PHYS852 Quantum Mechanics II, Fall 2008

HOMEWORK ASSIGNMENT 1:
Density Operator

1. [10pts] The trace of an operator is defined as $Tr\{A\} = \sum_m \langle m|A|m\rangle$, where $\{|m\rangle\}$ is an arbitrary basis set. Introduce a second arbitrary basis set, and use it to prove that the trace is independent of the choice of basis.

   Let $\{|\phi_n\rangle\}$ be an arbitrary second basis.
   In the basis $\{|m\rangle\}$, the trace is
   $$\mathrm{Tr}\{A\} = \sum_m \langle m|A|m\rangle \tag{1}$$
   In basis $\{|\phi_m\rangle\}$, it is
   $$\mathrm{Tr}\{A\} = \sum_n \langle \phi_n|A|\phi_n\rangle \tag{2}$$
   inserting the projector onto basis $\{|m\rangle\}$ then gives
   $$\mathrm{Tr}\{A\} = \sum_{m,n} \langle \phi_n|m\rangle\langle m|A|\phi_n\rangle \tag{3}$$
   re-ordering gives
   $$\mathrm{Tr}\{A\} = \sum_{m,n} \langle m|A|\phi_n\rangle\langle \phi_n|m\rangle \tag{4}$$
   recognizing that $\sum_n |\phi_n\rangle\langle\phi_n| = I$ leads to
   $$\mathrm{Tr}\{A\} = \sum_m \langle m|A|m\rangle \tag{5}$$

2. [10pts] Prove the linearity of the trace operation by proving $Tr\{aA+bB\} = aTr\{A\}+bTr\{B\}$.

$$\begin{aligned} \mathrm{Tr}\{aA+bB\} &= \sum_m \langle m|(aA+bB)|m\rangle \\ &= a\sum_m \langle m|A|m\rangle + b\sum_m \langle m|B|m\rangle \\ &= a\mathrm{Tr}\{A\} + b\mathrm{Tr}\{B\} \end{aligned} \tag{6}$$

3. [10pts] Prove the cyclic property of the trace by proving $Tr\{ABC\} = Tr\{BCA\} = Tr\{CAB\}$.

$$\begin{aligned}
\mathrm{Tr}\{ABC\} &= \sum_{m_1} \langle m_1|ABC|m_1\rangle \\
&= \sum_{m_1,m_2,m_3} \langle m_1|A|m_2\rangle\langle m_2|B|m_3\rangle\langle m_3|C|m_1\rangle \\
&= \sum_{m_1,m_2,m_3} \langle m_3|C|m_1\rangle\langle m_1|A|m_2\rangle\langle m_2|B|m_3\rangle = \mathrm{Tr}\{CAB\} \\
&= \sum_{m_1,m_2,m_3} \langle m_2|B|m_3\rangle\langle m_3|C|m_1\rangle\langle m_1|A|m_2\rangle = \mathrm{Tr}\{BCA\}
\end{aligned} \tag{7}$$

4. [10pts] Which of the following density matrices correspond to a pure state?

$$\rho_1 = \begin{pmatrix} \frac{2}{7} & 0 \\ 0 & \frac{5}{7} \end{pmatrix} \qquad \rho_2 = \begin{pmatrix} \frac{1}{4} & i\frac{\sqrt{3}}{4} \\ -i\frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix} \qquad \rho_3 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\rho_4 = \begin{pmatrix} \frac{1}{5} & \frac{\sqrt{2}}{5} \\ \frac{\sqrt{2}}{5} & \frac{4}{5} \end{pmatrix} \qquad \rho_5 = \begin{pmatrix} \frac{1}{9} & \frac{2}{9} & \frac{2}{9} \\ \frac{2}{9} & \frac{4}{9} & \frac{4}{9} \\ \frac{2}{9} & \frac{4}{9} & \frac{4}{9} \end{pmatrix}$$

A pure state must satisfy $\rho_{mn}\rho_{nm} = \rho_{mm}\rho_{nn}$ for every m and n.

ρ_1: $\frac{10}{49} \neq 0$, so NO.

ρ_2: $\frac{3}{16} = \frac{3}{16}$, so YES.

ρ_3: $0 = 0$, so YES

ρ_4: $\frac{4}{25} \neq \frac{2}{25}$, so NO

ρ_5: $m, n{=}1, 2 \rightarrow \frac{4}{81} = \frac{4}{81}$; $m, n{=}1, 3 \rightarrow \frac{4}{81} = \frac{4}{81}$; and $m, n{=}2, 3 \rightarrow \frac{16}{81} = \frac{16}{81}$, so YES.

5. [10 pts] Derive the equation of motion, $\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H, \rho(t)]$, using Schrödinger's equation and the most general form of the density operator, $\rho = \sum_j P_j |\psi_j\rangle\langle\psi_j|$.

$$\begin{aligned}
\frac{d}{dt}\rho &= \frac{d}{dt}\sum_j P_j|\psi_j\rangle\langle\psi_j| \\
&= \sum_j P_j\left[\left(\frac{d}{dt}|\psi_j\rangle\right)\langle\psi_j| + |\psi_j\rangle\frac{d}{dt}\langle\psi_j|\right] \\
&= \sum_j P_j\left[-\frac{i}{\hbar}H|\psi_j\rangle\langle\psi_j| + \frac{i}{\hbar}|\psi_j\rangle\langle\psi_j|H\right] \\
&= -\frac{i}{\hbar}H\sum_j P_j|\psi_j\rangle\langle\psi_j| + \frac{i}{\hbar}\left(\sum_j |\psi_j\rangle\langle\psi_j|\right)H \\
&= -\frac{i}{\hbar}\left[H, \rho\right] \qquad (8)
\end{aligned}$$