Fundamentals of Quantum Technology
Homework Sheet 3

1. Let $\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle\psi_i|$ be the density operator describing the state of some system.
   (a) Show that for a pure state, $\hat{\rho}^2 = \hat{\rho}$. Conclude that $\mathrm{Tr}\hat{\rho}^2 = 1$.
   (b) Show that, generally,
   $$\mathrm{Tr}\hat{\rho}^2 = \sum_{i,j} p_i p_j \left|\langle\psi_i \,|\, \psi_j\rangle\right|^2 .$$
   Conclude that, for *any* state, $\mathrm{Tr}\hat{\rho}^2 \leq 1$, and that $\mathrm{Tr}\hat{\rho}^2 = 1$ holds only for a pure state; that is, if the state is mixed then necessarily $\mathrm{Tr}\hat{\rho}^2 < 1$.
2. Let $\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle\psi_i|$ be the density operator describing the state of some system.
   (a) Show that for any normalized state $|\varphi\rangle$, the number $\langle\varphi| \hat{\rho} |\varphi\rangle$ is real and obeys $0 \leq \langle\varphi| \hat{\rho} |\varphi\rangle \leq 1$ (this means that the diagonal terms of a density matrix are always real numbers between 0 and 1, regardless of the choice of basis in which we write this matrix).
   (b) The ensemble average of some operator $\hat{O}$ is defined as
   $$\left\langle \hat{O} \right\rangle = \sum_i p_i \langle\psi_i| \hat{O} |\psi_i\rangle .$$
   Show that this is equivalent to writing
   $$\left\langle \hat{O} \right\rangle = \mathrm{Tr}\left(\hat{\rho}\hat{O}\right).$$
   (c) Suppose that the dynamics of the system is governed by a Hamiltonian $\hat{H}$. Prove that the time evolution of the density operator is given by
   $$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \frac{i}{\hbar}\left[\hat{\rho}, \hat{H}\right].$$
3. A prominent example of a mixed state is the thermal equilibrium state. Let $\hat{H}$ be the Hamiltonian of a certain system, and let $\{|\varphi_n\rangle\}$ be the corresponding basis of energy eigenstates, with $\hat{H}|\varphi_n\rangle = E_n |\varphi_n\rangle$. We introduce the following density operator, representing the thermal state:
   $$\hat{\rho} = \frac{1}{Z} e^{-\beta\hat{H}},$$
   where β is an inverse temperature and Z is a normalization constant which insures that $\mathrm{Tr}\hat{\rho} = 1$.
   (a) Calculate Z in terms of β and the energy levels E_n. What function did you obtain?
   (b) Let $\hat{O}$ be an operator representing some observable. Calculate $\left\langle \hat{O} \right\rangle$ with respect to the thermal state, using the result of Question 2(b).

4. Determine whether the following states of composite systems are entangled or not, by calculating the purity of the appropriate reduced density operator. If the state is not entangled, write it in the form
$$|\Psi\rangle = |\psi\rangle_{\text{Subsystem } A} |\phi\rangle_{\text{Subsystem } B} ,$$
where A and B are the two subsystems to which the full system is partitioned.

(a) Two $\frac{1}{2}$-spin particles in the state
$$|\Psi\rangle = -\frac{1}{2\sqrt{2}} |\uparrow\rangle_1 |\uparrow\rangle_2 + \frac{1}{2\sqrt{2}} |\uparrow\rangle_1 |\downarrow\rangle_2 - \frac{i\sqrt{3}}{2\sqrt{2}} |\downarrow\rangle_1 |\uparrow\rangle_2 + \frac{i\sqrt{3}}{2\sqrt{2}} |\downarrow\rangle_1 |\downarrow\rangle_2 .$$

(b) Two $\frac{1}{2}$-spin particles in the state
$$|\Psi\rangle = \frac{1}{2\sqrt{2}} |\uparrow\rangle_1 |\uparrow\rangle_2 + \frac{\sqrt{3}}{2\sqrt{2}} |\uparrow\rangle_1 |\downarrow\rangle_2 - \frac{\sqrt{3}}{2\sqrt{2}} |\downarrow\rangle_1 |\uparrow\rangle_2 + \frac{1}{2\sqrt{2}} |\downarrow\rangle_1 |\downarrow\rangle_2 .$$

(c) A $\frac{1}{2}$-spin particle and a photonic mode that can be occupied by up to 2 photons (that is, the available states for it are $|0\rangle, |1\rangle, |2\rangle$) in the state
$$|\Psi\rangle = \frac{1}{3} |\uparrow\rangle |0\rangle + \frac{2}{3} |\downarrow\rangle |1\rangle + \frac{2}{3} |\uparrow\rangle |2\rangle .$$