# Quantum Mechanics II

## Exercise 3: 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

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

   b) $\mathrm{Tr}\,\hat{\rho} = 1$.

   Solution: Using the linearity of trace we have

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

   where we have used the following property of projector $\mathrm{Tr}\,[|\psi_k\rangle\langle\psi_k|] = 1$.

   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 $\forall k$: $|\langle\phi|\psi_k\rangle|^2 \geq 0$ and $p_k \geq 0$.

   d) $1 - \hat{\rho} \geq 0$.

   Solution: For arbitrary state $|\phi\rangle$ we have

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

   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 $\rho_n$ (in full generality they are not $p_k$ because $|\psi_k\rangle$ may be not orthogonal) are real and have the following properties

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

Therefore $\rho_n$ may be interpreted as probabilities. They are probabilities to find the system in corresponding eigenstate $|\phi_n\rangle$.

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

Solution: Take a basis $\{|n\rangle\}$ then

$$
\begin{aligned}
\mathrm{Tr}\,\hat{\rho}^2 &= \sum_n \langle n| \left( \sum_k p_k |\psi_k\rangle\langle\psi_k| \sum_{k'} p_{k'} |\psi_{k'}\rangle\langle\psi_{k'}| \right) |n\rangle \\
&= \sum_{n,k,k'} p_k p_{k'} \langle n|\psi_k\rangle\langle\psi_k|\psi_{k'}\rangle\langle\psi_{k'}|n\rangle \\
&= \sum_{n,k,k'} p_k p_{k'}\rangle\langle\psi_{k'}|n\rangle\langle n|\psi_k\rangle\langle\psi_k|\psi_{k'}| \\
&= \sum_{k,k'} p_k p_{k'} \langle\psi_{k'}| \underbrace{\left( \sum_k |n\rangle\langle n| \right)}_{=\mathbb{I}} |\psi_k\rangle\langle\psi_k|\psi_{k'}\rangle \\
&= \sum_{k,k'} p_k p_{k'} \langle\psi_{k'}|\psi_k\rangle\langle\psi_k|\psi_{k'}\rangle \\
&= \sum_{k,k'} p_k p_{k'} \underbrace{||\langle\psi_{k'}|\psi_k\rangle||^2}_{\leq 1} \leq 1.
\end{aligned}
$$

The only possibility for the sum to be equal to one is if only one term in the mixture $\hat{\rho} = |\psi\rangle\langle\psi|$ does exist. Then the state is a projector which is a pure state.

3. Knowing that the evolution of $\rho(t)$ obeys Liouville's equation $i\hbar\frac{d}{dt}\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)]$, show that if the initial state $\rho(0)$ is pure, it stays pure for all $t$.

Solution: Using Liouville's equation consider time derivative

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

At the last step we used the invariance of trace under cyclic permutations. We conclude that the time derivative is zero for all states. This means that the value $\mathrm{Tr}\,[\hat{\rho}^2] = 1$ (for initial pure state) is constant under the 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 $\mathrm{Tr}\,[\hat{\rho}^2]$ 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 $\hat{\rho}(t)$ given by Liouville's equation.
   Solution: For any observable $\hat{A}$ we have:

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

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 $\alpha$ and $\beta$. 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 $\alpha$ 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 and therefore the states themselves as well although being differently prepared. The density matrices are equal in any basis, therefore no measurement can distinguish the two preparations.

The density matrix of state $\hat{\rho}_{\psi}$ is different. It is diagonal in the basis $\{|\psi\rangle, |\psi^{\perp}\rangle\}$ where it has only one nonzero element:

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

It is therefore a pure state. If a system being in this state $\hat{\rho}_{\psi}$ is measured in the basis $\{|\phi\rangle, |\psi^{\perp}\rangle\}$, no measurement outcome can correspond to the orthogonal state $|\psi^{\perp}\rangle$ because the corresponding probability is zero. This is not the case for two other mixtures $\hat{\rho}_{\psi}$ and $\hat{\rho}_{\psi\phi}$ having the density matrix with both diagonal elements greater than zero in any basis, because they are mixed states. If the system is prepared in this state the measurement outcome corresponding to state $|\phi^{\perp}\rangle$ is possible. Therefore one can unambigously discriminate state $\hat{\rho}_{\psi}$ from both states, $\hat{\rho}_{ab}$ and $\hat{\rho}_{\psi\phi}$, but not $\hat{\rho}_{ab}$ from $\hat{\rho}_{\psi\phi}$.