L15 Density Matrix

**M9: Trace of an Operator**

# Math Background: Trace

Operator

$$A \doteq \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1d} \\ a_{21} & a_{22} & \cdots & a_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ a_{d1} & a_{d2} & \cdots & a_{dd} \end{pmatrix}$$

Notation:
trace of A: Tr[ A ]

in bra-ket notation

$$Tr[A] = \sum_{i=1}^{d} \langle \phi_i | A | \phi_i \rangle$$

in coordinates:

$$Tr[A] = \sum_{i=1}^{d} a_{ii}$$

Trace operation is ***basis independent*** of the orthonormal basis $| \phi_i \rangle$ that is used to evaluate it!

Tr:
maps operator to complex number

A, B, C: operators
$\alpha$, $\beta$: complex numbers

Rules:

Cyclic Property
Tr[ A B C] = Tr [ B C A]

Linearity
Tr[$\alpha$ A + $\beta$ B] = $\alpha$ Tr[A] + $\beta$ Tr[B]

Examples:

1) $$Tr\left[|\Psi\rangle\langle\phi|\right] = \langle\phi|\Psi\rangle$$

2) A: normal operator
with eigenvalues $\lambda_i$

$$Tr[A] = \sum_{i=1}^{d} \lambda_i$$

## 4.8 Statistical Operator (density matrix)

### 4.8.1 Motivation and Definition

# Source: Mixed State vs. Pure State

Pure State Source
$|\Psi\rangle$

➔

**Prediction rules for superposition states:**

Pr("i") = $|\langle \phi_i | \Psi \rangle|^2$

**Mixed State Source**
$\{\Pr(\text{signal s}) \;\; , |\Psi_s\rangle\}_{s=1}^{n}$

➔

**Prediction rules for mixed states sources:**

$$\Pr(\text{"i"}) = \sum_{s=1}^{n} \Pr(\text{signal s}) \;\; |\langle \phi_i | \Psi_s \rangle|^2$$

**source side**

quantum states
+
a-priori probabilities

➔ statistical operator!!!!
(density matrix)

**measurement side:**

mean values

observed probabilities
+
assigned values

➔ observable operator!!!

**Mixed Source Expectation Value Prediction of Observable A:**

$$\langle A \rangle = \sum_s Pr(s) \langle \Psi_s | A | \Psi_s \rangle = Tr\left[ \underbrace{\sum_s Pr(s) |\Psi_s\rangle\langle\Psi_s|}_{\text{density matrix}} A \right]$$

density matrix
$$\rho := \sum_s Pr(s) |\Psi_s\rangle\langle\Psi_s|$$

$$\boxed{\langle A \rangle = \langle \Psi | A | \Psi \rangle}$$

Pure State Source $\rho = |\Psi\rangle\langle\Psi|$

$$\boxed{\langle A \rangle = Tr\left[\rho A\right]}$$

Mixed State Source

Intermediate steps leading to definition of density matrix:

$$\langle A \rangle = \sum_s Pr(s) \langle \Psi_s | A | \Psi_s \rangle$$
$$= \sum_s Pr(s)\, Tr\left[ |\Psi_s\rangle\langle\Psi_s| A \right]$$
$$= Tr\left[ \left( \sum_s Pr(s) |\Psi_s\rangle\langle\Psi_s| \right) A \right]$$

**4.8.2. Simple example with two situations:**

1. $\left.\begin{array}{ll} \frac{1}{2}, & |+\rangle \\ \frac{1}{2}, & |-\rangle \end{array}\right\} \Rightarrow \rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

2. $\left.\begin{array}{ll} \frac{1}{2}, & |+\rangle_x \\ \frac{1}{2}, & |-\rangle_x \end{array}\right\} \Rightarrow \rho = \frac{1}{2}\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Note that situation 1 and 2 are described by the same density matrix!
Therefore, all predictions using situation 1 or 2 will be identical!

**It does not matter how you prepare you source by mixing pure state sources: if the density matrix of different preparation method are identical, the mixed state sources are equivalent!**

### 4.8.3 Further Example:

observable: $A = |+\rangle\langle+|$

$$\Rightarrow \langle A\rangle = Pr(+)$$

source: $|\psi_1\rangle = |+\rangle_x, \; p_1 = \frac{1}{3}$

$$|\psi_2\rangle = |+\rangle, \; p_2 = \frac{2}{3}$$

$$\Rightarrow \langle A\rangle = Tr[A\rho] = Tr[A\rho]$$

with $A \doteq \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

$$\rho \doteq \frac{1}{3}\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{2}{3}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{6}+\frac{2}{3} & 1/6 \\ 1/6 & 1/6 \end{pmatrix} = \begin{pmatrix} 5/6 & 1/6 \\ 1/6 & 1/6 \end{pmatrix}$$

$$\Rightarrow A\rho = \begin{pmatrix} 5/6 & 1/6 \\ 0 & 0 \end{pmatrix}$$

$$\Rightarrow Tr[A\rho] = \frac{5}{6}$$

### 4.8.4 Density matrices and Global phase

$$|\psi\rangle \longrightarrow \rho = |\psi\rangle\langle\psi|$$

$$|\psi'\rangle = e^{i\phi}|\psi\rangle \rightarrow \rho = |\psi'\rangle\langle\psi'|$$

$$= e^{i\phi}|\psi\rangle\langle\psi|e^{-i\phi} = |\psi\rangle\langle\psi|$$

==> density matrix automatically eliminates global phases

### 4.8.5 General Properties of Density Matrices

1) **Hermitian** $\rho = \rho^{\dagger}$

2) **positive semi definite** $\rho \geq 0$

$$\langle \Psi | \rho | \Psi \rangle \geq 0 \quad \forall | \Psi \rangle$$

3) **Unit Trace**

$$Tr\left[\rho\right] = 1$$

Proofs:

1) $$\rho^{+} = \sum_{s} P_r(s)^{*} |\Psi_s\rangle\langle\Psi_s| = \sum_{s} P_r(s) |\Psi_s\rangle\langle\Psi_s|$$

$$= \rho$$

2) $$\langle \Psi | \rho | \Psi \rangle = \sum_{s} P_r(s) \langle \Psi | \Psi_s \rangle \langle \Psi_s | \Psi \rangle$$

$$= \underbrace{\sum_{s} \underbrace{P_r(s)}_{\geq 0} \underbrace{|\langle \Psi | \Psi_s \rangle|^2}_{\geq 0}}_{\geq 0}$$

3) $$Tr[\rho] = \sum_{s} P_r(s) \, Tr\left[|\Psi_s\rangle\langle\Psi_s|\right]$$

$$= \sum_{s} P_r(s) \langle \Psi_s | \Psi_s \rangle$$

$$= \sum_{s} P_r(s) = 1$$

### 4.8.6 Interpretation of Density Matrices

A source is completely characterized by its density matrix. Different sources and strategies can lead to the same density matrix, and are therefore equivalent in the quantum mechanical point of view (prediction of measurement outcome probabilities).

A) The density matrix completely describes the source!

B) several source preparations methods can yield same density matrix:

→ the sources are then completely equivalent

C) For given $\rho$, one can always find *one particular* source realization via the spectral decomposition!

**Inverse problem:**

Given any operator $\rho$ that is hermitian, positive semi-definite and has unit trace, then there is a strategy to build a source that has $\rho$ as its density matrix.

This strategy is not unique, there may be infinitely many approaches.

Canonical approach:

Write down the spectral decomposition of $\hat{\rho}$ :

$$\rho = \sum_i \lambda_i \, |\psi_i\rangle\langle\psi_i|$$

where the $|\psi_i\rangle$ are automatically orthonomal states. Moreover, as $\rho$ is positive semi-definite, the eigenvalues $\lambda_i$ must be non-negative. Finally, if $\rho$ has unit trace, we also have $\sum_i \lambda_i = 1$ .

Therefore, using a set of source which produce the pure states $|\psi_i\rangle$ each with a probability $\lambda_i$ will give an effective source described by density matrix $\rho$ .

$$\{\Pr(\text{signal s}) \ \ , |\Psi_s\rangle\}_{s=1}^{n}$$

eigenvalues $\lambda_i$
eigenvectors $|\lambda_i\rangle$

$$\rho := \sum_s Pr(s)|\Psi_s\rangle\langle\Psi_s|$$

$$\boldsymbol{\rho}$$

**<u>Use:</u>**

$$\boxed{\langle A\rangle = Tr\left[\rho A\right]}$$

Mixed State Source

**<u>4.8.7 Bloch Vector (special topic for 2-dimensional systems)</u>**

**4.8.7.1 Expansion into Pauli Operators**

The density matrix $\rho$ can be expanded in the operator basis formed by the identity operation $\mathbb{1}$ and Pauli operators $\sigma_x, \sigma_y, \sigma_z$

**Pauli Operators:**

$$\sigma_z \doteq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \sigma_x \doteq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y \doteq \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\rho = \alpha_0 \mathbb{1} + \alpha_x \sigma_x + \alpha_y \sigma_y + \alpha_z \sigma_z$$

Note: $\mathrm{tr}\, \mathbb{1} = \mathrm{Tr}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = 2$

$\mathrm{tr}\, \sigma_x = \mathrm{tr}\, \sigma_y = \mathrm{tr}\, \sigma_z = 0$

But: $\mathrm{Tr}(\rho) \overset{!}{=} 1$

$\Rightarrow \alpha_0 = \frac{1}{2}$

a more convenient parameterization then turns out to be

$$\rho = \frac{1}{2}\Big(\mathbb{1} + \underbrace{\vec{v}\cdot\vec{\sigma}}_{v_x\sigma_x + v_y\sigma_y + v_z\sigma_z}\Big)$$

## 4.8.7.2 Expansion Coefficients

Note:

$$\langle \sigma_x \rangle = \mathrm{Tr}\left[\frac{1}{2}(\mathbb{1} + \vec{v}\vec{\sigma})\,\sigma_x\right]$$

$$= \frac{1}{2}\mathrm{Tr}\left[(\mathbb{1} + v_x\sigma_x + v_y\sigma_y + v_z\sigma_z)\sigma_x\right]$$

$$= \frac{1}{2}\mathrm{Tr}\left[\sigma_x + v_x\mathbb{1} - v_y i\sigma_z + i v_z\sigma_y\right]$$

$$= v_x$$

So $\quad v_x = \langle \sigma_x \rangle = P_r(+in\,x) - P_r(-in\,x)$

Similar: $\quad v_y = \langle \sigma_y \rangle$

$$v_z = \langle \sigma_z \rangle$$

That means, that by performing the SG measurement in x, y and z direction, we can determine the Bloch vector $\vec{v}$ completely, and therefore determine also the density matrix of an arbitrary source completely.

This extends our earlier results regarding pure states to the case of mixed state sources.

### 4.8.7.3Properties of $\vec{v}$. (Bloch vector)

1) $\vec{v}$ is a three-dimensional vector over real numbers

Proof: $\rho, \sigma_x, \sigma_y, \sigma_z$ are hermitian, e.g. $\quad \rho = \rho^+$

Then $\quad \rho^+ = \frac{1}{2}(\mathbb{1} + \vec{v}^* \cdot \vec{\sigma})$

$$\parallel$$

$$\rho = \frac{1}{2}(\mathbb{1} + \vec{v}\cdot\vec{\sigma})$$

The decomposition into the operator basis of Pauli matrices and identity is unique, so therefore we have

$$\vec{v}^* = \vec{v}$$

That means, all elements of $\vec{v}$ must be real valued.

$$\boxed{2)\quad \|\vec{v}\| = \sqrt{\vec{v}\cdot\vec{v}} \leq 1}$$

Proof:
Write $\quad \vec{v} = \|\vec{v}\| \; \vec{e}_v$

$$\|\vec{e}_v\| = \sqrt{\vec{e}_v\cdot\vec{e}_v} = 1$$

Then

$$\rho = \frac{1}{2}\left(\mathbb{1} + \sqrt{\|\vec{v}\|}\; \vec{e}_v \cdot \hat{\vec{\sigma}}\right)$$

Eigenvalues:

$\vec{e}_v\cdot\vec{\sigma}$ : $\quad \pm 1$

(compare section 4.2 of Lecture 10 we are basically talking about a general spin component here!)

$\Rightarrow \rho$ : Eigenvalues $\quad \frac{1}{2}\left(1 \pm \sqrt{\|\vec{v}\|}\right)$

$\rho \geq 0$

Since we require $\quad 1 - \sqrt{\|\vec{v}\|} \geq 0$

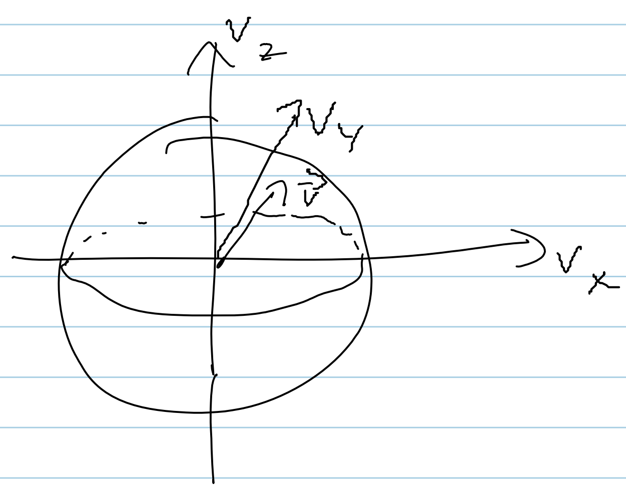
we also need to require

$$\Rightarrow \vec{v}\cdot\vec{v} \leq 1$$

$$\Rightarrow \sqrt{\vec{v}\cdot\vec{v}} \leq 1$$

**4.8.7.4 Graphical Representation: Bloch sphere**

Any density matrix $\rho$ of a two-dimensional quantum mechanical system is completely characterized by its Bloch vector $\vec{v}$ and can therefore be represented as vector with a 3-dimensional sphere :




Any vector within the unit sphere corresponds to a density matrix

Pure states are states on the surface!

If $\vec{v} \cdot \vec{v} = 1$

Then $\rho$ has eigenvalues 0 and 1, and its spectral decomposition is

$$\rho = |\psi\rangle\langle\psi|$$

for some vector $|\psi\rangle$ which is the eigenvector to eigenvalue 1.

**4.8.7.5 Example:**

Completely mixed state (thermal source)

$$\rho = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-| = \frac{1}{2}\mathbb{1}$$

$$\Rightarrow \quad \vec{v} = \begin{pmatrix} \langle\sigma_x\rangle \\ \langle\sigma_y\rangle \\ \langle\sigma_z\rangle \end{pmatrix} = \begin{pmatrix} \mathrm{Tr}[\rho\sigma_x] \\ \mathrm{Tr}[\rho\sigma_y] \\ \mathrm{Tr}[\rho\sigma_z] \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} \mathrm{Tr}[\sigma_x] \\ \mathrm{Tr}[\sigma_y] \\ \mathrm{Tr}[\sigma_z] \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$