Statistical Entropy

or information entropy

- define entropy of a probability distribution

  - probability distribution: P_m

$$P_m \geq 0 \rightarrow \sum_m P_m = 1$$

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

- complete knowledge of system:

$$P_n = 1 \qquad P_m = 0 \quad \forall m \neq n$$

$$S(P) = 0 \text{ in this case} \qquad \left(\lim_{x \to 0} x \ln x = 0\right)$$

- complete uncertainty of system

$$P_m = 1/M \Rightarrow S = -\sum_m \frac{1}{M} \ln \frac{1}{M} = \ln M$$

$\Downarrow$ $\qquad\qquad$ $\Downarrow$

the more information the less the entropy

in general, for an arbitrary prob. distribution:

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

- demonstrate this as:
  - optimize $S[P]$ as a function of $\{P_m\}$ under the normalization constraint

$$\tilde{S} = -\sum_m P_m \ln P_m + \lambda_0 \left(\sum_m P_m - 1\right)$$

$$\frac{\partial \tilde{S}}{\partial P_m} = 0 \Rightarrow -\ln P_m - 1 + \lambda_0 = 0 \Rightarrow P_m = \frac{1}{M}$$

- since $S=0$ for situation of complete certainty (2)

$\Rightarrow$ $P_n = 1/M$ is a maximum

- additivity of entropy for uncorrelated distributions:

in this case: $P_{mm'} = P_m Q_{m'}$ $\quad \sum_m P_m = 1$

$\sum_m Q_m = 1$

$$S = -\sum_{mm'} P_{mm'} \ln P_{mm'}$$

$$= -\sum_{mm'} P_m Q_{m'} \ln P_m Q_{m'}$$

$$= -\sum_m P_m \ln P_m - \sum_m Q_m \ln Q_m$$

$$= S[P] + S[Q]$$

- in general

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

$$S_{tot} \leq S[P] + S[Q]$$

equal sign holds for uncorrelated case

- completely correlated case

$$P_{mm'} = P_m \delta_{mm'}$$

$$S_{TOT} = -\sum_{mm'} P_{mm'} \ln P_{mm'}$$

$$= -\sum_{mm'} P_m \delta_{mm'} \ln P_m \delta_{mm'}$$

$$= -\sum_m P_m \ln P_m = S[P]$$

For mixed quantum states we will need the concept of tensor product (3)

Tensor Product

- two vectors: $|\Psi\rangle, |\phi\rangle$

$$|\Psi\rangle \otimes |\phi\rangle$$

expand $|\Psi\rangle = \sum_i c_i |\alpha_i\rangle$

$$|\varphi\rangle = \sum_i a_i |\alpha_i\rangle$$

$$|\Psi\rangle \otimes |\phi\rangle = \sum_{ij} c_i a_j |\alpha_i\rangle \otimes |\alpha_j\rangle$$

- two matrices

$$A \otimes B = \begin{matrix} A_{11} B_{11} & A_{11} B_{12} \cdots & A_{12} B_{N} & A_{12} B_{12} \cdots \\ \vdots & & & \\ A_{21} A_{11} & & & \\ \vdots & & & A_{NN} B_{11} \cdots \\ & & & \vdots \end{matrix}$$

ex

example: 2×2 matrix

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \otimes \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

$$= \begin{pmatrix} A_{11} B_{11} & A_{11} B_{12} & A_{12} B_{11} & A_{12} B_{12} \\ A_{11} B_{21} & A_{11} B_{22} & A_{12} B_{21} & A_{12} B_{22} \\ A_{21} B_{11} & A_{21} B_{12} & A_{22} B_{11} & A_{22} B_{12} \\ A_{21} B_{21} & A_{21} B_{22} & A_{22} B_{21} & A_{22} B_{22} \end{pmatrix}$$

can show that if A and B are $M \times M$ matrices and if C and D are $N \times N$ matrices

then $\Rightarrow$ $$[AB \otimes CD] = [A \otimes C][B \otimes D]$$

or:
$A \to M \times M$ matrix
$v \to M$ vector
$B \to N \times N$ matrix
$w \to N$ vector

$$Av \otimes Bw = [A \otimes B][v \otimes w]$$

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tensor products are useful to describe "compound" Hilbert spaces

example: System 1 $\Rightarrow$ Hamiltonian matrix $H^{(1)}$
M- dimensional

System 2 $\Rightarrow$ Hamiltonian matrix $H^{(2)}$
N - dimensional

$\Rightarrow$ the Hamiltonian of the compound system, if they are not interacting, is

$$H_{TOT} = H^{(1)} \otimes I^{(2)} + I^{(1)} \otimes H^{(2)}$$

$I^{(1)} \to$ M- dimensional identity
$I^{(2)} \to$ N - dimensional identity

if the two systems interact

$$H_{TOT} = H^{(1)} \otimes I^{(2)} + \cancel{H^{(2)} \otimes} \; I^{(1)} \otimes H^{(2)} + S^{(12)}$$

where $S^{(12)}$ is an $MN \times MN$ dimensional matrix

<u>example:</u> two spin-1/2 particles

particle-1: $S^2 = S_x^2 + S_y^2 + S_z^2$

$$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{1}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

$$S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

particle-2: same matrices

S_x for compound system

$$S_x^{(12)} = S_x \otimes I + I \otimes S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$S_y^{(12)} = S_y \otimes I + I \otimes S_y = \frac{1}{2}\begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}$$

$$S_z^{(12)} = S_z \otimes I + I \otimes S_z = \frac{1}{2}\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}$$

if the two systems interact

$$H_{TOT} = H^{(1)} \otimes I^{(2)} + I^{(1)} \otimes H^{(2)} + S^{(12)}$$

where in general $S^{(12)}$ is an NM by NM matrix

example: two spin-1/2 particles ~~coupled~~

$$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{1}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \qquad S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

combined spins for two particles

$$S_x^{(12)} = S_x \otimes I + I \otimes S_x$$

$$= \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

$$S_y^{(12)} = S_y \otimes I + I \otimes S_y$$

$$= \frac{1}{2}\begin{pmatrix} 0 & i & i & 0 \\ -i & 0 & 0 & i \\ -i & 0 & 0 & i \\ 0 & -i & -i & 0 \end{pmatrix}$$

$$S_z^{(12)} = \frac{1}{2}\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}$$

$$\left[S^{(12)}\right]^2 = S_x^{(12)} S_x^{(12)} + S_y^{(12)} S_y^{(12)} + S_z^{(12)} S_z^{(12)}$$

$$= \frac{1}{4}\begin{pmatrix} 2 & 0 & 0 & 2 \\ 0 & 2 & 2 & 0 \\ 0 & 2 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 2 & 0 & 0 & -2 \\ 0 & 2 & 2 & 0 \\ 0 & 2 & 2 & 0 \\ -2 & 0 & 0 & 2 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix}$$

$$= \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \Rightarrow \text{eigenvalues } 2, 0 \to$$ ~~not degenerate~~

eigenvalue $S_x^2 + S_y^2 + S_z^2 = 2 \Rightarrow$ 3-fold degenerate (triplet) 7

$$S = 1 \quad (S(S+1) = 2)$$

$S_x^2 + S_y^2 + S_z^2 = 0 \Rightarrow$ non-degenerate (singlet)

$$S = 0 \quad (S(S+1) = 0)$$

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density matrices:

~~given~~ given two systems 1 and 2 with density matrices

$$D^{(1)}_{ab}, \; D^{(2)}_{\alpha\beta}$$

- the density matrix for the combined system in the absence of interaction between the two will be

$$D_{TOT} = D^{(1)} \otimes D^{(2)}$$

$$\Rightarrow D^{TOT}_{a\alpha;b\beta} = D^{(1)}_{ab} D^{(2)}_{\alpha\beta}$$

- if there is interaction between the two systems: $D^{TOT}_{a\alpha;b\beta} \neq D^{(1)}_{ab} D^{(2)}_{\alpha\beta}$ in general

but the dimensionality of

$D^{TOT}_{a\alpha;b\beta}$ and $D^{(1)}_{ab} \otimes D^{(2)}_{\alpha\beta}$ is the same

- the tensor-product basis of the two systems is a complete orthonormal basis for the combined system

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suppose a system is coupled to a heat reservoir

$$\text{sys} - \text{res} \Rightarrow D^{(tot)}$$

in this case a useful quantity is the reduced density matrix

$$D^{(sys)} = Tr_{res}\, D^{(tot)}$$

$D^{(sys)}$ is obtained from $D^{(tot)}$ by tracing out the degrees of freedom associated with the reservoir

- if we have $D^{(tot)}_{a\alpha;b\beta}$

$$D^{(sys)}_{ab} = \sum_{\alpha} D^{(tot)}_{a\alpha;b\alpha}$$

- consider an operator acting in the Hilbert space of the system only $O^{(sys)}_{ab}$

the appropriate operator in the total Hilbert space is $O^{(tot)}_{a\alpha;b\beta} = O^{(sys)}_{ab}\,\delta_{\alpha\beta}$

$$O^{(tot)} = O^{(sys)} \otimes I^{(res)}$$

- the expectation value of $O^{(tot)}$ can be written in terms of $O^{(sys)}$ and the reduced density matrix

$$\langle O \rangle = \mathrm{Tr}\, D^{(tot)}\, O^{(tot)}$$

$$= \sum_{a\alpha}\sum_{b\beta} D^{(tot)}_{a\alpha;b\beta}\, O^{(tot)}_{b\beta;a\alpha}$$

$$= \sum_{a\alpha}\sum_{b\beta} D^{(tot)}_{a\alpha;b\beta}\, O^{(sys)}_{ba}\,\delta_{\alpha\beta}$$

$$= \sum_{ab}\sum_{\alpha} D^{(tot)}_{a\alpha;b\alpha}\, O^{(sys)}_{ba}$$

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

in general there are <u>reduced</u> operators

$O = \mathrm{Tr}_a O \Rightarrow$ in which part of the Hilbert space is traced out

Statistical Entropy of a Mixed Quantum State

$$\hat{D} = \sum_n p_n |\varphi_n\rangle\langle\varphi_n| \quad \Rightarrow |\varphi_n\rangle \text{ has to be an ortho-normal basis}$$

$$S_{st}[\hat{D}] = -k \, \mathrm{Tr}\, \hat{D} \ln \hat{D}$$

in general: $$\mathrm{Tr}\, f(\hat{D}) = \mathrm{Tr} \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \hat{D}^n$$

$$= \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \underline{\mathrm{Tr}[\hat{D}^n]}$$

$$\mathrm{Tr}[\hat{D}^n] = \mathrm{Tr}\left[\sum_{m_1} p_{m_1} |\varphi_{m_1}\rangle\langle\varphi_{m_1}|\right] \cdots \left[\sum_{m_n} p_{m_n} |\varphi_{m_n}\rangle\langle\varphi_{m_n}|\right]$$

$$= \mathrm{Tr}\left[\sum_m p_m^n |\varphi_m\rangle\langle\varphi_m|\right] = \underline{\sum_m p_m^n}$$

$$\mathrm{Tr}\, f(\hat{D}) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \sum_m p_m^n$$

$$= \sum_m \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} p_m^n$$

$$= \sum_m f(p_m)$$

$\mathrm{Tr}\, f(\hat{D}) = \sum_m f(p_m)$ for an orthonormal basis

$\Downarrow$

$$\boxed{-k \mathrm{Tr}\, \hat{D} \ln \hat{D} = -k \sum_m p_m \ln p_m = S[\hat{D}]}$$

$\Downarrow$

entropy of a quantum statistical system

additivity property

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

(a) and (α) are subsystems, non-interacting

~~independent~~ $D_{a\alpha:b\beta} = D^{(a)}_{ab}\, D^{(\alpha)}_{\alpha\beta}$

they can be diagonalized independently

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

$$\cancel{\mathrm{Tr}\, D \ln D = \sum_{a,\alpha} D}$$

for a diagonal matrix $\hat{A}$, $\mathrm{Tr} f(\hat{A}) =$

$$= \mathrm{Tr} \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} A^n = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \underline{\mathrm{Tr}\, A^n}$$

$$= \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \sum_i \lambda_i^n$$

λ_i - eigenvalues of matrix

$$= \sum_i \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \lambda_i^n$$

$$= \sum_i f(\lambda_i)$$

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

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

$$= \mathrm{Tr}\, D^{(a)} \ln D^{(a)} + \mathrm{Tr}\, D^{(\alpha)} \ln D^{(\alpha)}$$

$\Rightarrow$ for noninteracting case $\quad S_{tot} = S^{(a)} + S^{(\alpha)}$

$\Rightarrow$ in general $\quad S_{tot} \leq S^{(a)} + S^{(\alpha)}$

Time evolution of statistical entropy

$$S = -k\,\mathrm{Tr}\,\hat{D}\ln\hat{D}$$

in general $\frac{d}{dt}\mathrm{Tr}\,f(\hat{D}) = \mathrm{Tr}\,\frac{df(\hat{D})}{dt}$

$$f(\hat{D}) = \sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}\hat{D}^{n}$$

$$\frac{df(\hat{D})}{dt} = \sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}\left[\frac{d\hat{D}}{dt}\hat{D}^{n-1} + \hat{D}\frac{d\hat{D}}{dt}\hat{D}^{n-2} + \dots\right]$$

$$\mathrm{Tr}\,\frac{df(\hat{D})}{dt} = \sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}\left[\mathrm{Tr}\,\frac{d\hat{D}}{dt}\hat{D}^{n-1} + \mathrm{Tr}\,\hat{D}\frac{d\hat{D}}{dt}\hat{D}^{n-2} + \dots +\right]$$

cyclic invariance of trace

$$= \sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{(n-1)!}\,\underline{\mathrm{Tr}\,\frac{d\hat{D}}{dt}\hat{D}^{n-1}}$$

$$= \cancel{\sum_{n=0}^{\infty}}\,\mathrm{Tr}\,\frac{d\hat{D}}{dt}\left[\sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{(n-1)!}\hat{D}^{n-1}\right]$$

$$= \mathrm{Tr}\,\frac{d\hat{D}}{dt}f'(\hat{D})$$

$$i\hbar\frac{dS}{dt} = -i\hbar k\,\mathrm{Tr}\,(\ln\hat{D} + 1)\frac{d\hat{D}}{dt}$$

$$= -i\hbar k\,\mathrm{Tr}\,\ln\hat{D}\frac{d\hat{D}}{dt}$$

$$= -k\,\mathrm{Tr}\,\ln\hat{D}\,[\hat{D},\hat{H}] = -k\,\mathrm{Tr}\,\ln\hat{H}\,[\hat{D},\ln\hat{D}]$$

$= 0 \Rightarrow$ Hamiltonian dynamics