

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

$$Tr\{A\} = \sum_m \langle m|A|m\rangle \quad (1)$$

In basis  $\{|\phi_m\rangle\}$ , it is

$$Tr\{A\} = \sum_n \langle \phi_n|A|\phi_n\rangle \quad (2)$$

inserting the projector onto basis  $\{|m\rangle\}$  then gives

$$Tr\{A\} = \sum_{m,n} \langle \phi_n|m\rangle \langle m|A|\phi_n\rangle \quad (3)$$

re-ordering gives

$$Tr\{A\} = \sum_{m,n} \langle m|A|\phi_n\rangle \langle \phi_n|m\rangle \quad (4)$$

recognizing that  $\sum_n |\phi_n\rangle \langle \phi_n| = I$  leads to

$$Tr\{A\} = \sum_m \langle m|A|m\rangle \quad (5)$$

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

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

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

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

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

$$\begin{aligned}
 \rho_1 &= \begin{pmatrix} \frac{2}{7} & 0 \\ 0 & \frac{5}{7} \end{pmatrix} & \rho_2 &= \begin{pmatrix} \frac{1}{4} & i\frac{\sqrt{3}}{4} \\ -i\frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix} & \rho_3 &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\
 \rho_4 &= \begin{pmatrix} \frac{1}{5} & \frac{\sqrt{2}}{5} \\ \frac{\sqrt{2}}{5} & \frac{4}{5} \end{pmatrix} & \rho_5 &= \begin{pmatrix} \frac{1}{9} & \frac{2}{9} & \frac{2}{9} \\ \frac{2}{9} & \frac{4}{9} & \frac{4}{9} \\ \frac{2}{9} & \frac{4}{9} & \frac{4}{9} \end{pmatrix}
 \end{aligned}$$

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

$\rho_1$ :  $\frac{10}{49} \neq 0$ , so NO.

$\rho_2$ :  $\frac{3}{16} = \frac{3}{16}$ , so YES.

$\rho_3$ :  $0 = 0$ , so YES

$\rho_4$ :  $\frac{4}{25} \neq \frac{2}{25}$ , so NO

$\rho_5$ :  $m, n=1, 2 \rightarrow \frac{4}{81} = \frac{4}{81}$ ;  $m, n=1, 3 \rightarrow \frac{4}{81} = \frac{4}{81}$ ; 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,  $\rho = \sum_j P_j |\psi_j\rangle\langle\psi_j|$ .

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