Let's now consider a random variable. We then perform a series of observations on this random variable.

Let the set of possible outcomes be $\{e_m\}$ each of which whith probability P_m in such a way that

$$P_m \geq 0 \quad \forall m \qquad \sum_m^{M} P_m = 1$$

→ number of possible outcomes

We then define the entropy of the probability function

$$S[P] = - \sum_{m=1}^{M} P_m \ln P_m$$

typically in information theory one would use $\log_2$, but we can notice that a base change will only lead to a a multiplicative constant in the entropy (normalization)

Let's consider two cases

(i) $P_m = 1 \quad m=1$ (or one particular value of m)

$P_m = 0$ otherwise

The system is completely determined

$$\lim_{x \to 0} x \ln x = 0$$

$$\Rightarrow \boxed{S[P] = 0}$$

(ii) $P_m = \frac{1}{M} \quad \forall m$ (uniform distribution)

$$S[P] = - \sum_m^{M} \frac{1}{M} \ln M^{-1} = -\left(-\frac{1}{M} \ln M\right) \underbrace{\sum_{m=1}^{M}}_{M} = \ln M$$

↑ number of possible outcomes

$$\boxed{S[P] = \ln M}$$

Question: What is the maximum of entropy?

constraint : $\sum_m P_m = 1 \Rightarrow$ Lagrange multiplier

$$\tilde{S}[P] = S[P] - \lambda\left(\sum_m P_m - 1\right)$$

$$\frac{\partial \tilde{S}[P]}{\partial P_m} = \frac{\partial}{\partial P_m}\left[-\sum_{m=1} P_m \ln P_m\right] - \frac{\partial}{\partial P_m}\left[\lambda \sum_m P_m - 1\right]$$

$$= -\ln P_m - \overbrace{\cancel{\frac{P_m}{P_m}}}^{1} - \lambda = 0$$ extrema

This is valid for all m, so

$$P_m = 1/M \quad \forall m$$

Maximum or Minimum? $\Rightarrow$ Maximum because we've shown that

$S[P] = 0$ for $P_m = 1$ $m=1$; $P_m = 0$ otherwise

$$0 \leq S[P] \leq \ln M$$

uniform distribution

We note that complete knowledge about the system leads to zero entropy and the distribution that provides the least amount of information the larges entropy $\rightarrow$ in the uniform distribution all outcomes have equal probability.

If we now consider two random variables with possible outcomes

$$\{e_m, e_{m'}\}$$

If the variables are independent

$$P_{m,m'} = P_m \cdot P_{m'}$$

We then call $P \otimes P'$ the joint probability and

$$S[P \otimes P'] = -\sum_{m\,m'}^{M\,M'} P_{mm'} \ln P_{mm'} = -\sum_{m}^{M}\sum_{m'}^{M} P_m P_{m'} \ln P_m P_{m'}$$

$$= -\sum_{m}^{M}\sum^{M'} P_m P_{m'} (\ln P_m + \ln P_{m'})$$

$$= \underbrace{\left(-\sum_m P_m \ln P_m\right)}_{S[P']} \underbrace{\sum_{m'}^{M'} P_{m'}}_{1} - \underbrace{\sum_m P_m}_{1} \underbrace{\sum_{m'}^{M'} P_{m'} \ln P_{m'}}_{S[P']}$$

$$S[P \otimes P'] = S[P] + S[P']$$

In general for non independent events

$$S[P \otimes P'] \leq S[P] + S[P']$$ we will show this later.

Now, if the entropy is to be calculated from an ensemble of microstates, somehow we would like to use the information contained in the density matrix

$$D = \sum_n |\psi_n\rangle p_n \langle\psi_n|$$

to calculate the entropy

Intuitively we could state

$$S[D]_{tentative} = -\sum p_n \ln p_n$$

For a pure state

$D = |\psi\rangle\langle\psi|$ $\quad p_n = 1 \quad$ $S[D]_{tentative} = 0$

Ok! We have perfect knowledge about the system

We also remind ourselves that the entropy is a physical quantity and as such should be the average of some operator

$$\langle A\rangle = \sum_n p_n \underbrace{\langle\psi_n|A|\psi_n\rangle}_{-\ln p_n\ ?} = \mathrm{Tr}\, AD$$

If $A|a\rangle = a|a\rangle$
$f(A)|a\rangle = f(a)|a\rangle$

If $\{|\psi_n\rangle\}$ were eigenstates of D then $A = -\ln D$

and $S[D]_{tentative} = -k\,\mathrm{Tr}\, D \ln D = -k \sum_n p_n \ln p_n$

Ok!

The problem is that this is not generally the case

We can, however diagonalize $D = \sum_m |m\rangle P_m \langle m|$ where $\sum_m |m\rangle\langle m| = \mathbb{I}$

and $\sum_m P_m = 1$

because

$\mathrm{Tr}\, D = 1$

Let's now take the following example

Two level system

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

$$|\psi_1\rangle = |0\rangle \qquad |\psi_2\rangle = (1-\delta)^{1/2}|1\rangle + \delta|0\rangle$$

$$D = \frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2| = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}\left[\delta|0\rangle + (1-\delta^2)^{1/2}|1\rangle\right]\left[\delta\langle 0| + (1-\delta^2)^{1/2}\langle 1|\right]$$

$$D = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} + \frac{1}{2}\begin{pmatrix}\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & 1-\delta^2\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1+\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & 1-\delta^2\end{pmatrix}$$

$$\ln D = -\ln 2 + \ln\left[\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + \begin{pmatrix}\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & -\delta^2\end{pmatrix}\right]$$

$$\ln(\mathbb{I} + C) = \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}C^n$$

$$\approx \begin{pmatrix}\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & -\delta^2\end{pmatrix} - \underbrace{\underbrace{\frac{1}{2}\begin{pmatrix}\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & -\delta^2\end{pmatrix}\begin{pmatrix}\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & -\delta^2\end{pmatrix}}_{\frac{1}{2}\begin{pmatrix}\delta^4+\delta^2(1-\delta^2) & 0\\ 0 & \delta^4+\delta^2(1-\delta^2)\end{pmatrix}}}_{\frac{1}{2}\begin{pmatrix}\delta^2 & 0\\ 0 & \delta^2\end{pmatrix}}$$

$$D\ln D \approx -\ln 2\, D + \frac{1}{2}\begin{pmatrix}1+\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & 1-\delta^2\end{pmatrix}\begin{pmatrix}\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & -\delta^2\end{pmatrix} - \frac{1}{2}\begin{pmatrix}1+\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & 1-\delta^2\end{pmatrix}\frac{1}{2}\begin{pmatrix}\delta^2 & 0\\ 0 & \delta^2\end{pmatrix}$$

$$-D\ln 2 + \frac{1}{2}\begin{pmatrix}\delta^2+\delta^4+\delta^2(1-\delta^2) & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & 0\end{pmatrix} - \frac{\delta^2}{4}\begin{pmatrix}1+\delta^2 & \delta(1-\delta^2)^{1/2}\\ \delta(1-\delta^2)^{1/2} & 1-\delta^2\end{pmatrix}$$

$$\mathrm{Tr}\, D \ln D \sim -\ln 2 + \delta^2 - \frac{\delta^2}{2} = -\ln 2 + \frac{\delta^2}{2}$$

so $\mathrm{Tr}\, D \ln D \neq \sum_n p_n \ln p_n$ (to order δ^2)

But

$$+\sum p_n \ln_n = \frac{1}{2}\ln\frac{1}{2} + \frac{1}{2}\ln 1/2 = -\ln 2$$

—//—

Let's now diagonalize D $\Rightarrow$ D is Hermitian

$\mathrm{Tr}\, D = 1$

since the trace is invariant by rotations

$\sum_m P_m = 1$ where P_m are the eigenvalues of D for a basis ket $|m\rangle$

Diagonalizing D

$$\begin{vmatrix} \frac{1+\delta^2}{2} - \lambda & \frac{\delta}{2}(1-\delta^2)^{1/2} \\ \frac{\delta}{2}(1-\delta^2)^{1/2} & \frac{1-\delta^2}{2} - \lambda \end{vmatrix} = 0$$

$$\left(\frac{1+\delta^2}{2} - \lambda\right)\left(\frac{1-\delta^2}{2} - \lambda\right) - \frac{\delta^2}{4}(1-\delta^2) = 0$$

$$\left(\frac{1}{2} - \lambda\right)^2 - \cancel{\frac{\delta^4}{4}} - \frac{\delta^2}{4} + \cancel{\frac{\delta^4}{4}} = 0$$

$$\frac{1}{2} - \lambda = \pm\frac{\delta}{2}$$

$$\lambda = \frac{1}{2} \pm \frac{\delta}{2} \Rightarrow \quad P_1 = \frac{1}{2} - \frac{\delta}{2} \qquad P_2 = \frac{1}{2} + \frac{\delta}{2}$$

In the basis that diagonalizes D

$$D = |1\rangle P_1 \langle 1| + |2\rangle P_2 \langle 2| = \left(\frac{1}{2} - \frac{\delta}{2}\right)|1\rangle\langle 1| + \left(\frac{1}{2} + \frac{\delta}{2}\right)|2\rangle\langle 2| = \begin{pmatrix} \frac{1}{2} - \frac{\delta}{2} & 0 \\ 0 & \frac{1}{2} + \frac{\delta}{2} \end{pmatrix}$$

$$\mathrm{Tr}[D \ln D] = \sum_m \langle m| \Big[|1\rangle\langle 1| P_1 + |2\rangle P_2 \langle 2| \Big] \ln\Big[|1\rangle\langle 1| P_1 + |2\rangle\langle 2| P_2 \Big] |m\rangle$$

$A|a\rangle = a|a\rangle$

$f(A)|a\rangle = f(a)|a\rangle$

$$= P_1 \ln P_1 + P_2 \ln P_2$$

For our example

$$\mathrm{Tr}\, D \ln D = \left(\frac{1}{2}+\frac{\delta}{2}\right)\ln\left(\frac{1}{2}+\frac{\delta}{2}\right) + \left(\frac{1}{2}-\frac{\delta}{2}\right)\ln\left(\frac{1-\delta}{2}\right)$$

$$\left(\frac{1}{2}+\frac{\delta}{2}\right)\left(\ln\frac{1}{2} + \ln(1+\delta)\right) + \left(\frac{1}{2}-\frac{\delta}{2}\right)\left(\ln\frac{1}{2} + \ln(1-\delta)\right)$$

$$= \frac{1}{2}\ln\frac{1}{2} + \cancel{\frac{\delta}{2}\ln\frac{1}{2}} + \left(\frac{1}{2}+\frac{\delta}{2}\right)\underbrace{\ln(1+\delta)}_{\delta-\frac{\delta^2}{2}} + \frac{1}{2}\ln\frac{1}{2} - \cancel{\frac{\delta}{2}\ln\frac{1}{2}} + \left(\frac{1}{2}-\frac{\delta}{2}\right)\underbrace{\ln(1-\delta)}_{-\delta-\frac{\delta^2}{2}}$$

$$= -\ln 2 + \left(\frac{1}{2}+\frac{\delta}{2}\right)\left(\delta-\frac{\delta^2}{2}\right) - \left(\frac{1}{2}-\frac{\delta}{2}\right)\left(\delta+\frac{\delta^2}{2}\right)$$

$$\overset{O(\delta^2)}{=} -\ln 2 + \cancel{\frac{\delta}{2}} + \frac{\delta^2}{2} - \frac{\delta^2}{4} - \cancel{\frac{\delta}{2}} + \frac{\delta^2}{2} - \frac{\delta^2}{4} - \cancel{\frac{\delta^3}{4}} + \cancel{\frac{\delta^3}{4}}$$

$$= -\ln 2 + \delta^2 - \frac{\delta^2}{2} = -\ln 2 + \frac{\delta^2}{2}$$

So, by diagonalizing $D = \sum_m |m\rangle P_m \langle m|$ $\qquad \sum_m |m\rangle\langle m| = \mathbb{I}$

we recover

$$S[P] = -k\sum_m P_m \ln P_m = -k \,\mathrm{Tr}\, D \ln D$$ → correct

↳ normalization constant (will become important later)

Let's now assume that we have two separate Hilbert Spaces $\mathcal{H}^{(a)}$ and $\mathcal{H}^{(\alpha)}$ describing two systems

Total Hilbert space

$$\mathcal{H}^{(a)} \otimes \mathcal{H}^{(\alpha)}$$

A state $|\psi^{(a\alpha)}\rangle = \sum_{a\alpha} c_{a\alpha} |a\rangle \otimes |\alpha\rangle$

If the spaces do not "interact"

$$D^{(a\alpha)} = D^{(a)} \otimes D^{(\alpha)} \qquad D^{(a\alpha)}_{a\alpha;b\beta} = D^{(a)}_{ab} D^{(\alpha)}_{\alpha\beta}$$

If the two systems do not interact they can be diagonalized independently

$$D_{a\alpha;b\beta} = D^{(a)}_{aa} D^{(\alpha)}_{\alpha\alpha} \delta_{ab} \delta_{\alpha\beta}$$

$$\mathrm{Tr}\, D \ln D = \sum_{a\alpha} D^{(a)}_{aa} D^{(\alpha)}_{\alpha\alpha} \ln D^{(a)}_{aa} D^{(\alpha)}_{\alpha\alpha}$$

↳ already summing over the diagonal elements $\alpha = \beta$, $a = b$

$$= \sum_{a\alpha} D^{(a)}_{aa} D^{(\alpha)}_{\alpha\alpha} \left(\ln D^{(a)}_{aa} + \ln D^{(\alpha)}_{\alpha\alpha} \right)$$

$$= \underbrace{\sum_\alpha D^{(\alpha)}_{\alpha\alpha}}_{1} \underbrace{\sum_a D^{(a)}_{aa} \ln D^{(a)}_{aa}}_{S[D^{(a)}]} + \underbrace{\sum_a D^{(a)}_{aa}}_{1} \underbrace{\sum_\alpha D^{(\alpha)}_{\alpha\alpha} \ln D^{(\alpha)}_{\alpha\alpha}}_{S[D^{(\alpha)}]}$$

additivity of the entropy ⇒ equivalent to separable variables

If the two subspaces "interact" we define the partial trace

$$D^{(a)} = \mathrm{Tr}_\alpha D \qquad D^{(a)}_{(ab)} = \sum_\alpha D_{a\alpha;b\beta}$$

sum over the states of the other subspace.

Example: 2 spin-½ subsystems

$$D^{(1)} = p|1+\rangle\langle 1+| + (1-p)|1-\rangle\langle 1-|$$

$$D^{(2)} = q|2+\rangle\langle 2+| + (1-q)|2-\rangle\langle 2-|$$

$$D^{(12)} = \left(p|1+\rangle\langle 1+| + (1-p)|1-\rangle\langle 1-|\right) \otimes \left(q|2+\rangle\langle 2+| + (1-q)|2-\rangle\langle 2-|\right)$$

For simplicity

$$|1+\rangle \otimes |2+\rangle = |++\rangle$$
$$|1+\rangle \otimes |2-\rangle \equiv |+-\rangle$$
$$|1-\rangle \otimes |2+\rangle \equiv |+-\rangle$$
$$|1-\rangle \otimes |2-\rangle \equiv |--\rangle$$

$$D^{(12)} = pq|++\rangle\langle ++| + p(1-q)|+-\rangle\langle +-| + (1-p)q|-+\rangle\langle -+| + (1-p)(1-q)|--\rangle\langle --|$$

$$pq + p(1-q) + (1-p)q + (1-p)(1-q) =$$
$$\cancel{pq} + \cancel{p} - \cancel{pq} + \cancel{q} - \cancel{pq} + 1 - \cancel{p} - \cancel{q} + \cancel{pq} = 1$$

$$D^{(2)} = \mathrm{Tr}_1 D^{(12)} = \langle 1+|D^{12}|1+\rangle + \langle 1-|D^{12}|1-\rangle$$

$$= \underbrace{pq|2+\rangle\langle 2+| + p(1-q)|2-\rangle\langle 2-|}_{\langle 1+|} + \underbrace{(1-p)q|2+\rangle\langle 2+| + (1-p)(1-q)|2-\rangle\langle 2-|}_{\langle 1-|}$$

combining terms in $|2+\rangle$ and $|2-\rangle$

$$= q|2+\rangle\langle 2+| + (1-q)|2-\rangle\langle 2-| = D^{(2)}$$

The entropy

$$S[D^1] = -k\left[p\ln p + (1-p)\ln(1-p)\right]$$

$$S[D^2] = -k\left[q\ln q + (1-q)\ln(1-q)\right]$$

$S[D^{12}]$

$$D^{12} = \begin{array}{cc} \begin{array}{cccc} |++\rangle & |+-\rangle & |-+\rangle & |--\rangle \end{array} & \\ \begin{pmatrix} pq & 0 & 0 & 0 \\ 0 & p(1-q) & 0 & 0 \\ 0 & 0 & (1-p)q & 0 \\ 0 & 0 & 0 & (1-p)(1-q) \end{pmatrix} & \begin{array}{c} |++\rangle \\ |+-\rangle \\ |-+\rangle \\ |--\rangle \end{array} \end{array}$$

diagonal

$$S[D^{12}] = -k\left[\, pq\ln pq + p(1-q)\ln p(1-q) + (1-p)q\ln(1-p)q + (1-p)(1-q)\ln(1-p)(1-\right.$$

$$= -k\left[\, pq(\ln p + \ln q) + p(1-q)(\ln p + \ln(1-q)) + (1-p)q(\ln(1-p) + \ln q)\right.$$
$$\left. + (1-p)(1-q)(\ln(1-p) + \ln(1-q))\right]$$

$$= -k\left[\, pq\ln p + p(1-q)\ln p + pq\ln q + p(1-q)\ln(1-q) + (1-p)q\ln(1-p)\right.$$
$$\left. + (1-p)q\ln q + (1-p)(1-q)\ln(1-p) + (1-p)(1-q)\ln(1-q)\right]$$

$$= -k\left[p\ln p + q\ln q + (1-q)\ln(1-q) + (1-p)\ln(1-p)\right]$$

$$= -k\left[\underbrace{p\ln p + (1-p)\ln(1-p)}_{S[D^1]} + \underbrace{q\ln q + (1-q)\ln(1-q)}_{S[D^2]}\right]$$

Let's now suppose we have a pure 2-particle state given by

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left[|+-\rangle - |-+\rangle\right]$$

$\hat{S}_{Tot} = 0$
$S^2 = 0$ } eigenvalues
$S_z = 0$

$$D^{(12)} = \frac{1}{\sqrt{2}}\left[|+-\rangle - |-+\rangle\right]\left[\langle +-| - \langle -+|\right]\frac{1}{\sqrt{2}}$$

$$= \frac{1}{2}\left[|+-\rangle\langle +-| \underbrace{- |+-\rangle\langle -+|}_{0} \underbrace{- |-+\rangle\langle +-|}_{0} + |-+\rangle\langle -+|\right]$$

$$D^{(2)} = Tr_1 D^{(12)} = \langle 1+|D_{12}|1+\rangle + \langle 1-|D^{12}|1-\rangle$$

(only terms of the form $|+\sigma\rangle\langle +\sigma'|$ or $|-\sigma\rangle\langle -\sigma'|$ survive)

$$= \underbrace{\frac{1}{2}\left[|2-\rangle\langle 2-| + |2+\rangle\langle 2+|\right]}_{\text{diagonal}}$$

$$D^{(1)} = Tr_2 D^{(12)} = \underbrace{\frac{1}{2}\left[|1+\rangle\langle 1+| + |1-\rangle\langle 1-|\right]}_{\text{diagonal}}$$

$$S[D^{(1)}] = -k\left[\frac{1}{2}\ln\frac{1}{2} + \frac{1}{2}\ln\frac{1}{2}\right] = +k\ln 2$$

$$S[D^{(2)}] = k\ln 2$$

$$S[D^{(1)}] + S[D^{(2)}] = 2k\ln 2$$

We could diagonalize $D^{(12)}$ but we notice that $D^{(12)}$ is a pure state so $|\psi\rangle$ is an eigenstate with $P = 1$

all other states have $P = 0$

since $D^{(12)}$ is a pure state

$$S[D^{(12)}] = 0$$

Now we can ask ourselves, can we write

$$\mathcal{D}^{12} = \mathcal{D}^1 \otimes \mathcal{D}^2 \ ?$$

Let's assume the most general case

$$\mathcal{D}^i = a_i|+\rangle\langle+| + b_i|-\rangle\langle-| + c_i|+\rangle\langle-| + c_i^*|-\rangle\langle+| \qquad \text{with } a^i + b_i = 1$$

$$\Rightarrow \mathcal{D}^1\otimes\mathcal{D}^2 = \left[a_1|+\rangle\langle+| + b_1|-\rangle\langle-| + c_1|+\rangle\langle-| + c_1^*|-\rangle\langle+|\right] \otimes \left[a_2|+\rangle\langle+| + b_2|-\rangle\langle-| + c_2|+\rangle\langle-| + c_2^*|-\rangle\langle+|\right]$$

$$\begin{aligned}
= {} & \overbrace{a_1a_2}^{0}|++\rangle\langle++| + \overbrace{a_1b_2}^{1/2}|+-\rangle\langle+-| + \overbrace{a_1c_2}^{0}|++\rangle\langle+-| + \overbrace{a_1c_2^*}^{0}|+-\rangle\langle++| \\
& + \overbrace{b_1a_2}^{1/2}|-+\rangle\langle-+| + \overbrace{b_1b_2}^{0}|--\rangle\langle--| + \overbrace{b_1c_2}^{0}|-+\rangle\langle--| + \overbrace{b_1c_2^*}^{0}|--\rangle\langle-+| \\
& + \overbrace{c_1a_2}^{0}|++\rangle\langle-+| + \overbrace{c_1b_2}^{0}|+-\rangle\langle--| + \overbrace{c_1c_2}^{0}|++\rangle\langle--| + \overbrace{c_1c_2^*}^{1/2}|+-\rangle\langle-+| \\
& + \overbrace{c_1^*a_2}^{0}|-+\rangle\langle++| + \overbrace{c_1^*b_2}^{0}|--\rangle\langle+-| + \overbrace{c_1^*c_2}^{1/2}|-+\rangle\langle+-| + \overbrace{c_1^*c_2^*}^{0}|--\rangle\langle++|
\end{aligned}$$

From

$a_1a_2 = 0 \qquad a_1 = 0$ or $a_2 = 0$

if $a_1 = 0 \Rightarrow a_1b_2 = 0$, but it should give $a_1b_2 = 1/2$

if $a_2 = 0 \qquad b_1a_2 = 0$ but it should give $b_1a_2 = 1/2$

Even thought $\mathcal{D}^{12}$ is a pure state it cannot be separated into $\mathcal{D}^1\otimes\mathcal{D}^2$

In fact $|\Psi\rangle \neq |1\sigma\rangle\otimes|2\sigma'\rangle$

a tensor product between two single states

<u>entangled</u>

Let me now propose the following

$$\mathrm{Tr}\, X \ln Y - \mathrm{Tr}\, X \ln X \leq \mathrm{Tr}\, Y - \mathrm{Tr}\, X$$

where $\hat{X}$ and $\hat{Y}$ are Hermitian operators

Let $\hat{X}|m\rangle = X_m |m\rangle \qquad X_m > 0$

$\hat{Y}|m\rangle = Y_m |m\rangle \qquad Y_m > 0$

$$f(\hat{Y})|q\rangle = f(Y_q)|q\rangle$$

$$\mathrm{Tr}\, X \ln Y = \sum_m \langle m| \sum_{m'} X_{m'} |m'\rangle \underbrace{\langle m'|}_{\sum_{q''} |q''\rangle\langle q''|} \ln\left[\sum_{q'} Y_{q'} |q'\rangle\langle q'|\right] \underbrace{|m\rangle}_{\sum_q |q\rangle\langle q|}$$

$$= \sum_{mq} X_m \langle m|q\rangle \ln(Y_q) \langle q|m\rangle$$

$$= \sum_{mq} X_m |\langle q|m\rangle|^2 \ln(Y_q)$$

$$\mathrm{Tr}\, X \ln X = \sum_m \langle m| X \ln X |m\rangle = \sum_m X_m \ln X_m$$

since $\{|m\rangle\}$ and $\{|q\rangle\}$ are in the same Hilbert space

$$|m\rangle = \sum_q c_q^m |q\rangle \qquad \sum_q |c_q^m|^2 = 1$$

$$\langle q'|m\rangle = \sum_q c_q^m \langle q'|q\rangle = \sum_q c_q^m \delta_{q'q} = c_{q'}^m$$

$$\Rightarrow \quad \sum_q |\langle q|m\rangle|^2 = 1$$

$$\Rightarrow \quad \mathrm{Tr}\, X \ln X = \sum_m X_m \sum_q |\langle q|m\rangle|^2 \ln X_m = \sum_{mq} X_m |\langle q|m\rangle|^2 \ln X_m$$

$$\mathrm{Tr}\, X \ln Y - \mathrm{Tr}\, X \ln X = \sum_{mq} X_m |\langle q|m\rangle|^2 \ln(Y_q) - \sum_{mq} X_m |\langle q|m\rangle|^2 \ln X_m$$

$$= \sum_{mq} X_m |\langle q|m\rangle|^2 \ln\left(\frac{Y_q}{X_m}\right)$$

Now we notice that, since $\ln x$ is a concave function

$$\ln x \leqslant x-1 \qquad \text{for } x>0$$

and $\ln x = x-1$ for $x=1$

choosing

$$x = \frac{Y_q}{X_m}$$

$$\sum_{mq} |\langle q|m\rangle|^2 X_m \ln \frac{Y_q}{X_m} \leqslant \sum_{mq} |\langle q|m\rangle|^2 X_m \left(\frac{Y_q}{X_m} - 1\right) = \sum_{mq} |\langle q|m\rangle|^2 (Y_q - X_m)$$

but

$$\mathrm{Tr}\,\hat{Y} = \mathrm{Tr} \sum_q Y_q |q\rangle\langle q| = \sum_m \langle m| \left[\sum_q Y_q |q\rangle\langle q|\right] |m\rangle = \sum_{qm} |\langle q|m\rangle|^2 Y_q$$

or

$$\sum_{qm} |\langle q|m\rangle|^2 Y_q = \sum_q Y_q \underbrace{\sum_m |\langle q|m\rangle|^2}_{1} = \sum_q Y_q = \mathrm{Tr}\,\hat{Y}$$

the same is valid for $\hat{X}$

$$\mathrm{Tr}\,\hat{X} = \sum_{mq} |\langle q|m\rangle|^2 X_m$$

so

$$\mathrm{Tr}\,\hat{X}\ln\hat{Y} - \mathrm{Tr}\,\hat{X}\ln\hat{X} \leqslant \mathrm{Tr}\,\hat{Y} - \mathrm{Tr}\,\hat{X}$$

The equality is valid for

$$x=1 \quad \text{or} \quad X_m = Y_q$$

so $\quad |\langle m|q\rangle|^2 (Y_q - X_m) = 0 \qquad \forall\,(m,q)$

so $\quad \langle m|q\rangle = 0$

or $\quad Y = X$

since both $\{|m\rangle\}$ and $\{|q\rangle\}$ form a complete basis

$$Y = X$$

Returning

Let $\hat{A}$ an operator that acts only in the Hilbert space $\mathcal{H}^{(a)}$

$$\hat{A} = A^{(a)} \otimes \mathbb{I}^{(\alpha)}$$

$$\langle A \rangle = \mathrm{Tr}\, AD = \sum_{a\alpha} \sum_{b\beta} A^{(a)}_{ab} \delta_{\alpha\beta} D_{b\beta;a\alpha}$$

$$= \sum_{a\alpha} \sum_{b} A^{(a)}_{ab} D_{b\alpha;a\alpha}$$

$$= \sum_{a} \sum_{b} A^{(a)}_{ab} \underbrace{\sum_{\alpha} D_{b\alpha;a\alpha}}_{\mathrm{Tr}_\alpha D = D^{(a)}_{ba}}$$

$$= \sum_{ab} A^{(a)}_{ab} D^{(a)}_{ba} = \mathrm{Tr}\, A^{(a)} D^{(a)}$$

density operator for subsystem (a)

Let's take a system of two interacting subsystems

the

$$D \neq D^{(a)} \otimes D^{(\alpha)}$$ in general

Where we define

$$D^{(a)} = \sum_{\alpha} D = \mathrm{Tr}_{\alpha} D \rightarrow \text{acts only on } \mathcal{H}^{(a)}$$

$$D^{(\alpha)} = \sum_{a} D = \mathrm{Tr}_{a} D \rightarrow \text{acts only on } \mathcal{H}^{(\alpha)}$$

Then

$$D^{(a)} = D^{(a)} \otimes I^{(\alpha)}$$

$$D^{(\alpha)} = D^{(\alpha)} \otimes I^{(a)}$$

acting on the full Hilbert space

Defining

$$D \neq D' = D^{(a)} \otimes D^{(\alpha)} \quad \text{then}$$

$$\ln D' = \ln D^{(a)} \otimes D^{(\alpha)} = \underbrace{\ln D^{(a)} \otimes I^{(\alpha)}}_{\text{acts only on } (a)} + \underbrace{\ln D^{(\alpha)} \otimes I^{(a)}}_{\text{acts only on } (\alpha)}$$

Also

$$\mathrm{Tr}\, D \ln D^{(a)} \otimes I^{(\alpha)} = \sum_{a\alpha} \sum_{b\beta} D_{a\alpha; b\beta} \ln D^{(a)}_{ba} \delta_{\beta\alpha}$$

$$= \sum_{a} \underbrace{\sum_{\alpha} D_{a\alpha; b\alpha}}_{D^{(a)}_{ab}} \ln D^{(a)}_{ba} = \mathrm{Tr}_a D^{(a)} \ln D^{(a)}$$

Let me now use the inequality I just proved

using

$$D \equiv \hat{X}$$

$$D' \equiv \hat{Y}$$

$$\mathrm{Tr}\, D \ln D' - \mathrm{Tr}\, D \ln D \leq \underbrace{\mathrm{Tr}\, D}_{1} - \underbrace{\mathrm{Tr}\, D'}_{1}$$

$$\mathrm{Tr}\, D\left(\ln D^{(a)} \otimes I^{(\alpha)} + \ln I^{(a)} \otimes D^{(\alpha)}\right) - \mathrm{Tr}\, D \ln D \leq 0$$

$$\mathrm{Tr}_a D^{(a)} \ln D^{(a)} + \mathrm{Tr}_\alpha D^{(\alpha)} \ln D^{(\alpha)} - \mathrm{Tr}\, D \ln D \leq 0$$

$$\Rightarrow \quad \underbrace{\mathrm{Tr}\, D \ln D}_{-\frac{1}{k} S[D]} \geq \underbrace{\mathrm{Tr}_a D^{(a)} \ln D^{(a)}}_{-\frac{1}{k} S[D^{(a)}]} + \underbrace{\mathrm{Tr}_\alpha D^{(\alpha)} \ln D^{(\alpha)}}_{-\frac{1}{k} S[D^{(\alpha)}]}$$

$$S[D] \leq S[D^{(a)}] + S[D^{(\alpha)}]$$

■

The equality holds when

$$D = D' = D^{(a)} \otimes D^{(\alpha)} \equiv \text{isolated system.}$$