In this problem set we will explore various ways of characterizing and comparing states. Consider the following four 2-qubit density matrices $\rho_1$-$\rho_4$,

\[
\rho_1 = \frac{1}{2} \begin{pmatrix}
1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1
\end{pmatrix}, \quad \rho_2 = \frac{1}{2} \begin{pmatrix}
1 & 0 & 0 & 1/2 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1/2 & 0 & 0 & 1
\end{pmatrix}, \\
\rho_3 = \frac{1}{2} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}, \quad \rho_4 = \frac{1}{4} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}.
\]

   For the pure states $|\psi\rangle, |\chi\rangle$, we can define the fidelity in a couple equivalent ways;

   \[
   F_1 = |\langle \chi | \psi \rangle|^2 = |\langle \chi | \psi \rangle \langle \psi | \chi \rangle|,
   \]

   \[
   F_2 = |\langle \chi | \rho_\psi \rangle \rangle = \text{Tr} \rho_\psi \rho_\chi.
   \]

   Note that $F_2$ gives the correct answer for any $\rho_\psi$, i.e., even if $\rho_\psi$ is not a pure state. However, it turns out that this definition does not work if both $\rho_\psi$ and $\rho_\chi$ are not pure. Then we must use the more complicated

   \[
   F_3 = |\text{Tr} \sqrt{\rho_\psi \rho_\chi \rho_\psi}|^2
   \]

   Here $\sqrt{\rho_\psi}$ is defined such that $\sqrt{\rho_\psi} \sqrt{\rho_\psi} = \rho_\psi$.

   [You can calculate it, e.g., using Mathematica or Matlab. Hint: In Matlab, sqrt(rho) doesn’t work; use rho^0.5. In Mathematica rho^0.5 doesn’t do the trick; instead you need to use “MatrixPower”.]

   For all (10) independent combinations of the above matrices, calculate the fidelity between $\rho_i$ and $\rho_j$ [including $i = j$]. Note that $F(\rho_i, \rho_j) = F(\rho_j, \rho_i)$. To get practice with the different methods of calculating $F$, I recommend using the simplest definition that will work (e.g., $\rho_1$ can be written as pure state $\psi_1$, so $F_1$ may be used.)
2. [12] We can characterize the entropy (the opposite of the purity) of a state in one of two ways:
   
a) The normalized “linear entropy” \( S_L = \frac{4}{3}(1 - \text{Tr} \rho^2) \) [the factor \( \frac{4}{3} \) depends on the dimension of \( \rho \)].
   Calculate \( S_L \) for the four 2-qubit \( \rho \)’s listed before Problem 1. [4]

b) The von Neumann entropy \( S = -\text{Tr} (\rho \log_2 \rho) \).
   Calculate \( S \) for the four \( \rho \)’s. [8]
   [Hint: \( \text{Tr} (\rho \log_2 \rho) = \sum \lambda_k \log_2 \lambda_k \), where \( \lambda_k \) is the k-th eigenvalue of \( \rho \)].

3. [10] As (will be) discussed in class, in general the entanglement of formation present in a system may be defined as follows: If we have a state \( \rho \) of two qubits, one can consider all possible pure-state decomposition of \( \rho \), that is, all ensembles of state \( |\psi_i\rangle \) with probabilities \( p_i \) such that \( \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \). For each pure state, we can define \( \tilde{E}(\psi_i) \):
   \[
   \tilde{E} = -\text{Tr} [\rho_{\text{red}} \log_2 \rho_{\text{red}}],
   \]
   the von Neumann entropy of the reduced density matrix, obtained by tracing over \( |\psi_i\rangle \langle \psi_i| \) over either one of the subsystems. Then the entanglement of formation of the general state \( \rho \) is given by
   \[
   E(\rho) = \min \sum_i p_i \tilde{E}(\psi_i)
   \]
i.e., the minimum average entanglement of the pure states, minimized over all possible decompositions of \( \rho \). This minimization over decompositions of \( \rho \) is in general non-trivial to calculate, except by “brute-force” techniques. Fortunately, for pure states, we can simply use \( \tilde{E} \).
   
a) Calculate \( \tilde{E} \) for the four \( \rho \)’s. [4]

As indicated above, the above simple definition only works for pure states (this should be obvious from your answer in part a) for \( \rho_3 \). For a partially mixed state, a less trivial calculation is needed. One way is to perform the minimization of \( E \) over all possible decomposition of \( \rho \). However, it turns out that for two qubits (and \textit{only} for two qubits), there is in fact an analytic procedure:

1) Start with \( \rho \).

2) Calculate \( \tilde{\rho} \), defined as \( (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y) \), where \( \sigma_{y1,2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \), so that
   \[
   \sigma_y \otimes \sigma_y = \begin{pmatrix}
   0 & 0 & 0 & -1 \\
   0 & 0 & 1 & 0 \\
   0 & 1 & 0 & 0 \\
   -1 & 0 & 0 & 0
   \end{pmatrix}
   \]
   and \( \rho^* \) is the complex conjugate of \( \rho \) [all in the HH, HV, VH, VV basis].

3) Calculate the matrix \( R = \sqrt{\tilde{\rho} \tilde{\rho}^*} \).
4) Calculate the eigenvalues $\lambda_1, \ldots, \lambda_4$ of $R$, and order them such that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$.

5) Calculate the “concurrence” $C = \max \{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$. [Note that $C$ is already a measure of entanglement. The bigger $C$, the more entangled; $C = 0$ means not entangled. (A related measure is the “tangle”, defined as $T = C^2$.)]

6) Calculate $x = \left[1 + \sqrt{1 - C^2}\right]/2$.

7) Finally $E = h(x)$, where $h = -x \log_2 x - (1-x) \log_2 (1-x)$. [And this is the easy way!].

b) Calculate $E$ for $\rho_2$ and $\rho_3$. [6]

4. [8] Though, as we saw in the last problem, it is not always easy to calculate the amount of entanglement in a given state, it is fairly easy to determine whether there is any to begin with (or more precisely speaking, whether there is any to be gotten from the state). In particular, Perez and also the Horodecki’s have come up with the criterion of a positive partial transpose. Here’s how it works:
Start with $\rho$. Now, it is clear that the transpose of $\rho = \rho^T$ is also a legitimate density matrix. If $\rho$ can truly be separated into separate parts, then it follows that if only one of the parties takes the transpose (e.g., swaps the coefficients of the corresponding terms in the density matrix that have $|H}\langle V|$ and $|V\rangle\langle H|$), resulting in the partial transpose density matrix $\rho^\sim$, $\rho^\sim$ should still be a legitimate density matrix, i.e., should still have only non-negative eigenvalues. On the other hand, if $\rho$ cannot be separated, then it has been shown for all two qubit states (and also for all pure states with one qubit and one qu-trit) that the resulting $\rho^\sim$ will necessarily have at least one negative eigenvalue -- this, then, is a test for separability. {The Horodecki’s have further shown (I believe for all states), that passing this test delineates states with distillable entanglement, i.e., if the eigenvalues of the partial transpose are all non-negative, then there is no distillable entanglement in a system.}

a. For the 4 density matrices before problem 1, find the eigenvalues of the partial transpose density matrix $\rho^\sim$, thereby confirming your knowledge of the states, and your results from Prob. 3. [4]

Finally, we consider the so-called “Werner” states, which have the form

$$\rho_W(\lambda) \equiv \lambda \rho_{HH+VV} + (1 - \lambda) \rho_{\text{completely mixed}}$$

It is basically a “diluted” entangled state (the maximally entangled contribution could be any of the Bell states).

b) Write $\rho_W(\lambda)$ in matrix form [1].

c) Use the above separability criterion to show that there is entanglement in a Werner state as long as $\lambda > 1/3$. [3]