Quantum Mechanics II

Exercise 1: Density matrix – Solutions

1. Take a mixed state $\hat{\rho} = \sum_k p_k |\psi_k\rangle\langle\psi_k|$. Prove that

   a) $\hat{\rho}$ is hermitian (this means $\hat{\rho}^\dagger = \hat{\rho}$).
   Solution: Indeed, we have

   $$\hat{\rho}^\dagger \quad = \left(\sum_k p_k |\psi_k\rangle\langle\psi_k|\right)^\dagger = \sum_k p_k \left(|\psi_k\rangle\langle\psi_k|\right)^\dagger = \sum_k p_k |\psi_k\rangle\langle\psi_k| = \hat{\rho}.$$

   b) $\mathrm{Tr}\,\hat{\rho} = 1$.
   Solution: Using the linearity of trace we have

   $$\mathrm{Tr}\left[\hat{\rho}\right] = \mathrm{Tr}\left[\sum_k p_k |\psi_k\rangle\langle\psi_k|\right] = \sum_k p_k \mathrm{Tr}\left[|\psi_k\rangle\langle\psi_k|\right] = \sum_k p_k = 1,$$

   where we have used that for each projector $\mathrm{Tr}\left[|\psi_k\rangle\langle\psi_k|\right] = 1$.

   c) $\hat{\rho} \geq 0$ (this means $\forall|\phi\rangle$ from the Hilbert space we have $\langle\phi|\hat{\rho}|\phi\rangle \geq 0$).
   Solution: For arbitrary state $|\phi\rangle$ we have

   $$\langle\phi|\hat{\rho}|\phi\rangle = \sum_k p_k \langle\phi|\psi_k\rangle\langle\psi_k|\phi\rangle = \sum_k p_k |\langle\phi|\psi_k\rangle|^2 \geq 0,$$

   because all the terms in the sum are non-negative: $\forall k$: $|\langle\phi|\psi_k\rangle|^2 \geq 0$ and $p_k \geq 0$.

   d) $1 - \hat{\rho} \geq 0$. Solution: Let us choose a basis $\{|n\rangle\}$, then

   $$\langle\phi|(1-\hat{\rho})|\phi\rangle = \langle\phi|1|\phi\rangle - \sum_k p_k \langle\phi|\psi_k\rangle\langle\psi_k|\phi\rangle = 1 - \sum_k p_k |\langle\phi|\psi_k\rangle|^2 \geq 1 - \sum_k p_k = 1 - 1 = 0,$$

   where the inequality is due to the fact that $\forall k$: $|\langle\phi|\psi_k\rangle|^2 \leq 1$.

How can we interpret the eigenvalues of $\hat{\rho}$?

Solution: Properties (a) - (d) of $\hat{\rho}$ imply that its eigenvalues ρ_n (in full generality they are not p_k !!!) are real and have the following properties

1. $\forall n : 0 \leq \rho_n \leq 1$,
2. $\sum_n \rho_n = 1$.

Therefore ρ_n may be interpreted as probabilities.

2. Demonstrate (prove) that $\mathrm{Tr}\,\hat{\rho}^2 \leq 1$. When does the equality $\mathrm{Tr}\,\hat{\rho}^2 = 1$ hold?

Solution:

$$\langle\phi|\hat{\rho}|\phi\rangle = \sum_k p_k \langle\phi|\psi_k\rangle\langle\psi_k|\phi\rangle = \sum_k p_k |\langle\phi|\psi_k\rangle|^2 \leq \sum_k p_k = 1,$$

where inequality is due to the fact that $\forall k$: $|\langle\phi|\psi_k\rangle|^2 \leq 1$.

It is easy to see that when there is only one term in the mixture $\hat{\rho} = |\psi\rangle\langle\psi|$ we have $\mathrm{Tr}\,\hat{\rho}^2 = 1$. This corresponds to a pure state.

3. Knowing that the evolution of $\rho(t)$ obeys Liouville's equation

$$i\hbar \frac{d}{dt}\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)], \tag{1}$$

show that it the initial state $\rho(0)$ is pure, it stays pure for all t.

Solution: Using Liouville's equation consider time derivative

$$\begin{aligned}
\frac{d}{dt}\left(\mathrm{Tr}\left[\hat{\rho}^2\right]\right) &= \mathrm{Tr}\left[\left(\frac{d}{dt}\hat{\rho}\right)\hat{\rho} + \rho\left(\frac{d}{dt}\hat{\rho}\right)\right] = \frac{1}{i\hbar}\mathrm{Tr}\left[([H,\hat{\rho}]\hat{\rho} + \hat{\rho}[H,\hat{\rho}])\right] \\
&= \frac{1}{i\hbar}\mathrm{Tr}\left[\hat{H}\hat{\rho}\hat{\rho} - \hat{\rho}\hat{H}\hat{\rho} + \hat{\rho}\hat{H}\hat{\rho} - \hat{\rho}\hat{\rho}\hat{H}\right] = \frac{1}{i\hbar}\mathrm{Tr}\left[\left((\hat{H}\hat{\rho}\hat{\rho} - \hat{\rho}\hat{\rho}\hat{H}\right)\right] \\
&= \frac{1}{i\hbar}\mathrm{Tr}\left[\left((\hat{H}\hat{\rho}\hat{\rho} - \hat{H}\hat{\rho}\hat{\rho}\right)\right] = 0,
\end{aligned}$$

where at the last step we used the invariance of trace under cyclic permutations. Thus the considered time derivative is zero for all states. This means that the value $\mathrm{Tr}\left[\hat{\rho}^2\right] = 1$ (for initial pure state) is not changed in the course of evolution. Hence initially pure states stay pure for all t.

Another solution uses the fact that Liouville's equation was deduced from the time evolution of pure states given by the Schrödinger equation. Initial pure state may be written as $\hat{\rho}(0) = |\psi(0)\rangle\langle\psi(0)|$. Then the time evolution leads to $\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}(t)^\dagger$ where $\{\hat{U}(t)\}$ is a family of *unitary* operators ($\hat{U}^\dagger(t) = \hat{U}^{-1}(t)$) parametrized by t and determined by the Schrödinger equation so that $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$. Then our state $\hat{\rho}(t)$ is pure at any time, because it can always be expressed in the form of projector:

$$\hat{\rho}(t) = \hat{U}(t)|\psi(0)\rangle\langle\psi(0)|\hat{U}^\dagger(t) = |\psi(t)\rangle\langle\psi(t)|.$$

NB: The first proof is conceptually more useful, because the value of $\mathrm{Tr}\left[\hat{\rho}^2\right]$ may be considered as a measure of the degree of "purity" for quantum states. As we have seen in question 2, the maximum value "1" corresponds to pure states. One can show that the minimum value is $1/d$ where d is the dimension of the Hilbert space. The minimum value is achieved by *maximally mixed* state $\rho_{\mathrm{mm}} = \mathbb{I}/d$, where $\mathbb{I} = \sum_{k=1}^d |k\rangle\langle k|$ is the identity operator and vectors $|k\rangle$ form an orthonormal basis. One can conclude that the *unitary* evolution preserves the (degree of) purity of quantum states.

4. Prove Ehrenfest's theorem using the evolution of $\hat{\rho}(t)$ which is given by Eq. (1).
<u>Solution:</u> Consider the time derivative of the expectation value of observable $\hat{A}$:

$$\begin{aligned}
\frac{d}{dt}\langle\hat{A}\rangle &= \frac{d}{dt}\left(\mathrm{Tr}\left[\hat{A}\hat{\rho}\right]\right) = \mathrm{Tr}\left[\left(\frac{d}{dt}\hat{A}\right)\hat{\rho} + \hat{A}\left(\frac{d}{dt}\hat{\rho}\right)\right] = \left\langle\frac{d}{dt}\hat{A}\right\rangle + \frac{1}{i\hbar}\mathrm{Tr}\left[\hat{A}[\hat{H},\hat{\rho}]\right] \\
&= \left\langle\frac{d}{dt}\hat{A}\right\rangle + \frac{1}{i\hbar}\mathrm{Tr}\left[\hat{A}\hat{H}\hat{\rho} - \hat{A}\hat{\rho}\hat{H}\right] = \left\langle\frac{d}{dt}\hat{A}\right\rangle + \frac{1}{i\hbar}\mathrm{Tr}\left[\hat{A}\hat{H}\hat{\rho} - \hat{H}\hat{A}\hat{\rho}\right] \\
&= \left\langle\frac{d}{dt}\hat{A}\right\rangle + \frac{1}{i\hbar}\mathrm{Tr}\left[[\hat{A},\hat{H}]\hat{\rho}\right] = \left\langle\frac{d}{dt}\hat{A}\right\rangle + \frac{1}{i\hbar}\left\langle[\hat{A},\hat{H}]\right\rangle.
\end{aligned}$$

5. In two-dimensional Hilbert space with orthonormal basis $\{|a\rangle, |b\rangle\}$, is it possible to distinguish by measurements the preparations of quantum states defined below?

a) Superposition of two basis states $|a\rangle$ and $|b\rangle$ given by corresponding amplitudes α and β. The density matrix of the state $\hat{\rho}_\psi = |\psi\rangle\langle\psi|$ where $|\psi\rangle = \alpha|a\rangle + \beta|b\rangle$ is

$$\begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}.$$

b) Statistical mixture of basis states $|a\rangle$ and $|b\rangle$ taken with weights $|\alpha|^2$ and $|\beta|^2$ correspondingly. The density matrix of the mixture $\hat{\rho}_{ab} = |\alpha|^2|a\rangle\langle a| + |\beta|^2|b\rangle\langle b|$ is

$$|\alpha|^2\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + |\beta|^2\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}.$$

c) Equally weighted mixture of pure states $|\psi\rangle$ and $|\phi\rangle$ where state $|\psi\rangle$ is the same as in item a) and state $|\phi\rangle$ is given by the amplitudes α and $-\beta$. The density matrix of the mixture $\hat{\rho}_{\psi\phi} = \frac{1}{2}|\psi\rangle\langle\psi| + \frac{1}{2}|\phi\rangle\langle\phi|$ where $|\phi\rangle = \alpha|a\rangle - \beta|b\rangle$ is

$$\frac{1}{2}\begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} |\alpha|^2 & -\alpha\beta^* \\ -\alpha^*\beta & |\beta|^2 \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}.$$

The density matrices of all tree states in the basis $\{|a\rangle, |b\rangle\}$ have the same diagonal elements and therefore cannot be distinguished by measurement of any observable, which is diagonal in this basis. Moreover, the density matrixes of states $\hat{\rho}_{ab}$ and $\hat{\rho}_{\psi\phi}$ are equal. Note that equal matrices are equal in any basis, therefore no measurement in any basis can distinguish the two preparations.

The density matrix of state $\hat{\rho}_\psi$ is different. It is diagonal in the basis $\{|\psi\rangle, |\psi^\perp\rangle\}$:

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

where it has only one nonzero element. If the system being in state $\hat{\rho}_\psi$ is measured in the basis $\{|\phi\rangle, |\psi^\perp\rangle\}$ no measurement outcome can correspond to the orthogonal state $|\psi^\perp\rangle$. This is not the case for states $\hat{\rho}_\psi$ and $\hat{\rho}_{\psi\phi}$ which have both diagonal elements grater than nonzero in any basis, because they are mixed states and the measurement outcome corresponding to state $|\phi^\perp\rangle$ is possible. Thus state $\hat{\rho}_\psi$ can be distinguished from the other two.