
U_A \otimes U_B | \psi_\tau \rangle = \sqrt{p}|00\rangle + \sqrt{1-p}|11\rangle, \]  
(A2)

where \( 1/2 \leq p \leq 1 \). Meanwhile, \( \rho \) is transformed into
\[
\rho' = (U_A \otimes U_B)^\dagger \rho (U_A^\dagger \otimes U_B^\dagger) \]
\[
= \lambda \rho_\lambda + (1 - \lambda) \left( \begin{array}{cccc}
  p & 0 & 0 & \sqrt{p(1-p)} \\
  0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 \\
  \sqrt{p(1-p)} & 0 & 0 & 1 - p
\end{array} \right), \]  
(A3)

where \( \rho_\lambda \equiv U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger \) is still separable, and one partial transpose remains positive semi-definite.
Taking then, the partial transpose, the density matrix is transformed into
\[
\rho^{\mathcal T_n} = \lambda^*_n \rho_s^{\mathcal T_n} + (1-\lambda) \left( \begin{array}{cccc}
p & 0 & 0 & 0 \\
0 & \sqrt{p(1-p)} & 0 & 0 \\
0 & 0 & \sqrt{p(1-p)} & 0 \\
0 & 0 & 0 & 1-p \end{array} \right), \tag{A4}
\]
and we note that the last matrix has eigenvalues \(\lambda_1 = p, \lambda_2 = p(1-p), \lambda_3 = 1-p, \lambda_4 = (1-p)\) in (as \(p > 1/2\)) nonincreasing order. As the Hermitian matrix \(\rho^{\mathcal T_n}_s\) retains positive-semi-definiteness, we can employ a well-known result in matrix analysis [32] that for \(n \times n\) Hermitian matrices \(A\) and \(B\), with \(B\) being positive semi-definite, the eigenvalues of \((A + B)\) and \(A\), when arranged in non-ascending order, obey
\[
\lambda_k(A + B) \geq \lambda_k(A) \quad \text{for } k = 1, 2, \ldots, n. \tag{A5}
\]
Hence, identifying \(B\) with \(\lambda^*_n \rho_s^{\mathcal T_n}\) and \(A\) with the product of \((1-\lambda)\) and the matrix in Eq. (A4), we immediately see that \(\lambda_1(\rho^{\mathcal T_n}) \geq \lambda_2(\rho^{\mathcal T_n}) \geq \lambda_3(\rho^{\mathcal T_n}) \geq (1-\lambda)(1-p) \geq 0\) and, thus, \(\rho^{\mathcal T_n}\) (or equivalently \(\rho^{\mathcal T_n}_s\)) can have at most one negative eigenvalue. Thus, the negativity for \(C^2 \otimes C^2\) systems can then be written as \(N = \max \{0, -\lambda_4(\rho^{\mathcal T_n})\}\).

[11] By entropy we mean a measure of how mixed a state is (i.e., its mixedness). We shall focus on two measures: the linear entropy and the von Neumann entropy, defined in Sec. 11.
[20] A separable (or unentangled) state \((\text{bi-partite})\) \(\rho^{\mathcal T_n}\) can be expressed as \(\rho^{\mathcal T_n} = \sum_{ij} \rho_{ij}^A \otimes \rho_{ij}^B\), whereas an entangled state has no such decomposition.
[22] Suppose a bi-partite density matrix \(\rho\) is expressed in the following form: \(\rho = \sum_{ijkl} \rho_{ijkl}^A \otimes \rho_{ijkl}^B\). Then the partial transpose \(\rho^{\mathcal T_n}\) of the density matrix \(\rho\) is defined via
\[
\rho^{\mathcal T_n} = \sum_{ijkl} \rho_{ijkl}^A \otimes \rho_{ijkl}^B |e_A^i \otimes e_B^j\rangle |e_A^i \otimes e_B^j\rangle.
\]
We remark that the partial transpose depends on the basis chosen but the eigenvalues of the partial transposed matrix do not.
[27] By numerical exploration we mean the creation of a large set of random density matrices, for each of which we compute the relevant characteristics, in this case negativity and linear entropy.