Exercises 1: Quantum Mechanics

1.- Spin-$1/2$ Heisenberg model for two qubits: consider the Hamiltonian of two spins-$1/2$ (or *qubits*)

$$H = X_1 X_2 + Y_1 Y_2 + Z_1 Z_2 \ .$$

(a) Prove that $[H, \vec{S}] = 0$, where the total spin operator $\vec{S} = \vec{S}_1 + \vec{S}_2$ is defined such that

$$\vec{S}_1 \equiv \frac{1}{2}(X_1, Y_1, Z_1) \qquad \vec{S}_2 \equiv \frac{1}{2}(X_2, Y_2, Z_2)$$

(b) Compute the eigenbasis of operator $Z_1 Z_2$, and write H in this basis as a matrix.

(c) Compute the eigenvalues E_i and eigenvectors $|E_i\rangle$ of H, and check that $H = \sum_i E_i |E_i\rangle\langle E_i|$.

(d) Given a quantum state $|\psi\rangle$ of several parties, the *reduced density matrix* ρ of a susbsystem is defined by taking the *partial trace* over all the other systems on the state projector $|\psi\rangle\langle\psi|$. For instance, for a quantum state $|\psi\rangle$ of two qubits, the reduced density matrix of the first qubit is given by

$$\rho_1 \equiv \mathrm{tr}_2\left(|\psi\rangle\langle\psi|\right) = \sum_{i=0}^{1} \langle i_2|\psi\rangle\langle\psi|i_2\rangle \ ,$$

where $\{|i_2\rangle\}$ is some basis for the Hilbert space of the second qubit ($i_2 = 0, 1$). Also, the *von Neumann entropy or entanglement entropy* of a density matrix ρ is defined as

$$S(\rho) \equiv -\mathrm{tr}\left(\rho \log \rho\right) \ .$$

Compute the Schmidt decomposition, ρ_1, ρ_2, $S(\rho_1)$ and $S(\rho_2)$ for the eigenstate $|E_0\rangle$ of H with the lowest energy E_0 (ground state), and prove that $S(\rho_1)$ and $S(\rho_2)$ are maximal over the space of 2×2 trace-one Hermitian matrices.

(e) Compute the time evolution operator $U(t) = \exp(-iHt)$.

(f) Compute the state $|\psi(t)\rangle = U(t)|0_1\rangle|1_2\rangle$, where $\{|0\rangle, |1\rangle\}$ are the eigenstates of Z with ± 1 eigenvalue (spin up/down in the z-basis).

(g) Compute $\langle\psi(t)|Z_1|\psi(t)\rangle$, $\langle\psi(t)|X_1 Z_2|\psi(t)\rangle$, $\langle\psi(t)|H|\psi(t)\rangle$, and check that $\langle\psi(t)|H|\psi(t)\rangle \geq E_0$ always, with E_0 the lowest energy eigenvalue of H. This is an example of the *variational principle* for the ground state energy of a Hamiltonian.

2.- Bell Basis and CHSH inequality: consider the four quantum states

$$|\psi^{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|0_1 1_2\rangle \pm |1_1 0_2\rangle\right)$$
$$|\phi^{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|0_1 0_2\rangle \pm |1_1 1_2\rangle\right)$$

(a) Prove that they are an orthonormal basis of the Hilbert space of two qubits. This is called the *Bell basis.*

(b) Compute the Schmidt decomposition, ρ_1, ρ_2, $S(\rho_1)$ and $S(\rho_2)$ for these four states. Prove that $S(\rho_1)$ and $S(\rho_2)$ are always maximal over the space of 2×2 trace-one Hermitian matrices.

(c) Given the observables

$$Q = Z_1 \qquad S = \frac{-1}{\sqrt{2}}\left(Z_2 + X_2\right)$$
$$R = X_1 \qquad T = \frac{1}{\sqrt{2}}\left(Z_2 - X_2\right)$$

compute the quantity

$$|\langle QS\rangle + \langle RS\rangle + \langle RT\rangle - \langle QT\rangle|$$

where $\langle\ \cdot\ \rangle \equiv \langle\psi^-|\cdot|\psi^-\rangle$, and check that it is > 2.

(d) Compute the same combination of averages as above, but this time with $\langle\ \cdot\ \rangle \equiv \langle 0_1 1_2|\cdot|0_1 1_2\rangle$, and check that it is < 2. This is the *CHSH Bell inequality*: for classical (i.e. separable) bipartite probability distributions, the above combination of averages can *never* be larger than 2, whereas entangled quantum states can (and do) violate this. In fact, the states in the Bell basis maximally violate this inequality, and hence are also called *maximally entangled states of two qubits.*

3.- 3-qubit entanglement: consider the quantum states of 3 qubits

$$
\begin{aligned}
|GHZ\rangle &= \frac{1}{\sqrt{2}} \left(|+_1 +_2 +_3\rangle + |-_1 -_2 -_3\rangle \right) \\
|W\rangle &= \frac{1}{\sqrt{3}} \left(|0_1 0_2 1_3\rangle + |0_1 1_2 0_3\rangle + |1_1 0_2 0_3\rangle \right)
\end{aligned}
$$

(a) Imagine a bipartition of the system, where you take the first qubit versus the other two. For this bipartition, and for both states, compute the Schmidt decomposition, ρ_1 and $S(\rho_1)$. Which of the two states has more bipartite entanglement between qubit 1 and the rest of the system?

(b) Consider the closest product state to a given quantum state $|\psi\rangle$ of three qubits, i.e. the one that maximizes the squared overlap

$$
\Lambda^2 \equiv |\langle \phi_1 | \langle \phi_2 | \langle \phi_3 | \psi \rangle|^2 ,
$$

with $|\phi_i\rangle$ some state for qubit i. The *geometric entanglement* is defined as $E_g \equiv -\log \Lambda^2$, and is a measure of genuine *tripartite* entanglement, as opposed to bipartite measures like the entanglement entropy. In our case, the closest product states are given by $|+_1 +_2 +_3\rangle$ for the GHZ, and $|0_1 0_2 1_3\rangle$ for the W. Which of the two quantum states has more tripartite entanglement, as measured by E_g? How does this compare to $S(\rho_1)$ in the previous section?