HW8 Solutions

1. Using the CNOT and Hadamard gates, build a 3 qubit circuit that constructs the state
   \[ |\psi\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle) \]
   in analogy with the circuit described to build Bell states.

2. Find the Schmidt decomposition for the following
   \[ \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle), \quad \frac{1}{2} (|00\rangle + |11\rangle + |01\rangle + |10\rangle), \quad \frac{1}{\sqrt{3}} (|00\rangle + |01\rangle + |10\rangle) \]

   The first state is already Schmidt decomposed. For the second one, we observe that the state can be written as a product
   \[ \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \]
   which is the Schmidt decomposition for that state. For the third state, we use a general algorithm to find its Schmidt decomposition. Consider a Schmidt decomposed state
   \[ |\psi\rangle = \sum_i \sqrt{p_i} |i_A\rangle |i_B\rangle \]
   The reduced density matrices for this state are given by (since the Schmidt states can be extended to an orthonormal basis of the Hilbert space factors by using Gram-Schmidt)
   \[ \rho_A = \sum_i p_i |i_A\rangle \langle i_A|, \quad \rho_B = \sum_i p_i |i_B\rangle \langle i_B| \]
Observe that these are spectral decomposed, hence \( p_i \) are simply the eigenvalues of the reduced density matrices and the \(|i_A\rangle, |i_B\rangle\) are the eigenvectors. Hence, to find the Schmidt decomposition of a state, we need only find the eigenvalues and eigenvectors of the reduced density matrices. Applying this principle to the third state, we find

\[
\rho_A = \frac{1}{3}(|0_A\rangle + |1_A\rangle)(\langle 0_A| + \langle 1_A|) + \frac{1}{3} |0_A\rangle \langle 0_A| = \frac{1}{3} \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}
\]

\[
\rho_B = \frac{1}{3}(|0_B\rangle + |1_B\rangle)(\langle 0_B| + \langle 1_B|) + \frac{1}{3} |0_B\rangle \langle 0_B| = \frac{1}{3} \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}
\]

The eigenvalues of this matrix are given by

\[
p_{1,2} = \frac{1}{2} \pm \frac{\sqrt{5}}{6}
\]

and the eigenvectors are

\[
|I_A\rangle = \sqrt{\frac{1}{2} + \frac{\sqrt{5}}{2}} |0_A\rangle + \sqrt{\frac{2}{5 + \sqrt{5}}} |1_A\rangle
\]

\[
|II_A\rangle = \sqrt{\frac{1}{2} - \frac{\sqrt{5}}{2}} |0_A\rangle + \sqrt{\frac{2}{5 - \sqrt{5}}} |1_A\rangle
\]

\[
|I_B\rangle = \sqrt{\frac{1}{2} + \frac{\sqrt{5}}{2}} |0_B\rangle + \sqrt{\frac{2}{5 + \sqrt{5}}} |1_B\rangle
\]

\[
|II_B\rangle = \sqrt{\frac{1}{2} - \frac{\sqrt{5}}{2}} |0_B\rangle + \sqrt{\frac{2}{5 - \sqrt{5}}} |1_B\rangle
\]

which gives us the Schmidt decomposition of the state.

3 Prove that a state \(|\psi\rangle\) of a composite system \(AB\) is a product state iff it has Schmidt number 1. Also prove that \(|\psi\rangle\) is a product state iff the partial traces \(\rho_A\) and \(\rho_B\) are pure states.

If \(|\psi\rangle\) is a product state \(|\phi_A\rangle|\xi_B\rangle\), it is automatically in Schmidt decomposed form and hence has Schmidt number 1. Conversely, a state with Schmidt number 1 can be written in the form \(|\psi\rangle = \sqrt{1} |1_A\rangle |1_B\rangle\) which is a product state.

As shown in the previous problem, a Schmidt decomposed state gives spectral decomposed reduced density matrices. Hence, product states \(|\phi_A\rangle|\xi_B\rangle\), which have Schmidt number 1, give reduced density matrices of the form

\[
\rho_A = |\phi_A\rangle \langle \phi_A|, \quad \rho_B = |\xi_A\rangle \langle \xi_B|
\]

which are pure states. Conversely, if \(\rho_A\) and \(\rho_B\) are pure states, they must be of the form (3.1) and hence the Schmidt decomposition of the state \(|\psi\rangle\) must be a product.
4 A set $S$ is convex if for all points $x, y \in S$ the line segment joining the two points given by

$$y\lambda + x(1 - \lambda)$$

belongs to $S$ for $0 \leq \lambda \leq 1$

4.1 For a finite dimensional Hilbert space of dimension $N$, show that the density operators form a convex subset of the space of Hermitian operators. To do so we need to demonstrate that the convex linear combination $\sigma \lambda + \rho (1 - \lambda)$ of two density matrices $\rho, \sigma$ is also a density matrix. The combination is clearly Hermitian, the trace of the combination is

$$\text{tr}(\sigma)\lambda + \text{tr}(\rho)(1 - \lambda) = \lambda + 1 - \lambda = 1$$

which means that the combination is trace-normalized. Finally, to check positivity, we compute expectation value of the combination in an arbitrary state $|\psi\rangle$, which is given by

$$\langle \sigma \rangle \lambda + \langle \rho \rangle (1 - \lambda) \geq 0$$

since $\sigma$ and $\rho$ are both positive. Hence, we convex combination is also a Hermitian, trace-normalized, positive operator, which makes it a density matrix.

4.2 Show that the density matrix for a pure state cannot be written as a sum of two other density matrices.

No density matrix can be written as a sum of two other density matrices, because sums of density matrices aren’t trace-normalized. Instead we will show that a pure state density matrix can’t be written as a convex combination of density matrices. Let

$$\rho = \rho_1 \lambda + \rho_0 (1 - \lambda)$$

If $\rho$ is a pure state, it can be written as $|\psi\rangle \langle \psi|$ for some state $|\psi\rangle$. Consider an arbitrary state $|\psi_\perp\rangle$ orthogonal to $|\psi\rangle$. We have

$$0 = \langle \psi_\perp |\rho|\psi_\perp \rangle = \lambda \langle \psi_\perp |\rho_1|\psi_\perp \rangle + (1 - \lambda) \langle \psi_\perp |\rho_0|\psi_\perp \rangle$$

Since the right hand side is a sum of two non-negative terms, which adds to zero, both terms must individually vanish. One can have three possible solutions here. Two of them are

$$\lambda = 0, \rho_0 = \rho$$
$$\lambda = 1, \rho_1 = \rho$$

The third solution is to have

$$\langle \psi_\perp |\rho_{0,1}|\psi_\perp \rangle = 0$$

for all orthogonal states $\psi_\perp$. But then by constructing a Gram-Schmidt basis using $|\psi\rangle$ and other orthogonal states, one can see that in this basis the only non-zero matrix element of $\rho_{0,1}$ is $\langle \psi |\rho_{0,1}|\psi \rangle$. Hence, using this basis, we can write

$$\rho_0 = \rho_1 = |\psi\rangle \langle \psi | = \rho$$

Hence, pure states can’t be written as a convex combination of other density matrices.
4.3 Points in a convex set that cannot be expressed as a sum of other points are called extremal points. Pure states are extremal points in the set of density matrices. Show that only pure states are extremal.

We will prove the contrapositive of the question statement, i.e., any mixed state can always be written as a convex combination of two distinct density matrices.

By virtue of being Hermitian, any density matrix can be spectrally decomposed as

\[ \rho = \sum_{i=1}^{N} p_i |i\rangle \langle i| \]  

with \( \sum_i p_i = 1 \). \( \rho \) is a mixed state iff at least two of the \( p_i \) are non-zero. Let the number of non-zero \( p_i \)'s be \( m \geq 2 \). In this case we can find some integer \( k < m \) and define

\[ \rho_0 = \frac{1}{\sum_{i=1}^{k} p_i} \sum_{i=1}^{k} p_i |i\rangle \langle i| \]
\[ \rho_1 = \frac{1}{\sum_{i=k+1}^{m} p_i} \sum_{i=k+1}^{m} p_i |i\rangle \langle i| \]  

which are both density matrices and write \( \rho \) as a convex combination

\[ \rho = \lambda \rho_1 + (1 - \lambda) \rho_0, \quad \lambda = \sum_{i=k+1}^{m} p_i \]  

which means that it can’t be an extremal point.

4.4 For a single qubit system, show that the density matrix for an arbitrary mixed state can be written in the form:

\[ \rho = \frac{1}{2} (I + \vec{r} \cdot \vec{\sigma}) \]

where the real 3 dimensional vector \( \vec{r} \) satisfies \( |\vec{r}|^2 \leq 1 \). This is called the Bloch vector for \( \rho \). Show that this state is pure iff \( |\vec{r}|^2 = 1 \). Show that the definition of the Bloch vector coincides with the definition we gave at the beginning of the course.

Since \( \rho \) is a Hermitian operator, it can always be expanded in a basis of the identity and Pauli matrices, which form a basis for Hermitian operators in two dimensions. Since the Pauli matrices are traceless, the contribution to the trace of \( \rho \) comes solely from the coefficient of \( I \), and we must have

\[ \rho = \frac{1}{2} (I + \vec{r} \cdot \vec{\sigma}) \]  

All that remains is to show that \( |\vec{r}|^2 \leq 1 \). To do this, we shall use the positivity condition. Note that for two dimensions, positivity for density matrices is equivalent to saying that

\[ - 4 - \]
\[ \det \rho \geq 0, \]  
since the determinant is the product of eigenvalues and we already know that  
the eigenvalues must sum to 1. We find that  
\[ \det \rho = \frac{1}{4} (1 - |\vec{r}|^2) \quad (4.12) \]  
which gives us the condition \(|\vec{r}|^2 \leq 1\). Hence, the set of two dimensional density matrices  
forms a solid ball of unit radius in three dimensional Euclidean space. This ball is a convex  
set.

We have already shown that pure states and extremal points are equivalent, so all we  
need to do is find the extremal points of the solid ball, which are the set of points on its  
surface, given by \(|\vec{r}| = 1\), the Bloch sphere.

The definition of Bloch sphere used for pure states at the beginning of the course was  
the set of points parametrized by the polar angles \(\theta, \phi\)  
\[ |\psi\rangle = \cos(\theta/2) + e^{-i\phi} \sin(\theta/2) \quad (4.13) \]  
The corresponding density matrix can be put into the form  
\[ |\psi\rangle \langle \psi| = \frac{1}{2} (I + \vec{r} \cdot \vec{\sigma}) \quad (4.14) \]  
with  
\[ \vec{r} = (\sin \theta \cos \phi, \sin \theta, \sin \phi, \cos \theta) \quad (4.15) \]  
hence the two definitions of the Bloch sphere agree.

4.5 Consider an arbitrary tripartite state  
\[ |\psi\rangle_{ABC} \in H_A \otimes H_B \otimes H_C. \]  
Does a Schmidt decomposition exist? Namely, are there orthonormal bases  
\([|i_A\rangle], [|i_B\rangle], [|i_C\rangle]\) such that  
\[ |\psi\rangle_{ABC} = \sum_i \lambda_i |i_A\rangle |i_B\rangle |i_C\rangle \]  
We will show that there isn’t a Schmidt decomposition for such states by providing a  
counter-example. Consider the state  
\[ |\psi\rangle_{ABC} = \frac{1}{\sqrt{2}} (|0_A0_B\rangle + |1_A1_B\rangle) |0_C\rangle \quad (4.16) \]  
i.e., the Bell state tensored with the state \(|0\rangle_C\) (or any other vector in \(C\) would work for  
this argument). The property we shall be using here is that for any orthonormal bases of  
the three factors of the Hilbert spaces, the Bell state retains it’s form, i.e.,  
\[ \frac{1}{\sqrt{2}} (|0_A0_B\rangle + |1_A1_B\rangle) = \frac{1}{\sqrt{2}} (|0'_A0'_B\rangle + |1'_A1'_B\rangle) \quad (4.17) \]  
Hence, whatever orthonormal basis we pick, our state will necessarily be of the form  
\[ \frac{1}{\sqrt{2}} (|0'_A0'_B\rangle + |1'_A1'_B\rangle) \otimes (\alpha |0'_C\rangle + \beta |1'_C\rangle) \quad (4.18) \]  
The only choice we have is that of the complex numbers \(\alpha\) and \(\beta\) above and for no values  
of these is the above state in a Schmidt decomposed form.
4.6 A density matrix is separable if it can be written in the form

\[ \rho = \sum_k p_k \rho_i^k \otimes \cdots \otimes \rho_n^k \]

with \( \sum_k p_k = 1 \) where \( \rho_i^k \) is a pure state of the subsystem \( i \). Consider the density matrix

\[ \rho = p |\beta_{11}\rangle \langle \beta_{11}| + (1 - p) \frac{I}{4} \]

with \( 0 \leq p \leq 1 \). For what values of \( p \) is \( \rho \) separable?

The simplest way of checking whether the density matrix is separable or not is to use the positive-partial-transpose (PPT) or the Peres-Horodecki criterion\(^1\), which is necessary in general and sufficient in two dimensions, which is the case for us.

We first define the partial transpose of a density matrix. Suppose we have, in a basis

\[ \rho = \sum_{ijkl} \rho_{ij}^{kl} |ij\rangle \langle kl| \]

we can define its partial transpose with respect to either factors of the Hilbert space as

\[ \rho^T_A = \sum_{ijkl} \rho_{ij}^{kl} |kj\rangle \langle il| \]

\[ \rho^T_B = \sum_{ijkl} \rho_{ij}^{kl} |il\rangle \langle kj| \]

The PPT criterion states that for separable density matrices, the partial transposes have positive eigenvalues. It suffices to check for only one partial transpose. For the given state, we have

\[ \rho = \frac{p}{2} (|01\rangle \langle 01| - |10\rangle \langle 10|) + \frac{1 - p}{4} (|00\rangle \langle 00| + |01\rangle \langle 01| + |10\rangle \langle 10| + |11\rangle \langle 11|) \]

\[ = \frac{1 - p}{4} (|00\rangle \langle 00| + |11\rangle \langle 11|) + \frac{1 + p}{4} (|01\rangle \langle 01| + |10\rangle \langle 10|) - \frac{p}{2} (|01\rangle \langle 10| + |10\rangle \langle 01|) \]

(4.21)

The partial transpose of this state is given by

\[ \rho^T_B = \frac{1 - p}{4} (|00\rangle \langle 00| + |11\rangle \langle 11|) + \frac{1 + p}{4} (|01\rangle \langle 01| + |10\rangle \langle 10|) - \frac{p}{2} (|00\rangle \langle 11| + |11\rangle \langle 00|) \]

(4.22)

which in matrix form in the ordered basis \{ |00\rangle, |01\rangle, |10\rangle, |11\rangle \} is given by

\[ \rho^T_B = \frac{1}{4} \begin{pmatrix} 1 - p & 0 & 0 & -2p \\ 0 & 1 + p & 0 & 0 \\ 0 & 0 & 1 + p & 0 \\ -2p & 0 & 0 & 1 - p \end{pmatrix} \]

(4.23)

Its eigenvalues are \((1 - 3p)/4, (1 + p)/4\). For the eigenvalues to be all positive, we need

\[ p \leq \frac{1}{3} \]

(4.24)

For these values, the density matrix is separable. Otherwise, it isn’t separable.

\(^1\)See the lecture notes by John Preskill or https://en.wikipedia.org/wiki/Peres\-Horodecki\_criterion for more details.