

1. Entanglement

Entanglement Involves Multipartite States!

- Let $\mathcal{H}_A, \mathcal{H}_B$ be vector spaces for *two* quantum 2-state systems.
 - The state space for the combined "bipartite" system is represented by the *product vector space* $\mathcal{H}_A \otimes \mathcal{H}_B$.
- Suppose $\{|0_A\rangle, |1_A\rangle\}$ is a basis for $\mathcal{H}_A$ and $\{|0_B\rangle, |1_B\rangle\}$ is a basis for $\mathcal{H}_B$.
 - Then: $\{|0_A\rangle|0_B\rangle, |0_A\rangle|1_B\rangle, |1_A\rangle|0_B\rangle, |1_A\rangle|1_B\rangle\}$ is a basis for $\mathcal{H}_A \otimes \mathcal{H}_B$.
 - And: Any bipartite state $|Q\rangle$ in $\mathcal{H}_A \otimes \mathcal{H}_B$ can be expanded in this basis:

$$|Q\rangle = a|0_A\rangle|0_B\rangle + b|0_A\rangle|1_B\rangle + c|1_A\rangle|0_B\rangle + d|1_A\rangle|1_B\rangle$$

Def. 1 (*Product/non-product vector state*). A **product vector state** in a product vector space $\mathcal{H}_A \otimes \mathcal{H}_B$ is a vector $|\psi\rangle$ that can be written as a product of two vectors $|\psi\rangle = |v_A\rangle \otimes |v_B\rangle$, where $|v_A\rangle \in \mathcal{H}_A$ and $|v_B\rangle \in \mathcal{H}_B$. A **non-product vector state** in $\mathcal{H}_A \otimes \mathcal{H}_B$ is a vector that is not a product vector.

Examples

- *Non-product*: $|\Psi^+\rangle = \sqrt{1/2} \{ |0_A\rangle |0_B\rangle + |1_A\rangle |1_B\rangle \}$

- *Product*:

$$|Q\rangle = \sqrt{1/4} \{ |0_A\rangle |0_B\rangle + |0_A\rangle |1_B\rangle + |1_A\rangle |0_B\rangle + |1_A\rangle |1_B\rangle \}$$

$$= \sqrt{1/4} \{ |0_A\rangle + |1_A\rangle \} \{ |0_B\rangle + |1_B\rangle \}$$

$$|Q'\rangle = \sqrt{1/2} \{ |0_A\rangle |0_B\rangle + |1_A\rangle |0_B\rangle \} = \sqrt{1/2} \{ |0_A\rangle + |1_A\rangle \} |0_B\rangle$$

$$|Q''\rangle = |0_A\rangle |0_B\rangle$$

- Suppose $|0\rangle$ and $|1\rangle$ are eigenstates of Hardness ($|0\rangle = |hard\rangle$ and $|1\rangle = |soft\rangle$).

According to the Eigenvalue-Eigenvector Rule:

- In vector states $|\Psi^+\rangle$ and $|Q\rangle$, both electrons have no determinate Hardness value.

 Both are in superposed states

- In vector state $|Q'\rangle$, electron *A* has no determinate Hardness value, but electron *B* *does* (i.e., hard).

 Electron *A* is in a superposed state

- In vector state $|Q''\rangle$, both electrons have determinate Hardness values.

Examples

- *Non-product*: $|\Psi^+\rangle = \frac{1}{\sqrt{2}} \{ |0_A\rangle |0_B\rangle + |1_A\rangle |1_B\rangle \}$

- *Product*:

$$|Q\rangle = \frac{1}{\sqrt{4}} \{ |0_A\rangle |0_B\rangle + |0_A\rangle |1_B\rangle + |1_A\rangle |0_B\rangle + |1_A\rangle |1_B\rangle \}$$

$$= \frac{1}{\sqrt{4}} \{ |0_A\rangle + |1_A\rangle \} \{ |0_B\rangle + |1_B\rangle \}$$

$$|Q'\rangle = \frac{1}{\sqrt{2}} \{ |0_A\rangle |0_B\rangle + |1_A\rangle |0_B\rangle \} = \frac{1}{\sqrt{2}} \{ |0_A\rangle + |1_A\rangle \} |0_B\rangle$$

$$|Q''\rangle = |0_A\rangle |0_B\rangle$$

- Suppose $|0\rangle$ and $|1\rangle$ are eigenstates of Hardness ($|0\rangle = |hard\rangle$ and $|1\rangle = |soft\rangle$).

According to the Projection Postulate:

- In the non-product vector state $|\Psi^+\rangle$, when a measurement is performed on electron A, its state collapses (to either $|0_A\rangle$ or $|1_A\rangle$), *and this instantaneously affects the state of electron B!*
- In any of the product vector states, a measurement performed on electron A will not affect the state of electron B.

*Spooky action
at a distance?*

*Can this be
detected?*

Entanglement Involves Correlations!

- Idea: When a bipartite system is in an entangled vector state, its subsystems can have properties that are correlated in a non-classical way.


*Can't be explained
by a direct cause!* *Can't be explained by
a common cause!*

- Quantum Information Theory: How to exploit entanglement correlations to solve computational problems.

Task #1: *How can we represent correlated observables with respect to vector states?*

Task #2: *How can we represent correlations that cannot be due to either a direct cause or a common cause?*

Def. 2 (*Expectation value for vector state*). The **expectation value** $\langle O \rangle_\psi$ of an observable represented by an operator O with respect to a vector state $|\psi\rangle$ is given by $\langle O \rangle_\psi \equiv \langle \psi | O | \psi \rangle$.

- Idea: $\langle O \rangle_\psi$ is the average value of O in the vector state $|\psi\rangle$.
 - Suppose: O has eigenvectors $|b_i\rangle$ and eigenvalues b_i , and let $|\psi\rangle = \sum_i \alpha_i |b_i\rangle$, $\langle \psi | = \sum_j \alpha_j^* \langle b_j |$.
 - Then:

$$\begin{aligned}
 \langle O \rangle_\psi &= \langle \psi | O | \psi \rangle = \sum_j \alpha_j^* \langle b_j | O \sum_i \alpha_i | b_i \rangle \\
 &= \sum_{i,j} b_i \alpha_j^* \alpha_i \langle b_j | b_i \rangle \quad \leftarrow \begin{array}{l} \langle b_j | b_i \rangle = 1 \text{ for } i = j, \text{ and } 0 \text{ otherwise.} \\ \alpha_i^* \alpha_i = |\alpha_i|^2 = \text{Pr}_{|\psi\rangle}(b_i | O) \end{array} \\
 &= \sum_i b_i \text{Pr}_{|\psi\rangle}(b_i | O)
 \end{aligned}$$

The average value of the set of values $\{b_1, \dots, b_n\}$ with the Born probabilities $\{\text{Pr}_{|\psi\rangle}(b_1 | O), \dots, \text{Pr}_{|\psi\rangle}(b_n | O)\}$ assigned to its members.

Def. 3 (*Product operator*). Let O_A and O_B be operators on vector spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, and let $|\psi_A\rangle \in \mathcal{H}_A$, $|\psi_B\rangle \in \mathcal{H}_B$, and $|\psi_A \otimes \psi_B\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. The **product operator** $O_A \otimes O_B$ is defined by

$$(O_A \otimes O_B)|\psi_A \otimes \psi_B\rangle \equiv O_A|\psi_A\rangle \otimes O_B|\psi_B\rangle$$

- *Idea*: The "A" part of $O_A \otimes O_B$ only acts on the "A" part of $|\psi_A \otimes \psi_B\rangle$, and the "B" part of $O_A \otimes O_B$ only acts on the "B" part of $|\psi_A \otimes \psi_B\rangle$.
- O_A and O_B represent observables (properties) of the two subsystems of a composite bipartite system.

What does it mean to say these observables are correlated with each other?

Def. 4 (*Correlated observables for vector states*). Let O_A and O_B be operators on vector spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ with identity operators I_A and I_B , and let $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. Then the observables represented by O_A and O_B are **correlated in vector state $|\psi\rangle$** just when

$$\langle O_A \otimes O_B \rangle_\psi \neq \langle O_A \otimes I_B \rangle_\psi \langle I_A \otimes O_B \rangle_\psi$$

 The expectation value of $O_A \otimes O_B$ cannot be factored into a product of the expectation values of its "parts"

- Motivation: The observables O_A and O_B are correlated in the sense of Def. 4 *if and only if* they are *statistically dependent*; i.e.,

$$\Pr_{|\psi\rangle}(a_i, b_j | O_A, O_B) \neq \Pr_{|\psi\rangle}(a_i | O_A) \Pr_{|\psi\rangle}(b_j | O_B), \quad \text{for all } i, j$$

$$\left(\begin{array}{l} \text{The joint probability of getting} \\ \text{the value } a_i \text{ of } O_A \text{ and the} \\ \text{value } b_j \text{ of } O_B \text{ in the state } |\psi\rangle \end{array} \right) \neq \left(\begin{array}{l} \text{The probability of} \\ \text{getting the value } a_i \\ \text{of } O_A \text{ in the state } |\psi\rangle \end{array} \right) \times \left(\begin{array}{l} \text{The probability of} \\ \text{getting the value } b_j \\ \text{of } O_B \text{ in the state } |\psi\rangle \end{array} \right)$$

Task #1 accomplished!

Claim. Observables represented by the operators O_A and O_B that appear in a product operator $O_A \otimes O_B$ are uncorrelated in a product vector state and correlated in a non-product vector state.

- Example: Let $|\psi_{\text{prod}}\rangle = |\psi_A \psi_B\rangle$ and $|\psi_{\text{non}}\rangle = \sqrt{1/2}\{|\psi_A \phi_B\rangle + |\phi_A \psi_B\rangle\}$ be a product vector and a non-product vector in $\mathcal{H}_A \otimes \mathcal{H}_B$.

$$\begin{aligned}
 \langle O_A \otimes O_B \rangle_{\psi_{\text{prod}}} &= \langle \psi_A \psi_B | (O_A \otimes O_B) | \psi_A \psi_B \rangle \\
 &= \langle \psi_A \psi_B | (O_A | \psi_A \rangle \otimes O_B | \psi_B \rangle) \quad \leftarrow \text{def. of product operator} \\
 &= \langle \psi_A | O_A | \psi_A \rangle \langle \psi_B | O_B | \psi_B \rangle \quad \leftarrow \text{def. of product space inner-product} \\
 &= \langle \psi_A | O_A | \psi_A \rangle (\langle \psi_B | I_B | \psi_B \rangle) (\langle \psi_A | I_A | \psi_A \rangle) \langle \psi_B | O_B | \psi_B \rangle \quad \leftarrow \text{insertion of identity} \\
 &= \langle \psi_A \psi_B | (O_A \otimes I_B) | \psi_A \psi_B \rangle \langle \psi_A \psi_B | (I_A \otimes O_B) | \psi_A \psi_B \rangle \quad \leftarrow \text{rearranging...} \\
 &= \langle O_A \otimes I_B \rangle_{\psi_{\text{prod}}} \langle I_A \otimes O_B \rangle_{\psi_{\text{prod}}}
 \end{aligned}$$

No correlation between O_A and O_B in $|\psi_{\text{prod}}\rangle$!

Claim. Observables represented by the operators O_A and O_B that appear in a product operator $O_A \otimes O_B$ are uncorrelated in a product vector state and correlated in a non-product vector state.

- Example: Let $|\psi_{\text{prod}}\rangle = |\psi_A \psi_B\rangle$ and $|\psi_{\text{non}}\rangle = \sqrt{1/2}\{|\psi_A \phi_B\rangle + |\phi_A \psi_B\rangle\}$ be a product vector and a non-product vector in $\mathcal{H}_A \otimes \mathcal{H}_B$.

$$\begin{aligned}\langle O_A \otimes O_B \rangle_{\psi_{\text{non}}} &= \frac{1}{2} \{ \langle \psi_A \phi_B | + \langle \phi_A \psi_B | \} (O_A \otimes O_B) \{ |\psi_A \phi_B\rangle + |\phi_A \psi_B\rangle \} \\ &= \frac{1}{2} \{ \langle O_A \rangle_{\psi_A} \langle O_B \rangle_{\phi_B} + \langle \phi_A | O_A | \psi_A \rangle \langle \psi_B | O_B | \phi_B \rangle + \langle \psi_A | O_A | \phi_A \rangle \langle \phi_B | O_B | \psi_B \rangle \\ &\quad + \langle O_A \rangle_{\phi_A} \langle O_B \rangle_{\psi_B} \}\end{aligned}$$

$$\begin{aligned}\langle O_A \otimes I_B \rangle_{\psi_{\text{non}}} \langle I_A \otimes O_B \rangle_{\psi_{\text{non}}} &= \frac{1}{4} \{ \langle O_A \rangle_{\psi_A} \langle O_B \rangle_{\phi_B} + \langle O_A \rangle_{\psi_A} \langle O_B \rangle_{\psi_B} + \langle O_A \rangle_{\phi_A} \langle O_B \rangle_{\phi_B} + \langle O_A \rangle_{\phi_A} \langle O_B \rangle_{\psi_B} \}\end{aligned}$$

$$\underline{\text{So:}} \quad \langle O_A \otimes O_B \rangle_{\psi_{\text{non}}} \neq \langle O_A \otimes I_B \rangle_{\psi_{\text{non}}} \langle I_A \otimes O_B \rangle_{\psi_{\text{non}}}$$

Correlation between O_A and O_B in $|\psi_{\text{non}}\rangle$!

So: *Non-product vector states exhibit correlations between observables.*

- *Can these correlations be explained by direct causes and/or common causes?*

- In $|\psi_{\text{non}}\rangle = \frac{1}{\sqrt{2}}\{|0_A 1_B\rangle - |1_A 0_B\rangle\}$, there is a *correlation* between the Hardness properties of electron A & electron B: When one is *hard*, the other is *soft*.

- Direct cause explanation?

- No! Projection Postulate entails that when a measurement is performed on electron A, its state collapses (to either $|0_A\rangle$ or $|1_A\rangle$), and this *instantaneously affects the state of electron B!*

"Spooky action at a distance"!



- Common cause explanation?

- No! Can show that in $|\psi_{\text{non}}\rangle$ there are pair-wise correlations between four spin- $\frac{1}{2}$ observables such that a particular sum of their expectation values violates a "Bell" inequality that it must satisfy if the correlations are due to a common cause.



John Stewart Bell
(1928-1990)



A bit messy to demonstrate! Ultimately due to the way we represent expectation values of bipartite properties in a non-product vector state.

So: *Non-product vector states exhibit correlations between observables that cannot be explained either by a direct cause or a common cause.*

- *Classical* correlations can always be explained by a direct cause and/or a common cause.
- This suggests that the correlations exhibited by non-product vector states are unique to quantum mechanics.
 - *Call them "entanglement correlations".*
 - *Call the vector states in quantum mechanics that support them, "entangled vector states".*

Def. 5 (*Entangled vector state*). A state represented by a multipartite vector $|\psi\rangle$ is **entangled** just when $|\psi\rangle$ is a non-product vector state.

Task #2 accomplished!

2. Density Operators

- Motivation: Suppose a quantum system is associated with an *ensemble* $\{|\psi_i\rangle, p_i\}$ of vector states $|\psi_i\rangle$, each with a probability p_i .



Suppose we don't know what state our quantum system is in; suppose all we know are its possible states.

- Recall: In Gibbs' approach to classical statistical mechanics, we considered an ensemble of *classical* states to be a *classical* phase space Γ with a probability distribution $\rho(x, t)$ defined on it.
 - *In QM, we use a vector space $\mathcal{H}$ instead of a classical phase space Γ .*
 - *What should we use instead of the function $\rho(x, t)$?*

Answer: An operator...

Def. 6 (Density operator). The density operator ρ for a system in an ensemble $\{|\psi_i\rangle, p_i\}$ of m vector states $|\psi_i\rangle \in \mathcal{H}$ each with probability p_i , is defined by

$$\rho = \sum_{i=1}^m p_i |\psi_i\rangle\langle\psi_i|, \text{ where } \sum_{i=1}^m p_i = 1.$$

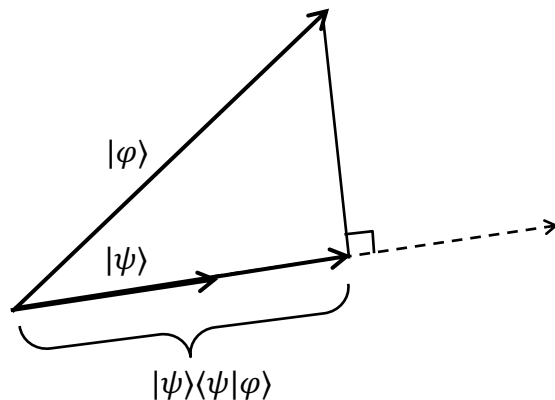
*Warning! Same notation but different mathematical objects:
 ρ in QM is an operator.
 $\rho(x, t)$ in classical Stat Mech is a function.*

• Note 1: $|\psi\rangle\langle\psi|$ is a *projection operator*.

- It acts on a vector $|\varphi\rangle$ and gives you another vector $|\psi\rangle\langle\psi|\varphi\rangle$.
- It projects $|\varphi\rangle$ in the direction of $|\psi\rangle$.

vector $|\psi\rangle$!

- inner product (number) $\langle\psi|\varphi\rangle$!
- the magnitude of $|\varphi\rangle$ in the direction of $|\psi\rangle$!



Def. 6 (*Density operator*). The density operator ρ for a system in an ensemble $\{|\psi_i\rangle, p_i\}$ of m vector states $|\psi_i\rangle \in \mathcal{H}$ each with probability p_i , is defined by

$$\rho = \sum_{i=1}^m p_i |\psi_i\rangle \langle \psi_i|, \quad \text{where } \sum_{i=1}^m p_i = 1.$$

*Warning! Same notation but different mathematical objects:
 ρ in QM is an operator.
 $\rho(x, t)$ in classical Stat Mech is a function.*

- Note 2: The vector states $\{|\psi_i\rangle\}$ are not necessarily orthogonal to each other, and m is not necessarily the dimension n of $\mathcal{H}$.

But: ρ can always be expressed in terms of a basis $\{|\phi_i\rangle\}$ of $\mathcal{H}$ as

$$\rho = \sum_{i=1}^n \lambda_i |\phi_i\rangle \langle \phi_i|$$

where $|\phi_i\rangle$ are eigenvectors of ρ with eigenvalues $\lambda_i \geq 0$.

← Because ρ is Hermitian!

- And: Since ρ is supposed to represent an ensemble of vector states, in this case $\{|\phi_i\rangle, \lambda_i\}$, we require $\sum_{i=1}^n \lambda_i = 1$. ← The sum of the eigenvalues of a density operator is 1!

Def. 6 (Density operator). The density operator ρ for a system in an ensemble $\{|\psi_i\rangle, p_i\}$ of m vector states $|\psi_i\rangle \in \mathcal{H}$ each with probability p_i , is defined by

$$\rho = \sum_{i=1}^m p_i |\psi_i\rangle \langle \psi_i|, \quad \text{where } \sum_{i=1}^m p_i = 1.$$

*Warning! Same notation but different mathematical objects:
 ρ in QM is an operator.
 $\rho(x, t)$ in classical Stat Mech is a function.*

- Note 3: A density operator can describe more than one ensemble of vector states.

Example:

Let: $|a\rangle = \sqrt{3/4}|0\rangle + \sqrt{1/4}|1\rangle$

$|b\rangle = \sqrt{3/4}|0\rangle - \sqrt{1/4}|1\rangle$

Then: $|0\rangle = \sqrt{1/3}|a\rangle + \sqrt{1/3}|b\rangle$

$|1\rangle = |a\rangle - |b\rangle$

So: $\rho = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b|$ corresponds to $\rightsquigarrow \{|a\rangle, |b\rangle; \frac{1}{2}, \frac{1}{2}\}$

$= \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$ corresponds to $\rightsquigarrow \{|0\rangle, |1\rangle; \frac{3}{4}, \frac{1}{4}\}$

*distinct ensembles,
same density
operator*

Def. 7 (*Pure/mixed density operator state*). If a density operator can be expressed as $\rho = |\psi\rangle\langle\psi|$, then it is called a **pure density operator state**. Otherwise, it is called a **mixed density operator state**.

- Note 1: An "ignorance" interpretation of a mixed density operator state is not always appropriate!

$$\rho = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2| + \dots$$

← Ignorance as to what vector state the system is in?

- Concern 1: ρ can describe more than one ensemble of vector states.

Let: $|a\rangle = \sqrt{3/4}|0\rangle + \sqrt{1/4}|1\rangle$

$|b\rangle = \sqrt{3/4}|0\rangle - \sqrt{1/4}|1\rangle$

Then: $\rho = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b|$ corresponds to $\{|a\rangle, |b\rangle; \frac{1}{2}, \frac{1}{2}\}$
 $= \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$ corresponds to $\{|0\rangle, |1\rangle; \frac{3}{4}, \frac{1}{4}\}$

← If the system is in the density operator state ρ , which ensemble is it in?

- Concern 2: An ignorance interpretation cannot be applied to a mixed density operator state of a subsystem of a composite system in a pure *entangled* density operator state.

Def. 7 (*Pure/mixed density operator state*). If a density operator can be expressed as $\rho = |\psi\rangle\langle\psi|$, then it is called a **pure density operator state**. Otherwise, it is called a **mixed density operator state**.

- Note 2: A mixed density operator state is not the same thing as a superposed vector state!

Example:

- The mixed density operator state $\rho = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b|$ corresponds to an *ensemble* of vector states $\{|a\rangle, |b\rangle; \frac{1}{2}, \frac{1}{2}\}$.
- The pure density operator state $\rho = \frac{1}{2}\{|a\rangle + |b\rangle\}\{\langle a| + \langle b|\}$ corresponds to a *single* vector state $\frac{1}{\sqrt{2}}\{|a\rangle + |b\rangle\}$.

3. von Neumann Entropy

- Recall: A density operator $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ that characterizes an ensemble $\{|\psi_i\rangle, p_i\}$ of quantum vector states is the correlate of a Gibbs distribution $\rho(x, t)$ that characterizes an ensemble of classical states.
- And: The Gibbs entropy is given by $S_{\text{Gibbs}}(\rho) = -k \int_{\Gamma} \rho(x, t) \ln \rho(x, t) dx$



Recall: ρ in QM is an operator; $\rho(x, t)$ in classical Stat Mech is a function.



The ensemble average of $-k \ln \rho(x, t)$

What is the quantum correlate of S_{Gibbs} ?

Def. 8 (*von Neumann entropy*). The **von Neumann entropy** $S_{\text{vN}}(\rho)$ of a density operator state ρ is defined by

$$S_{\text{vN}}(\rho) \equiv -\text{Tr}(\rho \ln \rho)$$



John von Neumann
(1903-1957)

- Note 1: What is " $\ln \rho$ "? *We know what $\ln$ does to a number, but what does it do to an operator?*

- Let B be an operator such that $B|\psi_i\rangle = b_i|\psi_i\rangle$.
- Let $f(x)$ be a function on the real numbers.
- Then $f(B)|\psi_i\rangle \equiv f(b_i)|\psi_i\rangle$

If B is an operator with eigenvalues b_i , then " $f(B)$ " is the name for the operator with eigenvalues $f(b_i)$.

- Recall: Can always express ρ as $\rho = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$, where $\rho|\phi_i\rangle = \lambda_i|\phi_i\rangle$

- So: $\ln \rho |\phi_i\rangle = \ln \lambda_i |\phi_i\rangle$



$\ln \rho$ is an operator with eigenvalues $\ln \lambda_i$.



- ρ is an operator with eigenvalues λ_i
- $\{|\phi_i\rangle\}$ is a basis for $\mathcal{H}$

Def. 8 (*von Neumann entropy*). The **von Neumann entropy** $S_{\text{vN}}(\rho)$ of a density operator state ρ is defined by

$$S_{\text{vN}}(\rho) \equiv -\text{Tr}(\rho \ln \rho)$$



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- Note 2: If ρ is a density operator state on an n -dim vector space $\mathcal{H}$, then the maximum value of $S_{\text{vN}}(\rho)$ is $\ln n$.

Proof: Note first:

$$S_{\text{vN}}(\rho) = -\text{Tr}(\rho \ln \rho) = -\sum_{i=1}^n \langle \phi_i | (\rho \ln \rho) | \phi_i \rangle = -\sum_{i=1}^n \lambda_i \ln \lambda_i \quad \{\phi_i\} \text{ is an eigen-vector basis of } \rho$$

- Now recall $(d/d\lambda_i)S_{\text{vN}}(\lambda_i^*) = 0$ for the λ_i^* that maximizes S_{vN} :

$$dS_{\text{vN}}(\lambda_i^*) = -\sum_{i=1}^n (\ln \lambda_i^* - \alpha) d\lambda_i = 0 \quad \leftarrow \text{constrained by } \sum_{i=1}^n d\lambda_i = 0$$

- Solve for λ_i^* :

$$\lambda_i^* = e^\alpha \Rightarrow \sum_{i=1}^n \lambda_i = ne^\alpha = 1 \Rightarrow \alpha = \ln(1/n) \Rightarrow \lambda_i^* = (1/n)$$

- Thus: $S_{\text{vN}}(\lambda_i^*) = -\sum_{i=1}^n (1/n) \ln(1/n) = -n(1/n) \ln(1/n) = \ln n$

Def. 8 (*von Neumann entropy*). The **von Neumann entropy** $S_{\text{vN}}(\rho)$ of a density operator state ρ is defined by

$$S_{\text{vN}}(\rho) \equiv -\text{Tr}(\rho \ln \rho)$$



John von Neumann
(1903-1957)

• Claim: $\text{Tr}(\rho O)$ is the expectation value $\langle O \rangle_\rho$ of the operator O in the density operator state ρ .

- So: $S_{\text{vN}}(\rho)$ is the expectation value of the operator $-\ln \rho$ in the density operator state ρ .

← Analogous to ensemble average in Gibbs approach!

Proof: Let $\{|\psi_j\rangle, p_j\}$ be associated with ρ , and let $|b_i\rangle$ and b_i be eigenvectors and values of O .

- Then: We can expand each $|\psi_j\rangle$ in the $|b_i\rangle$ basis as $|\psi_j\rangle = \sum_k \alpha_{jk} |b_k\rangle$, and express ρ as $\rho = \sum_j p_j |\psi_j\rangle \langle \psi_j| = \sum_{j,k,l} p_j \alpha_{jk} \alpha_{jl}^* |b_k\rangle \langle b_l|$.

- So: $\text{Tr}(\rho O) = \sum_i \langle b_i | \rho O | b_i \rangle$

$$= \sum_{i,j,k,l} p_j b_i \alpha_{jk} \alpha_{jl}^* \langle b_i | b_k \rangle \langle b_l | b_i \rangle$$

$\langle b_i | b_k \rangle = 1$ for $i = k$, and 0 otherwise.
 $\langle b_l | b_i \rangle = 1$ for $l = i$, and 0 otherwise.

$$= \sum_j p_j \sum_i b_i \alpha_{ji} \alpha_{ji}^*$$

$\alpha_{ji} \alpha_{ji}^* = |\alpha_j|^2 = \text{Pr}_{|\psi_j\rangle}(b_i | B)$

$$= \sum_j p_j \sum_i b_i \text{Pr}_{|\psi_j\rangle}(b_i | B)$$

$$= \sum_j p_j \langle O \rangle_{\psi_j}$$

- The weighted sum of the ave. value of O in each vector state $|\psi_j\rangle$ in the ensemble $\{|\psi_j\rangle, p_j\}$.
- Which is the ave. value of O in the density operator state ρ !

What does $S_{\text{vN}}(\rho)$ measure?

Def. 9 (*Maximally mixed density operator state*). Let ρ be a density operator on an n -dim vector space $\mathcal{H}$ with identity operator I_n . Then ρ is **maximally mixed** just when it can be expressed by $\rho = (1/n)I_n$.

- Recall: A mixed density operator can be expressed by $\rho = \sum_{i=1}^n \lambda_i |\phi_i\rangle\langle\phi_i|$ where the $|\phi_i\rangle$ form a basis for $\mathcal{H}$, and $\sum_{i=1}^n \lambda_i = 1$.
 - And: ρ is pure just when one λ_i is 1 and all the rest are 0.
- Intuition: The more mixed ρ is, the "farther away" it is from the pure case.
 - And: The maximum "distance" ρ is from the pure case occurs when all the λ_i are equal; i.e., when $\lambda_i = 1/n$.
- So:
$$\begin{aligned}\rho_{\max} &= \sum_{i=1}^n (1/n) |\phi_i\rangle\langle\phi_i| \\ &= (1/n) \sum_{i=1}^n |\phi_i\rangle\langle\phi_i| \\ &= (1/n) I_n\end{aligned}$$

$S_{\text{vN}}(\rho)$ is a measure of the degree to which ρ is mixed!

Claim 1. Let ρ be a density operator on an n -dim vector space $\mathcal{H}$. Then $S_{\text{vN}}(\rho)$ varies from zero, if ρ is a pure density operator state, to $\ln n$, if ρ is a maximally mixed density operator state.

- Proof: Suppose ρ is a pure density operator state.
 - Then: $S_{\text{vN}}(\rho) = -\sum_{i=1}^n \lambda_i \ln \lambda_i = -\ln(1) = 0$
- Now Suppose ρ is a maximally mixed density operator state.
 - Then: $S_{\text{vN}}(\rho) = -\sum_{i=1}^n \lambda_i \ln \lambda_i = -\sum_{i=1}^n (1/n) \ln(1/n)$
 $= -\ln(1/n)$
 $= \ln n \quad \leftarrow \text{The maximum value of } S_{\text{vN}}!$