Statistical physics 2, homework 1

1. Check which of the following matrices can be a density matrix and which describes a pure state:

$$\rho_1 = \begin{pmatrix} 2/7 & 0 \\ 0 & 5/7 \end{pmatrix}, \qquad \rho_2 = \begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix}, \qquad \rho_3 = \frac{1}{4}\begin{pmatrix} 1 & i\sqrt{3} \\ -i\sqrt{3} & 3 \end{pmatrix}$$
$$\rho_4 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \rho_5 = \frac{1}{5}\begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 4 \end{pmatrix}, \qquad \rho_6 = \frac{1}{9}\begin{pmatrix} 1 & 2 & 2 \\ 2 & 4 & 4 \\ 2 & 4 & 4 \end{pmatrix} \tag{1}$$

2. **Density matrix**
   - Consider a spin 1 system in the following state:
   $$|\alpha\rangle = i|1\rangle - |-1\rangle$$
   - construct the density matrix
   - check if the system is in a pure state
   - What is the expectation value of the spin?

3. **Duble spin**
   - A sorce emits two spins at the same time which may have two different polarications:
   $$|LL\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |LR\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |RL\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |RR\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$
   - The source can produce two different states:
   $$\rho_1 = \frac{1}{2}(|LL\rangle + |RR\rangle)(\langle LL| + \langle RR|)$$
   $$\rho_2 = \frac{1}{2}(|LL\rangle\langle LL| + |RR\rangle\langle RR|) \tag{2}$$
   - Calculate the density matrices and show which one of them is in a pure state.
   - Alice can measure only the first spin, Bob the second. What is the probability that Bob measures L if Alice has already measured L in both cases?

4. **Density matrix after transition**:
   - Let us consider a spin 1/2 system. We have two orthogonal pure states: $|\psi_1\rangle$ and $|\psi_2\rangle$. Choose an apropriate basis.
   - Using your basis write the density operator for the following states:
   $$\rho_1 = \frac{1}{2}(|\psi_1\rangle + |\psi_2\rangle)(\langle\psi_1| + \langle\psi_2|)$$
   $$\rho_2 = \frac{1}{2}(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|) \tag{3}$$
   - The system undergoes a transition according to the following:
   $$|\psi_1\rangle \to \frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle) = |\varphi_1\rangle$$
   $$|\psi_2\rangle \to \frac{1}{\sqrt{2}}(|\psi_1\rangle - |\psi_2\rangle) = |\varphi_2\rangle \tag{4}$$

- Write the transition operator in your basis
- Calculate the density matrix after the transition for both cases.
- What is the probability of observing $|\varphi_1\rangle$ and $|\varphi_2\rangle$?

5. **Thermal density matrix**: Consider a 1/2-spin system in an external field: $\mathcal{H} = h\sigma_z$.
   - Write doen the thermal density operator of the system.
   - Evaluate the density matrix for large and small temperatures.
   - Which of them is a pure state?
6. **I**sing model density matrix: Consider the Ising Hamiltonian:
$$\mathcal{H} = -J\sum_{(i,j)} \sigma_i\sigma_j - h\sum_i \sigma_i$$
   - Write down the density matrix for a simple spin in the mean field limit using the magnetization of the system.
   - Calculate the density matrix of the while system
   - Calculate the expected magnetization using the density matrix and show that it is equal to the magnetization used for the density matrix.
   - Calculate the expectatino value of the energy
7. **Neumann equation** Describe the time evolution of an 1/2 spin in an external magnetic field $\vec{B}$.
   - Write up a Zeeman Hamiltonian using Pauli matrices and an external field $\vec{B}$.
   - Write up the expectation value of the spin using the density matrix.
   - Using the invariance of the trace with respect to cyclic permutation of tensor product show that the Neumann equation of the above system reduces to:
$$i\frac{dP_i}{dt} = -\frac{1}{2}\gamma\sum_j B_j \mathrm{Tr}([\sigma_i, \sigma_j]\rho) \tag{5}$$
     , where $\vec{P}$ is the polarization of the spin
   - Show that the density matrix of the spin polarization is
$$\rho = \frac{1}{2}(I_2 + \vec{P}\vec{\sigma}), \tag{6}$$
     where I_2 is the 2×2 identity matrix and $\vec{\sigma}$ is the Pauli vector.
   - Show that using Eq. (6) in Eq. (5) gives
$$\frac{d\vec{P}}{dt} = \gamma\vec{P} \times \vec{B}$$
8. **Neumann equation for separable Hamiltonian**: Suppose that your Hamiltonian can be split into two parts: $\mathcal{H} = \mathcal{H}_0 + V$, where $\mathcal{H}_0$ is time independent. Define the time evolution operator operator:
$$U_I(t) = e^{-i\hbar\mathcal{H}_0 t},$$
   with
$$|\psi\rangle_I = U_I^+|\psi\rangle, \text{ and } A_I = U_I^+ A U_I.$$
   Show that the von Neumann equation translates to
$$i\hbar\frac{\partial}{\partial t}\rho_I(t) = [V(t), \rho_I(t)]$$
9. **The maximum entropy principle – simple example** Consider a random variable $X \in 1, 2, 3$ which can take 3 values. We know that the expectation value of $\langle X\rangle = \bar{x}$. The probability p_i of outcome i is unknown.
   - Write up the maximum entropy principle

- Derive the general solution for p_i.
- Determine the lagrange multipliers
- Determine p_i for the cases: $\bar{x} = 1$, $\bar{x} = 2$, and $\bar{x} = 3$.

10. **Closed system** A completely uncinstrained system has N states. Calculate the probability of finding the system in state i using the principle of maximum entropy.

11. **Boltzmann factor** Let us have a set of states i with energy E_i. We know that the total energy in the system is E.

    - Using the principle of maximum entropy show that the probability of state i is

    $$p_i \propto e^{-\beta E_i}, \tag{7}$$

    where β is the Lagrange multiplier for the energy.
    - Calculate the normalization factor
    - Calculate the relation between E and β

12. **Grand canonical ensemble** Let us have a set of states i with energy E_i and particle number N_i. We know that the total energy and the number of particles in the system are E and N respectively. Using the principle of maximum entropy show that the probability of state i is

    $$p_i \propto e^{-\beta E_i - \mu N_i}, \tag{8}$$

    where β is the Lagrange multiplier for the energy and μ is that of the particle number

13. **The principle of maximum entropy** Show that if the variance of a system is constrained than the probabilities of the states can be described by a Gaussian.

14. **The principle of maximum entropy – example** Consider a six sided loaded die with the sides numbered 1 through 6. [Note: A die is said to be loaded if the probabilities of the six possible outcomes are not uniform.] Using the principle of maximum entropy find the probabilities of outcomes (i.e., 1, 2, 3, 4, 5 and 6) for each of the given constraints.

    - The probability of an odd numbered outcome is 1/3.
    - The probability of obtaining a 2, 4 or 6 is zero and the expected value of the outcome is 4.
    - The probability of an odd numbered outcome is 1/3 and the probability of an outcome that is a multiple of three is 1/6.

15. **Maxwell-Boltzmann distribution**

    - Consider a set of states where $\sum_i x_i^2 = E$.
    - The density of states with outcome x goes as x^2
    - Show that the probability of a state with outcome x is proportional to:

    $$p(x) \propto x^2 \exp(-\lambda x^2)$$