Problem. Density Matrix

Problem Statement

An alternative (and more general) way of describing a quantum system is through the density operator:

$$\rho = \sum_i w_i \left|\alpha^{(i)}\right\rangle \left\langle\alpha^{(i)}\right|, \quad \sum_i w_i = 1 \tag{124}$$

where the states $\alpha^{(i)}$ need not be orthogonal. A state where only one $w_i \neq 0$ is called a *pure state*. Otherwise it's called a mixture. Note that w_i is not parametrizing a superposition of states - the $|\alpha\rangle$'s themselves could also be superpositions.

1. Show that the trace of the density matrix $\text{Tr}(\rho) = 1$. (it is useful top remember the definition of the matrix elements)
2. Show that for a pure state $\rho^2 = \rho$ and $\text{Tr}(\rho^2) = 1$
3. Define the *ensemble average* for an operator $[A]$:

$$[A] = \sum_i w_i \left\langle\alpha^{(i)}\right| A \left|\alpha^{(i)}\right\rangle \tag{125}$$

   Now show that this may be written as

$$[A] = \text{Tr}(\rho A) \tag{126}$$

4. Show that, generally, $\text{Tr}(ABC...)$ is invariant under cyclic permutations. Use this to demonstrate that the trace does not depend on the basis used to represent the matrix.
5. Given a spin 1/2 particle, show that an equal superposition of states $|+\rangle + |-\rangle$, where $|\pm\rangle \equiv \left|S_z = \pm\frac{\hbar}{2}\right\rangle$ is not equivalent to the mixture of states proportional to $|+\rangle\langle+| + |-\rangle\langle-|$. Do this by explicitly evaluating $[S_x]$, where $S_x = \frac{\hbar}{2}(|+\rangle\langle-| + |-\rangle\langle+|)$. Do not forget to normalize your states and mixtures.
6. Given that the states $\left|\alpha^{(i)}\right\rangle$ obey the time-dependent Schrodinger equation, derive the equation of motion for ρ in the case where $w_i(t)$ are also time-dependent.

Solution 1.

$$\text{Tr}(\rho) = \sum_i \rho_{ii} \tag{127}$$

Let us define what do we mean by "ρ_{ii}",

$$\begin{aligned}
\rho_{ij} &= \langle i| \rho |j\rangle && (128)\\
&= \langle i| \left(\sum_k w_k \left|\alpha^{(k)}\right\rangle \left\langle\alpha^{(k)}\right|\right) |j\rangle && (129)\\
&= \sum_k w_k \left\langle i\middle|\alpha^{(k)}\right\rangle \left\langle\alpha^{(k)}\middle|j\right\rangle && (130)\\
&= \sum_k w_k \left\langle\alpha^{(k)}\middle|j\right\rangle \left\langle i\middle|\alpha^{(k)}\right\rangle && (131)
\end{aligned}$$

Using this definition in the first equation here,

$$\begin{aligned}
\text{Tr}(\rho) &= \sum_i \rho_{ii} && (132)\\
&= \sum_i \sum_k w_k \left\langle\alpha^{(k)}\middle|i\right\rangle \left\langle i\middle|\alpha^{(k)}\right\rangle && (133)
\end{aligned}$$

Now, using the fact that $\left|\alpha^{(i)}\right\rangle$ are complete states, i.e. $\sum_i |i\rangle\langle i| = 1$, we get

$$\mathrm{Tr}(\rho) = \sum_k w_k \left\langle \alpha^{(k)} \middle| \alpha^{(k)} \right\rangle \tag{134}$$

The $\left|\alpha^{(k)}\right\rangle$ may not be orthogonal, but we can assume wlog that they are normalized, i.e. $\left\langle \alpha^{(k)} \middle| \alpha^{(k)} \right\rangle = 1$,

$$\mathrm{Tr}(\rho) = \sum_k w_k = 1 \tag{135}$$

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Solution 2.

Let us now prove that $\rho^2 = \rho$ is indeed true for a pure state.

For a pure state, we can always find $|i\rangle \in \mathcal{H}$. We can again wlog assume that this state is normalized to unity, i.e. $\langle i|i\rangle = 1$ such that $\rho = |i\rangle\langle i|$ (As defined in the question, a pure state is where only one $w_i \neq 0$).

$$\rho^2 = \rho\rho = |i\rangle\langle i|i\rangle\langle i| = |i\rangle\langle i| = \rho \tag{136}$$

As we saw $\rho^2 = \rho$ for a pure state,

$$\mathrm{Tr}\left(\rho^2\right) = \mathrm{Tr}(\rho) = 1 \tag{137}$$

from the previous proof.

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Solution 3.

This could be one of those proofs where going RHS to LHS might be quicker. Let's see.
Let $A_{ij} = \langle i| A |j\rangle$ is the matrix elements of A with respect to an orthonormal basis $|i\rangle$.

$$\begin{aligned}
\mathrm{Tr}(\rho A) &= \sum_i \sum_j \rho_{ij} A_{ji} && (138)\\
&= \sum_i \sum_j \left(\sum_k w_k \left\langle \alpha^{(k)} \middle| j \right\rangle \left\langle i \middle| \alpha^{(k)} \right\rangle \right) (\langle j| A |i\rangle) && (139)\\
&= \sum_i \sum_j \sum_k w_k \left\langle \alpha^{(k)} \middle| j \right\rangle \langle j| A |i\rangle \left\langle i \middle| \alpha^{(k)} \right\rangle && (140)\\
& && (141)
\end{aligned}$$

Taking $|i\rangle, |j\rangle$ to be a complete set of states the sum over i, j will give us a one,

$$\mathrm{Tr}(\rho A) = \sum_k w_k \left\langle \alpha^{(k)} \middle| A \middle| \alpha^{(k)} \right\rangle = [A] \tag{142}$$

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Solution 4.

To prove the cyclic property of trace mathematically rigorously, induction should do the job. Although, as physcicists we could right now make a base case and a strong argument to generalize it.

$$\begin{aligned}
\mathrm{Tr}(AB) &= \sum_i \langle \psi_i| AB |\psi_i\rangle && (143)\\
&= \sum_{i,j} \langle \psi_i| A |\phi_j\rangle \langle \phi_j| B |\psi_i\rangle && (144)\\
&= \sum_{i,j} \langle \phi_j| B |\psi_i\rangle \langle \psi_i| A |\phi_j\rangle && (145)\\
&= \sum_j \langle \phi_i| BA |\phi_i\rangle && (146)\\
&= \mathrm{Tr}(BA) && (147)
\end{aligned}$$

Assuming one of the operator above is made of mutiple operators multiplying each other, we can do the exact same proofs by squeezing in more fat unities ($\sum_i |\psi_i\rangle \langle\psi_i| = 1$ into them and playing out the exact same proof. We also saw that we went from ψ basis to ϕ basis and still get back the original trace. Hence, the trace does is basis independent.

Solution 5.

$$|+\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \quad |-\rangle = \begin{bmatrix}0\\1\end{bmatrix} \tag{148}$$

$$\begin{aligned}
\rho = |+\rangle\langle+| + |-\rangle\langle-| &= \begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} + \begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} && (149)\\
&= \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix} && (150)\\
&= \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} && (151)
\end{aligned}$$

$$\begin{aligned}
[S_x] &= \mathrm{Tr}\left(\rho S_x\right) && (152)\\
&= \frac{\hbar}{2}\left(\langle+|\,\rho\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}|+\rangle + \langle-|\,\rho\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}|-\rangle\right) && (153)\\
&= \frac{\hbar}{2}\left(\begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} + \begin{bmatrix}0 & 1\end{bmatrix}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}\right) && (154)\\
&= 0 && (155)
\end{aligned}$$

Now same computation for the superposition state (already normalized),

$$|\psi_{\text{sup}}\rangle = |+\rangle + |-\rangle \equiv \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \tag{156}$$

$$\rho_{\text{sup}} = |\psi_{\text{sup}}\rangle\langle\psi_{\text{sup}}| = \frac{1}{2}\begin{bmatrix}1\\1\end{bmatrix}\begin{bmatrix}1 & 1\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix} \tag{157}$$

$$\begin{aligned}
[S_x]_{\text{sup}} &= \mathrm{Tr}\left(\rho_{\text{sup}} S_x\right) && (158)\\
&= \frac{\hbar}{4}\left(\langle+|\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}|+\rangle + \langle-|\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}|-\rangle\right) && (159)\\
&= \frac{\hbar}{4}\left(\begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} + \begin{bmatrix}0 & 1\end{bmatrix}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}\right) && (160)\\
&= \frac{\hbar}{4}(2) && (161)\\
&= \frac{\hbar}{2} && (162)
\end{aligned}$$

We can clearly see a difference between $[S_x]$ and $[S_x]_{\text{sup}}$ showing us the difference between the mixed and superposition states.

Solution 6.

$$\frac{d}{dt}\rho = \frac{d}{dt}\sum_i w_i(t)\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right| \tag{163}$$

$$= \sum_i \left(\frac{dw_i(t)}{dt}\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right|\right) + \sum_i w_i(t)\left(\left(\frac{d}{dt}\left|\alpha^{(i)}\right\rangle\right)\left\langle\alpha^{(i)}\right| + \left|\alpha^{(i)}\right\rangle\left(\frac{d}{dt}\left\langle\alpha^{(i)}\right|\right)\right) \tag{164}$$

$$= \sum_i \left(\frac{dw_i(t)}{dt}\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right|\right) + \sum_i w_i(t)\left[\left(-\frac{i}{\hbar}H\left|\alpha^{(i)}\right\rangle\right)\left\langle\alpha^{(i)}\right| + \left|\alpha^{(i)}\right\rangle\left(\frac{i}{\hbar}\left\langle\alpha^{(i)}\right|H\right)\right] \tag{165}$$

$$= \sum_i \left(\frac{dw_i(t)}{dt}\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right|\right) + \left[-\frac{i}{\hbar}H\sum_i w_i(t)\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right| + \frac{i}{\hbar}\sum_i w_i(t)\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right|H\right] \tag{166}$$

$$= \sum_i \left(\frac{dw_i(t)}{dt}\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right|\right) + \left[-\frac{i}{\hbar}H\rho + \frac{i}{\hbar}\rho H\right] \tag{167}$$

$$= \sum_i \left(\frac{dw_i(t)}{dt}\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right|\right) - \frac{i}{\hbar}\left[H,\rho\right] \tag{168}$$

$$\tag{169}$$