1 Traces, Traces Everywhere (5 points)

(a.) Okay, so the time evolved state is given by,
\[ \hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t), \]  
from which we can compute \( \hat{\rho}^n(t) \) using the fact that \( \hat{U} \) is unitary i.e. \( \hat{U}(t)\hat{U}^\dagger(t) = \hat{I} \),
\[ \hat{\rho}^n(t) = \hat{U}(t)\hat{\rho}^n(0)\hat{U}^\dagger(t). \]
Now we trace over this and use the cyclic property of trace \( \text{Tr}(ABC) = \text{Tr}(CAB) = \text{Tr}(BCA) \) to get,
\[ \text{Tr}(\hat{\rho}^n(t)) = \text{Tr}(\hat{\rho}^n(0)) = \sum_i \lambda_i^n, \]
where \( \{\lambda_i\} \) is the set of eigenvalues of \( \hat{\rho}(0) \).

(b.) While one can compute the asked traces and determinant explicitly by considering a generic qubit state and its corresponding \( 2 \times 2 \) density operator, we will follow a much compact approach, harnessing properties of traces. In what follows, denote \( \lambda_1 \) and \( \lambda_2 \) to be the eigenvalues of the density matrix of the qubit state \( \hat{\rho} \).
It is easily seen that,
\[ \text{Tr}(\hat{\rho}^n) = \lambda_1^n + \lambda_2^n. \]
In particular we have \( \text{Tr}(\hat{\rho}) = \lambda_1 + \lambda_2 = 1 \) since the density operator has unit trace and \( \text{Tr}(\hat{\rho}^2) = \lambda_1^2 + \lambda_2^2 \). Also, one can notice that \( \text{det}(\rho) = \lambda_1\lambda_2 \). Okay, now let’s use some kindergarden arithmetic: \( (\lambda_1+\lambda_2)^2 = \lambda_1^2 + \lambda_2^2 + 2\lambda_1\lambda_2 \), which in our context is gives us the determinant we are looking for,
\[ \text{det}(\rho) = \frac{1}{2} \left( \text{Tr}^2(\hat{\rho}) - \text{Tr}(\hat{\rho}^2) \right) = \frac{1}{2} \left( \text{Tr}(\hat{\rho}) - \text{Tr}(\hat{\rho}^2) \right). \]
Now, consider \( \lambda_1^3 + \lambda_2^3 = (\lambda_1 + \lambda_2)(\lambda_1^2 + \lambda_2^2 - \lambda_1\lambda_2) \), from which one can directly write,
\[ \text{Tr}(\hat{\rho}^3) = \text{Tr}(\rho)\left( \text{Tr}(\hat{\rho}^2) - \text{det}(\rho) \right) = \text{Tr}(\rho)\left( \frac{3}{2} \text{Tr}(\hat{\rho}^2) - \frac{1}{2} \text{Tr}(\hat{\rho}) \right). \]
Of course, \( \text{Tr} \hat{\rho} = 1 \) everywhere above. If you feel like, you can also compute these by considering a generic qubit state \( \hat{\rho} = \hat{I}/2 + \vec{a} \cdot \hat{\sigma}/2 \) and find \( \hat{\rho}^2 \) and \( \hat{\rho}^3 \) and find the traces and determinant asked for.

2 More on von Neumann Entropy (5 points)

(a.) This one can be argued simply by observing the fact that a unitary transformation of \( \hat{\rho} \) simply corresponds to a global basis change and eigenvalues of a matrix are left invariant under a basis change/unitary transformation and hence, the von Neumann entropy, which can
be constructed using only the eigenvalues of $\hat{\rho}$ only is invariant too.

(b.) Onto proving concavity now. First, it is important to mention that, in general, $\hat{\rho}$, $\hat{\rho}_1$ and $\hat{\rho}_2$ will not commute and hence will not be simultaneously diagonalizable. Let us work in the eigenbasis of $\hat{\rho}$ which we label $\{|\rho_m\rangle\}$ with corresponding eigenvalue $\rho_m$ (We will use single subscripts for eigen properties and double indices will be used to denote matrix elements.) The von Neumann entropy of $\hat{\rho}$ is simply given by,

$$S(\hat{\rho}) = \sum_m -\rho_m \log (\rho_m) \equiv \sum_m s(\rho_m), \tag{7}$$

where the function $s(x) = -x \log(x)$. This is a concave in the domain $[0, 1]$ since its second derivative $f'' \leq 0$ and hence it satisfies a concavity condition, for any $\alpha \in [0, 1]$

$$s((1 - \alpha)x + \alpha y) \geq (1 - \alpha)s(x) + \alpha s(y). \tag{8}$$

We will use this property heavily in this proof. Notice how the eigenvalue $\rho_m$ of $\hat{\rho}$ can be written as,

$$\rho_m = \langle \rho_m | \hat{\rho} | \rho_m \rangle = p_1 \langle \rho_m | \hat{\rho}_1 | \rho_m \rangle + p_2 \langle \rho_m | \hat{\rho}_2 | \rho_m \rangle, \tag{9}$$

where we used $\hat{\rho} = p_1 \hat{\rho}_1 + p_2 \hat{\rho}_2$ as given in the question. Now since each of the terms in the summand of Eq. (7) is concave, we can use the concavity property of Eq. (8) to write,

$$s(\rho_m) \geq p_1 s(\langle \rho_m | \hat{\rho}_1 | \rho_m \rangle) + p_2 s(\langle \rho_m | \hat{\rho}_2 | \rho_m \rangle), \tag{10}$$

and a simple sum over $m$ reads,

$$S(\hat{\rho}) \geq p_1 \sum_m s(\langle \rho_m | \hat{\rho}_1 | \rho_m \rangle) + p_2 \sum_m s(\langle \rho_m | \hat{\rho}_2 | \rho_m \rangle). \tag{11}$$

Now life would have been nice and simple had $\hat{\rho}_1$ and $\hat{\rho}_2$ been diagonal in the $\{|\rho_m\rangle\}$ (eigenbasis of $\hat{\rho}$) basis and we could have identified the sums on the right side of Eq. (11) as the von Neumann entropies $S(\hat{\rho}_1)$ and $S(\hat{\rho}_2)$, but well, in general $s(\langle \rho_m | \hat{\rho}_1 | \rho_m \rangle)$ and $s(\langle \rho_m | \hat{\rho}_1 | \rho_m \rangle)$ are not the eigenvalues of $\hat{\rho}_1$ and $\hat{\rho}_2$, but just the diagonal entries of the density matrices of $\hat{\rho}_1$ and $\hat{\rho}_2$ in the $\{|\rho_m\rangle\}$ basis. Let us now try and make contact with the von Neumann entropies of $\hat{\rho}_1$ and $\hat{\rho}_2$ using these diagonal entries.

Let me state and prove a general result that we will end up needing. We will now show that,

$$- \sum_n \lambda_{nn} \log (\lambda_{nn}) \geq S(\hat{\rho}), \tag{12}$$

where $\hat{\rho}$ is any density operator and $\lambda_{nn}$ are its diagonal entries in any basis, not necessarily its eigenbasis (The inequality will become an equality when we work in the eigenbasis). Let us write $\hat{\rho}$ in both its eigenbasis $\{|\rho_m\rangle\}$ and some other basis $\{|\lambda_n\rangle\}$,

$$\hat{\rho} = \sum_m \rho_m |\rho_m\rangle \langle \rho_m | = \sum_{n,n'} \lambda_{nn'} |\lambda_n\rangle \langle \lambda_n |. \tag{13}$$

To connect these two and be able to write the diagonal entries $\lambda_{nn}$ in terms of the eigenvalues $\rho_m$, let’s introduce two complete set of states as follows,

$$\hat{\rho} = \sum_m \rho_m \sum_{n,n'} |\lambda_n\rangle \langle \lambda_n | \langle \rho_m | \rho_m \rangle |\lambda_{n'}\rangle \langle \lambda_{n'} |. \tag{14}$$
from which we can read the diagonal entries $\lambda_{nn}$ simply,

$$
\lambda_{nn} = \sum_m \rho_m |\langle \lambda_n | \rho_m \rangle|^2 .
$$

These overlaps are expansion coefficients of eigenstates $|\rho_m\rangle$ in the $\{ |\lambda_n\rangle \}$ basis and one can easily they verify they satisfy,

$$
\sum_n |\langle \lambda_n | \rho_m \rangle|^2 = 1 .
$$

Hence, we notice, each diagonal term is a weighted sum of eigenvalues as shown by Eq. (15) with all weights summing to unity and hence we can invoke concavity again to write,

$$
-\lambda_{nn} \log (\lambda_{nn}) \geq \sum_m |\langle \lambda_n | \rho_m \rangle|^2 (-\rho_m \log (\rho_m))
$$

This concludes our digression proof. Return to where we left off for concavity and now we simply apply this general inequality result to each of the $\hat{\rho}_1$ and $\hat{\rho}_2$ diagonal terms of Eq. (11) and perform the sum to get the desired concavity answer,

$$
S(\hat{\rho}) \geq p_1 S(\hat{\rho}_1) + p_2 S(\hat{\rho}_2) .
$$

(c.) Consider the separable state $\hat{\rho}_{AB} = \hat{\rho}_A \otimes \hat{\rho}_B$. For concreteness take $\dim (A) = d_A$ and $\dim (B) = d_B$ and hence the dimension of Hilbert space on which $\hat{\rho}_{AB}$ lives is simply $d = d_A d_B$. Let’s label the $d$ eigenvalues of $\hat{\rho}_{AB}$ as $\lambda_k$ with $k = 1, 2, \cdots, d$. Also, label the eigenvalues of $\hat{\rho}_A$ as $\alpha_i$, $i = 1, 2, \cdots, d_A$ and those of $\hat{\rho}_B$ as $\beta_j$, $j = 1, 2, \cdots, d_B$. One can now construct a bijective map which relates the $d = d_A d_B$ eigenvalues of $\hat{\rho}_{AB}$ with those of $\hat{\rho}_A$ and $\hat{\rho}_B$,

$$
\lambda_k = \alpha_i \beta_j , \; k \equiv (i, j) \text{ with } i = 1, 2, \cdots, d_A \text{ and } k = 1, 2, \cdots, d_B .
$$

Now, let’s get to the entropy.

$$
S(\hat{\rho}_{AB}) = \sum_{k=1}^d \lambda_k \log (\lambda_k) = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} (\alpha_i \beta_j) \log (\alpha_i \beta_j) .
$$

We can now split the log to get,

$$
S(\hat{\rho}_{AB}) = \sum_{j=1}^{d_B} \beta_j \sum_{i=1}^{d_A} \alpha_i \log (\alpha_i) + \sum_{i=1}^{d_A} \alpha_i \sum_{j=1}^{d_B} \beta_j \log (\beta_j) .
$$

Now notice, $S(\hat{\rho}_A) = \sum_{i=1}^{d_A} \alpha_i \log (\alpha_i)$ and $S(\hat{\rho}_B) = \sum_{j=1}^{d_B} \beta_j \log (\beta_j)$ and also that the sum of eigenvalues of any density operator is its trace which is unity, i.e. $\sum_{i=1}^{d_A} \alpha_i = \sum_{j=1}^{d_B} \beta_j = 1$, which gives us the required result,

$$
S(\hat{\rho}_{AB}) = S(\hat{\rho}_A) + S(\hat{\rho}_B) .
$$
3 Let’s measure a GHZ! (5 points)

(a.) Let us construct the projection operators corresponding to measurement in the \{\ket{\pm x}\} basis,

\[
\hat{P}_+ = \ket{+x}\bra{+x}, \quad \hat{P}_- = \ket{-x}\bra{-x}. \tag{23}
\]

One can now easily see that this set of projection operators satisfies all the required conditions for being a Projective Value Measurement (PVM). The set of projection operators are

1. Hermitian: \(\hat{P}_+^\dagger = \hat{P}_+\), \(\hat{P}_-^\dagger = \hat{P}_-\),
2. Complete: \(\hat{P}_+ + \hat{P}_- = \ket{0}\bra{0} + \ket{1}\bra{1} = \hat{I}\),
3. Orthogonal Projectors: \(\hat{P}_+\hat{P}_+ = \hat{P}_+, \hat{P}_-\hat{P}_- = \hat{P}_-\), \(\hat{P}_+\hat{P}_- = \hat{P}_-\hat{P}_+ = 0\)
4. Positive: eigenvalues of \(\hat{P}_+\) and \(\hat{P}_-\) are 0 and 2 which are \(\geq 0\)

(b.) The pre-measurement GHZ density operator is simply,

\[
\hat{\rho}_0 = |\text{GHZ}\rangle \langle \text{GHZ}| = \frac{1}{2} (|000\rangle \langle 000| + |000\rangle \langle 111| + |111\rangle \langle 000| + |111\rangle \langle 111|), \tag{25}
\]

where the convention I am following labels subsystems in states and their duals as \(|ABC\rangle\) and \(\langle ABC|\), respectively.

Okay, let’s compute some projections now, but first notice the following overlaps which will be useful,

\[
\langle +x|0\rangle = \langle +x|1\rangle = \frac{1}{\sqrt{2}}, \tag{26}
\]
\[
\langle -x|0\rangle = -\langle -x|1\rangle = \frac{1}{\sqrt{2}}. \tag{27}
\]

The following projections can now be easily computed,

\[
\hat{P}_+\hat{\rho}_0\hat{P}_+ = \frac{1}{4} \ket{+x}\bra{+x} \otimes (|000\rangle \langle 000| + |000\rangle \langle 111| + |111\rangle \langle 000| + |111\rangle \langle 111|), \tag{28}
\]
\[
\hat{P}_-\hat{\rho}_0\hat{P}_- = \frac{1}{4} \ket{-x}\bra{-x} \otimes (|000\rangle \langle 000| - |000\rangle \langle 111| - |111\rangle \langle 000| + |111\rangle \langle 111|), \tag{29}
\]

which we can write more compactly as,

\[
\hat{P}_+\hat{\rho}_0\hat{P}_+ = \frac{1}{2} \ket{+x}\bra{+x} \otimes \left( \frac{|000\rangle + |111\rangle}{\sqrt{2}} \right) \left( \frac{|000\rangle + |111\rangle}{\sqrt{2}} \right), \tag{30}
\]
\[
\hat{P}_-\hat{\rho}_0\hat{P}_- = \frac{1}{2} \ket{-x}\bra{-x} \otimes \left( \frac{|000\rangle - |111\rangle}{\sqrt{2}} \right) \left( \frac{|000\rangle - |111\rangle}{\sqrt{2}} \right). \tag{31}
\]

It’s a good idea to express the first qubit, on which the PVM projectors have been applied, in the measurement basis; in this case the \{\ket{\pm x}\} basis since the outcome of such a measurement will be in the said basis. Expressing it in the standard \{\ket{0}, \ket{1}\} basis is somewhat obscuring the interpretation of the PVM. Let us also compute the traces of these projections which will serve as normalization factors and probabilities as well,

\[
\Tr(\hat{P}_+\hat{\rho}_0\hat{P}_+) = \Tr(\hat{P}_-\hat{\rho}_0\hat{P}_-) = \frac{1}{2}. \tag{32}
\]
This can be easily seen from Eqs. (30) and (31) since \( \text{Tr}(\hat{P}_+) = \text{Tr}(\hat{P}_-) = 1 \) and also the residual states of the second and third qubits \( \left( \frac{|00\rangle + |11\rangle}{\sqrt{2}} \right) \) are normalized too. The measurement interpretation of the PVM is that with probability \( p_+ = \text{Tr}(\hat{P}_+ \hat{\rho}_0 \hat{P}_+) \), the outcome of the measurement on the first qubit is observed to be “+x” and the post-measurement state in this case will be,

\[
\hat{\rho}_+ = \frac{\hat{P}_+ \hat{\rho}_0 \hat{P}_+}{\text{Tr}(\hat{P}_+ \hat{\rho}_0 \hat{P}_+)},
\]

and with probability \( p_- = \text{Tr}(\hat{P}_- \hat{\rho}_0 \hat{P}_-) \), the outcome observed it,

\[
\hat{\rho}_- = \frac{\hat{P}_- \hat{\rho}_0 \hat{P}_-}{\text{Tr}(\hat{P}_- \hat{\rho}_0 \hat{P}_-)},
\]

Okay, now we can simply state the questions asked for in the homework.

If the post-measurement state is not known to the observer, the density operator describing the GHZ will be given by,

\[
\hat{\rho}_1 = p_+ \hat{\rho}_+ + p_- \hat{\rho}_- ,
\]

\[
\hat{\rho}_1 = \frac{1}{2} |+x\rangle \langle +x| \otimes \left( \frac{|00\rangle + |11\rangle}{\sqrt{2}} \right) \left( \frac{|00\rangle + |11\rangle}{\sqrt{2}} \right) + \frac{1}{2} |-x\rangle \langle -x| \otimes \left( \frac{|00\rangle - |11\rangle}{\sqrt{2}} \right) \left( \frac{|00\rangle - |11\rangle}{\sqrt{2}} \right).
\]

On the other hand, for part (c.) with probability \( p_+ = 1/2 \) we will observe the post-measurement state to be \( \hat{\rho}_+ \) of Eq. (33) in which case the residual state of the second and third qubits can simply be “read-off” as,

\[
|\psi^+_{23}\rangle = \left( \frac{|00\rangle + |11\rangle}{\sqrt{2}} \right).
\]

The other possibility of the measurement outcome is observing the “-x” outcome for the first qubit with probability \( p_- = 1/2 \), in which case the GHZ state is given by \( \hat{\rho}_- \) of Eq. (34) and the residual state of the other two qubits will be,

\[
|\psi^-_{23}\rangle = \left( \frac{|00\rangle - |11\rangle}{\sqrt{2}} \right).
\]

It is worth pointing out here that even though we found pure residual states for the other two qubits; in general, the residual state of sub-systems on which measurement is not performed will be mixed.

\section{Thermal Spins in a B-field (5 points)}

In this question, for all our matrix representations, we will exclusively work in the \( \hat{\sigma}_z \) basis. The Hamiltonian of the spin 1/2 particle in the B-field is simply,

\[
\hat{H} = -\frac{\gamma B}{2} \hat{\sigma}_z \equiv \begin{bmatrix} -\frac{\omega}{2} & 0 \\ 0 & \frac{\omega}{2} \end{bmatrix},
\]

where we have defined \( \omega = \gamma B \) for convenience. Now since the particle is a part of a thermal ensemble at temperature \( T \equiv 1/k_B \beta \) with \( k_B \) being the Boltzmann constant, its density operator is thermal,

\[
\hat{\rho} = \frac{\exp(-\beta \hat{H})}{\text{Tr}(\exp(-\beta \hat{H}))}.
\]
Since we are asked to work in the $\hat{\sigma}_z$ basis in which $\hat{H}$ is diagonal, hence $\exp(-\beta \hat{H})$ will be diagonal in this basis too, given by,

$$\exp(-\beta \hat{H}) \equiv \begin{bmatrix} e^{\beta \omega/2} & 0 \\ 0 & e^{-\beta \omega/2} \end{bmatrix},$$

whose trace is simply $\text{Tr}(\exp(-\beta \hat{H})) = e^{\beta \omega/2} + e^{-\beta \omega/2}$ and hence,

$$\rho = \frac{1}{e^{\beta \omega/2} + e^{-\beta \omega/2}} \begin{bmatrix} e^{\beta \omega/2} & 0 \\ 0 & e^{-\beta \omega/2} \end{bmatrix}.$$ (41)

(b.) Now we compute the expectation values of $\hat{\sigma}$ for the particle in this thermal ensemble. For $\hat{\sigma}_l$, the expectation value is given by,

$$\langle \hat{\sigma}_l \rangle = \text{Tr}(\hat{\sigma}_l \hat{\rho}).$$ (43)

It can now be seen rather straightforwardly by matrix multiplication and taking the trace that

$$\langle \hat{\sigma}_x \rangle = \langle \hat{\sigma}_y \rangle = 0$$

and,

$$\langle \hat{\sigma}_z \rangle = \frac{e^{\beta \omega/2} - e^{-\beta \omega/2}}{e^{\beta \omega/2} + e^{-\beta \omega/2}} = \tanh \left( \frac{\beta \omega}{2} \right).$$ (44)

(c.) Now we can compute the average magnetization of $N$ such particles in the thermal ensemble,

$$\hat{M} = \frac{N\gamma}{2} \left( \langle \hat{\sigma}_x \rangle \hat{i} + \langle \hat{\sigma}_y \rangle \hat{j} + \langle \hat{\sigma}_z \rangle \hat{k} \right),$$ (45)

where the expectations are the single particle expectations computed in part (b) above and $\{\hat{i}, \hat{j}, \hat{k}\}$ are spatial unit vectors along $x, y$ and $z$ directions, respectively. This gives us,

$$\hat{M} = \frac{N\gamma}{2} \tanh \left( \frac{\beta \omega}{2} \right) \hat{z}. $$ (46)

Now we consider the high temperature or the small $\beta$ limit and Taylor expand the magnitude of $\hat{M}$ to linear order in $\beta$ to get the characteristic Curie’s Law $1/T$ dependence of the magnetization,

$$M = \frac{N\gamma^2 B}{4k_B} \left( \frac{1}{T} \right) + \mathcal{O} \left( \left( \frac{1}{T^3} \right) \right).$$ (47)